NUREG/CR-6844, Vol. 3

TRISO-Coated Particle Fuel Phenomenon Identification and Ranking Tables (PIRTs) for Fission Product Transport Due to Manufacturing, Operations, and Accidents

Appendices E through I

U.S. Nuclear Regulatory Commission
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Appendices E through I

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ABSTRACT

TRISO-coated particle fuel is to be used in the next generation of gas-cooled reactors. In anticipation of future licensing applications for gas-cooled reactors, the United States Nuclear Regulatory Commission (NRC) seeks to fully understand the significant features of TRISO-coated particle fuel design, manufacture, and operation, as well as behavior during accidents. The objectives of the TRISO Phenomena Identification and Ranking Table (PIRT) program are to (1) identify key attributes of gas-cooled reactor fuel manufacture which may require regulatory oversight, (2) provide a valuable reference for the review of vendor fuel qualification plans, (3) provide insights for developing plans for fuel safety margin testing, (4) assist in defining test data needs for the development of fuel performance and fission product transport models, (5) inform decisions regarding the development of NRC's independent reactor fuel performance code and fission product transport models, (6) support the development of NRC's independent models for source term calculations, and (7) provide insights for the review of vendor fuel safety analyses. To support these objectives, the NRC commissioned a PIRT panel to identify and rank the factors, characteristics, and phenomena associated with TRISO-coated particle fuel. PIRTs were developed for (1) Manufacturing, (2) Operations, (3) a Depressurized Heatup Accident, (4) a Reactivity Accident, (5) a Depressurization Accident with Water Ingress, and (6) a Depressurization Accident with Air Ingress.

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FOREWORD

In anticipation of future licensing applications for gas-cooled reactors, the United States Nuclear Regulatory Commission (NRC) seeks to fully understand the significant features of TRISO-coated particle fuel design, manufacture, and operation, as well as behavior during accidents.

To address this objective, the NRC convened the formation of a panel of experts to identify and rank the factors, characteristics, and phenomena associated with the life-cycle phases of TRISO-coated particle fuel. The products of the panel are Phenomena Identification and Ranking Tables (PIRTs) and the associated documentation.

Six phenomena identification and ranking tables (PIRTs) were developed by the panel and are presented in this report. They are: (1) Manufacturing, (2) Operations, (3) Depressurized Heatup Accident, (4) Reactivity Accident, (5) Depressurization Accident with Water Ingress, and (6) Depressurization Accident with Air Ingress.

Analyses and summaries for each of the six PIRTs are presented. A total of 327 factors, characteristics and phenomena are identified in the six PIRT tables. The importance of each factor, characteristic, process or phenomenon was assessed relative to the magnitude of its influence on fission product release or in a more accident consequence-related term, the source term. One hundred-ten (110) factors, characteristics and phenomena were assigned an importance rank of "High" by each panel member. The panel concluded that these 110 factors, characteristics and phenomena had the most significant impact on fission product release. Each panel member prepared a written rationale supporting the importance rank assigned to each highly ranked factor, characteristic or phenomenon. These rationales are included in this report. The level of knowledge for each factor, characteristic or phenomenon was also assessed and documented. Of particular interest to the agency are those factors, characteristics or phenomena assessed by the panel as being of high importance but not yet adequately understood.

The PIRT results will be used by the agency to (1) identify key attributes of gas-cooled reactor fuel manufacture, (2) provide a valuable reference for the review of vendor gas-cooled reactor fuel qualification plans, (3) provide insights for developing plans for fuel safety margin testing, (4) assist in defining test data needs for the development of fuel performance and fission product transport models, (5) inform decisions regarding the development of NRC's independent gas-cooled reactor fuel performance code and fission product transport models, (6) support the development of NRC's independent models for source term calculations, and (7) provide insights for the review of vendor gas-cooled fuel safety analyses.

This report is consistent with the NRC strategic performance goals (NUREG-1614, Vol. 2)

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APPENDIX E

PANEL MEMBER DETAILED PIRT SUBMITTALS FOR TRISO FUEL DEPRESSURIZATION ACCIDENT WITH WATER INGRESS

The INEEL submittal is provided in Appendix E.1 (pages E-2 through E-79).

The ORNL submittal is provided in Appendix E.2 (pages E-80 through E-160).

The SNL submittal is provided in Appendix E.3 (pages E-161 through E-238).

Appendix E.1

Detailed PIRT Submittal by the INEEL Panel Member

E. A. Petti

TRISO Fuel PIRT: Accident with Subsequent Water Intrusion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Fuel Element Irradiation history	The temperature, burnup and fast fluence history of the layer

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	7	Remedy:
Rationale: Irradiation history determines inventory at risk and initial conditions in particle relative to internal pressure in the particle and stress state.	Rationale:	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Fuel Element Condensed phase diffusion	Inter granular diffusion and/or intra-grannular solid-state diffusion

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	6	Remedy:
Rationale: Mechanism describing the transport of fission products in matrix of the fuel element. Important to understanding source term for the reactor.	Rationale: Air or water ingress can change the microstructure of the matrix, which can influence the surface diffusion of fission products by making transport easier. At very low partial pressures, air and water oxidation rates can be determined by the number of active sites in the matrix at which the oxidation can occur. In some cases oxidation can be catalyzed by impurity elements that are trapped at adsorption sites in the graphitic matrix. Thus there can be competition between fission product adsorption and the reaction between the air or steam and the matrix. The isotherms are fairly well known. The key issue is whether the internal surface area of the matrix has been changed by the air or water oxidation event and thus the amount of material available for release. Dislocations and/or defects can act as trapping sites for fission products as they transport through the matrix. If the number of dislocations is about the same as the number of fission products then the effect may be important. If the fission product concentration is much greater than the dislocation density then the effect is probably second order. Exact values have not been measured nor has any transport behavior been directly correlated with these parameters. The influence of the oxidation event may be to provide enough energy to the matrix to release fission products from the traps. Sensitivity analysis can be performed to scope this out.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Fuel Element Gas phase diffusion	Diffusion of gaseous fission products through layer (Knudsen and bulk diffusion through pore structure, and pressure driven permeation through structure). Other factors include holdup, cracking, adsorption, site poisoning, permeability, sintering and annealing.

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: II	5	Remedy:
Rationale: Gas phase diffusion is thought to be the mechanism for gaseous fission product transport in the matrix.	Rationale: Air or water ingress can change the microstructure and porosity of the matrix, which can influence the gas diffusion of fission products by making transport easier. The interconnected porosity can be a transport path for the air or water intrusion. The reaction of air or water with the matrix can change the microstructure, porosity, tortuosity, and permeability, and hence affect gaseous fission product transport in the matrix.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Fuel Element: Transport of metallic FPs through fuel element	Chemical stoichiometry of the chemical species that includes the radioisotope of interest
	Chemical form	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	7	Remedy:
Rationale: Transport has been assumed to be elemental for the major fission products (Cs, Ag, I, Xe, Sr). Potential changes in chemical form due to the presence of air or water can be calculated.	Rationale:	Closure Criterion:

<u>Additional Discussion</u>

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Fuel Element: Chemical attack by water Kinetics	Rate of reaction per unit surface area as a function of temperature and partial pressure of steam

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: II	6	Remedy:
Rationale: Very important to determining the overall course of the oxidation transient.	Rationale: Some reaction rate data exists and sensitivity analysis can be used to address uncertainties.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Fuel Element: Chemical attack by water Catalysis	Modification of the reaction rate by fission products or impurities

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	5	Remedy:
Rationale: Impurities can alter reaction rate and thus behavior expected in the reactor.	Rationale: Oxidation rate data have been determined for actual pebbles and compacts and thus implicitly include the effects of impurities. The effects of fission products have not been included because oxidation testing has not been performed on irradiated material. In principle sensitivity calculations can be performed with variations in the oxidation rate to bound this effect.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Fuel Element: Chemical attack by water	Changes in chemical form resulting from oxidizing or reducing fission products
	Changes in chemical form of fission products	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: II	7	Remedy:
Rationale: This can be important because the transport behavior is dependent on the chemical form.	Rationale: This can also be calculated for a range of oxygen potentials to determine if any of the key fission products change in chemical form during the air or water ingress accident.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Fuel Element: Chemical attack by water	Changes in diffusivity, porosity, adsorptivity, etc.
	Changes in graphite properties	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	6	Remedy:
Rationale: The oxidation can change the microstructure of the graphite by creating tunnels or pathways in the matrix. Thus, because the microstructure changes, the porosity, adsorptivity, etc. can also change.	Rationale: No measurements have been made on this effect. Conservative assumptions on such changes may allow sensitivity studies in this area.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Fuel Element: Chemical attack by water	Release of graphite FP inventory
	Holdup reversals	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	6	Remedy:
Rationale: As the oxidation process continues, any fission products trapped at sites in the matrix may be released because of the thermal energy associated with the oxidation.	Rationale: This can be accounted for in a very simplistic, yet conservative manner if details are not well known or more sophisticated models with detrapping can be used if the fundamental data needed for such models exist.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Fuel Element: Chemical attack by water Temperature distribution	Impact of graphite oxidation on temperature distribution through material

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	8	Remedy:
Rationale: Very important in doing an oxidation calculation is to make sure the temperature response of the material, as a result of the energy generation, is properly calculated.	Rationale: This is well known and can be done in most of the safety codes used by NRC (e.g. MELCOR). The degree of fine detail in the model may be an open question but can be handled with sensitivity studies.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Outer PyC Layer Gas-phase diffusion	Diffusion of gaseous fission products through layer (Knudsen and bulk diffusion through pore structure, and pressure driven permeation through structure)

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	6	Remedy:
Rationale: Release from intact particles is less important than from particles with exposed kernels in the presence of water.	Rationale: Effective diffusion coefficients for noble gases through PyC exist for both German and U.S. PyC. The Knudsen diffusion formalism has not been historically used in the modeling. The effect of oxidation on changes in the transport behavior has not been studied. Sensitivity studies can be performed to bound potential changes to determine the impact on the overall source term.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Outer PyC Layer Condensed-phase diffusion	Inter-granular diffusion an/or intra-grannular solid state diffusion.

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	6	Remedy:
Rationale: Release from intact particles is less important than from particles with exposed kernels in the presence of water.	Rationale: Data exist on the effective diffusivity of Cs, Ag, and Sr through the PyC layer. The mechanism responsible for the transport has not been definitively identified. The effect of oxidation on transport properties has not been studied. Sensitivity studies can be performed to bound potential changes to determine the impact on the overall source term.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Outer PyC Layer Layer oxidation	Uptake of oxygen by the layer through a chemical reaction

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	7	Remedy:
Rationale: Oxidation of OPyC is needed to understand thermal response of the particles in the fuel element.	Rationale: Reaction rates for PyC are known at these temperatures.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Outer PyC Layer Stress state (compression/tension)	The state of the forces induced by external forces that are acting across the layer to resist movement

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	8	Remedy:
Rationale: The stress state is judged to be of low importance for a chemical oxidation event.	Rationale: Stress state is easily calculated using current finite element models for coated particles.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Outer PyC Layer Intercalation	Trapping of species between crystallite planes of the graphite structure

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	4	Remedy:
Rationale: In an intact particle, little diffusion of fission products is expected. If the level of adsorption or defect sites is high in the OPyC due to neutron irradiation, for example, then these sites may be effective in holding up fission products if they are not annealed out during the oxidation event. In a failed particle, the number of fission product atoms is so large that such a mechanism is very small. This is based on diffusion and trapping modeling performed for tritium under the NPR program in the early 1990s. The oxidation event if severe enough could probably liberate any adsorbed or trapped fission products. Sensitivity studies with a diffusion and trapping model can study this in more detail to determine overall significance in the core for the oxidation event.	Rationale:	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Outer PyC Layer Trapping	Adsorption of fission products on defects

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	4	Remedy:
Rationale: In an intact particle, little diffusion of fission products is expected. If the level of adsorption or defect sites is high in the OPyC due to neutron irradiation, for example, then these sites may be effective in holding up fission products if they are not annealed out during the oxidation event. In a failed particle, the number of fission product atoms is so large that such a mechanism is very small. This is based on diffusion and trapping modeling performed for tritium under the NPR program in the early 1990s. The oxidation event if severe enough could probably liberate any adsorbed or trapped fission products. Sensitivity studies with a diffusion and trapping model can study this in more detail to determine overall significance in the core for the oxidation event.	Rationale:	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Outer PyC Layer Cracking	Lengths, widths and numbers of cracks produced in layer during operation or an accident

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	6	Remedy:
Rationale: A cracked OPyC will not retain fission gases and would act as a fast transport path for oxidation of the SiC.	Rationale: Models can be used to calculate the stress state in the OPyC layer.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Outer PyC Layer: Chemical attack by water Kinetics	Rate of reaction per unit surface area as a function of temperature and partial pressure of steam

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	7	Remedy:
Rationale: Oxidation of OPyC is needed to understand thermal response of the particles in the fuel element.	Rationale: Reaction rates for PyC are known at these temperatures.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Outer PyC Layer: Chemical attack by water Catalysis	Modification of the reaction rate by fission products or impurities

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	4	Remedy:
Rationale: Impurities can change reaction rates and thus influence course of the ingress event.	Rationale: Reaction rate testing of PyC would implicitly include the effects of any impurities on the overall oxidation. No chemical reaction rate measurements have been performed using irradiated PyC where fission products may be in the layer. In principle sensitivity calculations can be performed with variations in the oxidation rate to bound this effect.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Outer PyC Layer: Chemical attack by water	Changes in chemical form resulting from oxidizing or reducing fission products
	Changes in chemical form of fission products	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	7	Remedy:
Rationale: This can be important because the transport behavior is dependent on the chemical form.	Rationale: This can be calculated for a range of oxygen potentials to determine if any of the key fission products change in chemical form during the air or water ingress accident.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Outer PyC Layer: Chemical attack by water Changes in graphite properties	Changes in diffusivity, porosity, adsorptivity, etc.

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	6	Remedy:
Rationale: The oxidation can change the microstructure of the PyC by creating tunnels or pathways in the matrix. Thus, because the microstructure changes, the porosity, adsorptivity, etc. can also change.	Rationale: No measurements have been made on this effect. Conservative assumptions on such changes may allow sensitivity studies in this area.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Outer PyC Layer: Chemical attack by water Holdup reversal	Release of graphite FP inventory

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	6	Remedy:
Rationale: As the oxidation process continues any fission products trapped at sites in the PyC may be released because of the thermal energy associated with the oxidation.	Rationale: This can be accounted for in a very simplistic yet conservative manner if details are not well known or more sophisticated models with detrapping can be used if the fundamental data needed for such models exist.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Outer PyC Layer: Chemical attack by water Temperature distribution	Impact of graphite oxidation on temperature distribution through material

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	8	Remedy:
Rationale: Very important in doing an oxidation calculation is to make sure the temperature response of the material as a result of the chemical reaction is properly calculated.	Rationale: This is well known and can be done in most of the safety codes used by NRC (e.g. MELCOR). The high conductivity of the PyC should make the gradient quite small in general. The degree of fine detail in the model may be an open question but can be handled with sensitivity studies.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	SiC Layer Gas-phase diffusion	Diffusion of gaseous fission products through layer (Knudsen and bulk diffusion through pore structure, and pressure driven permeation through structure)

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	7	Remedy:
Rationale: As the primary fission product barrier understanding the transport is very important.	Rationale: Effective diffusion coefficients exist in both the U.S. and Germany for the fission gases through the SiC. They are probably a combination of bulk diffusion and Knudsen diffusion at these high temperatures but the two mechanisms have never been individually sorted out in any experiment. The parameters needed for such detailed models and the changes in microstructure of the SiC particle to particle and/or across the layer and/or as a result of the oxidation make such an effort very expensive and time consuming. The use of effective diffusion coefficients although less scientifically satisfying is more pragmatic and may be completely acceptable in system safety analysis when accompanied by proper sensitivity studies.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	SiC Layer Condensed-phase diffusion	Inter-granular diffusion and/or intra-grannular solid-state diffusion

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: II	7	Remedy:
Rationale: As the primary fission product barrier understanding the transport is very important.	Rationale: Effective diffusion coefficients exist in both the U.S. and Germany for the metallic fission products through the SiC. They are probably a combination of bulk diffusion and grain boundary diffusion at these high temperatures but the two mechanisms have never been individually sorted out in any experiment. The parameters needed for such detailed models and the changes in microstructure of the SiC particle to particle and/or across the layer and/or as a result of the oxidation process make such an effort very expensive and time consuming. The use of effective diffusion coefficients although less scientifically satisfying is more pragmatic and may be completely acceptable in system safety analysis when accompanied by proper sensitivity studies.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	SiC Layer Thermal deterioration/decomposition	Decline in the quality of the layer due to thermal loading

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	8	Remedy:
Rationale: Less important in oxidation events than in the longer term traditional heatup event. (See similar factor in heatup PIRT table for more information).	Rationale:	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	SiC Layer Fission product corrosion	Attack of layer by fission products, e.g., Pd

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	7	Remedy:
Rationale: The deterioration of the SiC layer via Pd attack has been postulated as a key failure mechanism because Pd forms silicides based on phase diagram and experimental measurements. This is very important for the high burnup fuel being proposed in new reactor designs since the Pd yield from Pu fission is much greater (~ 25 x) that from U fission. Overall, it is judged to be of less importance in the oxidation event since it is assumed that the chemical energy associated with the oxidation event would dominate the subsequent fission product behavior in the particle.	Rationale: Various research institutions have performed many measurements. The kinetics of this mechanism is not known with enough certainty since extrapolations from the database are required. More testing would help develop a better understanding of the phenomena and its impact above 1600°C. Synergistic effects between oxidation and Pd attack (e.g., increase in temperature due to oxidation and its impact on greater Pd corrosion) have never been studied experimentally, but can be examined use computer models with appropriate sensitivity studies.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	SiC Layer Heavy metal diffusion	Diffusion of heavy metals through the intact layer

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	3	Remedy:
Rationale: Although higher oxides of uranium (UO_{2+x}) can be volatile, this factor is judged to be of low importance in air or water ingress events since the ability of air or water to get to the kernel to mobilize the uranium is quite small given the large amount of carbon in the system available to react with air or steam.	Rationale: Heavy metal diffusion has never been observed in German accident heating tests.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	SiC Layer Layer oxidation	Uptake of oxygen by the layer through a chemical reaction

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	5	Remedy:
Rationale: Oxidation by air or water is important to understand the response of the fuel.	Rationale: Some data exist, but the database is incomplete.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	SiC Layer Fission product release through undetected defects	Passage of fission products from the buffer region through defects in the SiC layer

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	5	Remedy:
Rationale: As the primary fission product barrier understanding the transport is very important.	Rationale: Effective diffusion coefficients exist in both the U.S. and Germany for the fission gases through the SiC. Release via defects has never been individually sorted out from the other transport mechanisms in any experiment. The parameters needed to model release via defects and the presence or absence of defects in the SiC layer particle to particle, and/or across the layer, and/or changes in the defect structure as a result of oxidation makes such an effort very expensive and time consuming. The use of effective diffusion coefficients although less scientifically satisfying is more pragmatic and may be completely acceptable in system safety analysis when accompanied by proper sensitivity studies that assume some percentage of defective SiC layers present in the core.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	SiC Layer Fission product release through failures, e.g., cracking	Passage of fission products from the buffer region through regions in the SiC layer that fail during operation or an accident

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: II	7	Remedy:
Rationale: A particle with a failed SiC layer, but intact PyC layers, will not release fission gas. The PyC layers must fail in order to have fission gas release. A failed layer sometimes is modeled as having no fission product retention characteristics in fuel performance models. This conservative assumption is reasonable assuming that the code can adequately calculate when an SiC layer can fail. The oxidation event may cause failure of the layer, which would then result in fission product release.	Rationale: Such a causal relationship can be modeled and sensitivity studies performed to determine the overall impact in an oxidation event.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	SiC Layer Thermodynamics of the SiC-fission product system	Chemical form of fission products including the effects of solubility, intermetallics, and chemical activity.

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	7	Remedy:
Rationale: Critical to understanding transport behavior of fission products	Rationale: Thermodynamic calculations have been performed for both the UO_2 and UCO systems over a broad temperature, burnup and enrichment range to establish the chemical forms of the fission products. Similar calculations can be performed in the presence of steam or air to determine the changes in chemical form of the fission products.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	SiC Layer Sintering	Change of SiC microstructure as a function of temperature

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	2	Remedy:
Rationale: The CVD SiC is very high density almost theoretical, so it is difficult to see that there would be much of a role for sintering to change the microstructure. Chemical effects from the oxidation event are much more important.	Rationale:	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	SiC Layer: Chemical attack by water	Rate of reaction per unit surface area as a function of temperature and partial pressure of steam
	Kinetics	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: II	6	Remedy:
Rationale: Oxidation by air or water is important to understand the response of the fuel.	Rationale: Some data exist, but the database is incomplete.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	SiC Layer: Chemical attack by water Catalysis	Modification of the reaction rate by fission products or impurities

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	5	Remedy:
Rationale: Impurities can modify the reaction rate and thus impact the course of the event.	Rationale: Some air oxidation rate data have been determined for SiC and thus implicitly include the effects of impurities. The effects of fission products have not been included because oxidation testing has not been performed on irradiated SiC material with fission products. In principle sensitivity calculations can be performed with variations in the oxidation rate to bound this effect.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	SiC Layer: Chemical attack by water	Changes in chemical form resulting from oxidizing or reducing fission products
	Changes in chemical form of fission products	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	7	Remedy:
Rationale: This can be important because the transport behavior is dependent on the chemical form.	Rationale: This can also be calculated for a range of oxygen potentials to determine if any of the key fission products change in chemical form during the air or water ingress accident.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	SiC Layer: Chemical attack by water	Changes in diffusivity, porosity, adsorptivity, etc.
	Changes in SiC properties	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	2	Remedy:
Rationale: The oxidation can change the microstructure of the SiC by creating tunnels or pathways in the matrix. Thus, because the microstructure changes, the porosity, adsorptivity, etc. can also change.	Rationale: No measurements have been made on this effect. Conservative assumptions on such changes may allow sensitivity studies in this area.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	SiC Layer: Chemical attack by water Holdup reversals	Release of SiC FP inventory

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue *Closure Criteria*
Rank: M	6	Remedy:
Rationale: As the oxidation process continues, any fission products trapped at sites in the SiC may be released because of the thermal energy associated with the oxidation.	Rationale: This can be accounted for in a very simplistic yet conservative manner if details are not well known or more sophisticated models with detrapping can be used if the fundamental data needed for such models exist.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	SiC Layer: Chemical attack by water Temperature distributions	Impact of SiC oxidation on temperature distribution through material

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: II	8	Remedy:
Rationale: Very important in doing an oxidation calculation is to make sure the temperature response of the material, as a result of the chemical reaction, is properly calculated.	Rationale: This is well known and can be done in most of the safety codes used by NRC (e.g. MELCOR). The degree of fine detail in the model may be an open question but can be handled with sensitivity studies.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Inner PyC Layer Gas-phase diffusion	Diffusion of gaseous fission products through layer (Knudsen and bulk diffusion through pore structure, and pressure driven permeation through structure)

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	6	Remedy:
Rationale: Transport through intact particles is less important than those with exposed kernels in ingress events.	Rationale: PyC effectively retain fission gases. Effective diffusion coefficients for noble gases through PyC exist for both German and U.S. PyC. The Knudsen diffusion formalism has not been historically used in the modeling. The effect of oxidation on changes in the transport behavior has not been studied. Sensitivity studies can be performed to bound potential changes to determine the impact on the overall source term.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Inner PyC Layer Condensed phase diffusion	Inter-granular diffusion and/or intra-grannular solid-state diffusion

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	6	Remedy:
Rationale: Transport through intact particles is less important than those with exposed kernels in ingress events.	Rationale: Data exist on the effective diffusivity of Cs, Ag, and Sr through the PyC layer. The mechanism responsible for the transport has not been definitively identified. The effect of oxidation on transport properties has not been studied. Sensitivity studies can be performed to bound potential changes to determine the impact on the overall source term.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Inner PyC Layer Pressure loading (Fission products)	Stress loading of the layer by increased pressure from fission products

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	8	Remedy:
Rationale: A key parameter to determine stress in coating layer	Rationale: Noble gases contribute to the pressure loading in the particle. The effect of temperature due to the oxidation event on the pressure is easily calculated.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Inner PyC Layer Pressure loading (Carbon monoxide)	Stress loading of the layer by carbon monoxide by increased pressure

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H for UO_2 and L for UCO	8	Remedy:
Rationale: A key parameter to determine stress in coating layer	Rationale: Co (for UO_2 only) contributes to the pressure loading in the particle. The effect of temperature due to the oxidation event on the pressure is easily calculated.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Inner PyC Layer Layer oxidation	Reaction of pyrolytic graphite with oxygen released from the kernel

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	3	Remedy:
Rationale: At high temperatures, oxygen release from kernel increases over that in normal operations because of instability of some oxidic fission products at high temperatures.	Rationale: Known at these temperatures	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Inner PyC Layer Stress state (compression/tension)	The state of the forces induced by external forces that are acting across the layer to resist movement

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	8	Remedy:
Rationale: The stress state is judged to be of low importance for a chemical oxidation event.	Rationale: Stress state is easily calculated using current finite element models for coated particles.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Inner PyC Layer Cracking	Lengths, widths and numbers of cracks produced in layer during accident

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	5	Remedy:
Rationale: A cracked IPyC will not retain fission gases and would act as a fast transport path for metallic fission products to the SiC layer. Furthermore, a cracked IPyC will allow CO to attack the SiC layer.	Rationale:	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Inner PyC Layer Intercalation	Trapping of species between sheets of the graphite structure

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	6	Remedy:
Rationale: Surface and bulk diffusion with intercalation of Cs and Sr (trapping) is probably the underlying mechanism of transport through the PyC. Given the large number of Cs atoms, the trapping may be somewhat less important in the IPyC than in the OPyC where fewer Cs atoms are expected and their concentration may be more on the order of the number of trapping sites.	Rationale: Transport models do not consider intercalation. Effective diffusion coefficients exist in both the U.S. and Germany for the Cs and Sr through IPyC. The data are probably a combination of diffusion and trapping via intercalation at these high temperatures but the two mechanisms have never been individually sorted out in any experiment. Furthermore, the models do not consider effects that oxidation could have on changing the microstucture and the intercalation behavior. The parameters needed for such detailed models and the changes in microstructure of the IPyC particle to particle and/or sometimes across the layer and/or as a result of oxidation make such an effort very expensive and time consuming. The use of effective diffusion coefficients although less scientifically satisfying is more pragmatic and may be completely acceptable in system safety analysis when accompanied by proper sensitivity studies.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Inner PyC Layer: Chemical attack by water Kinetics	Rate of reaction per unit surface area as a function of temperature and partial pressure of steam

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	7	Remedy:
Rationale: Oxidation of IPyC is needed to understand thermal response of the particles in the fuel element.	Rationale: Reaction rates for PyC are known at these temperatures.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Inner PyC Layer: Chemical attack by water Catalysis	Modification of the reaction rate by fission products or impurities

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	4	Remedy:
Rationale: Impurities can alter reaction rates and change course of the ingress event.	Rationale: Reaction rate testing of PyC would implicitly include the effects of any impurities on the overall oxidation. No chemical reaction rate measurements have been performed using irradiated PyC where fission products may be in the layer. In principle, sensitivity calculations can be performed with variations in the oxidation rate to bound this effect.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Inner PyC Layer: Chemical attack by water Changes in chemical form of fission products	Changes in chemical form resulting from oxidizing or reducing fission products

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: II	7	Remedy:
Rationale: This can be important because the transport behavior is dependent on the chemical form.	Rationale: This can also be calculated for a range of oxygen potentials to determine if any of the key fission products change in chemical form during the air or water ingress accident.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Inner PyC Layer: Chemical attack by water Changes in graphite properties	Changes in diffusivity, porosity, adsorptivity, etc.

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	6	Remedy:
Rationale: The oxidation can change the microstructure of the PyC by creating tunnels or pathways in the matrix. Thus, because the microstructure changes, the porosity, adsorptivity, etc., can also change.	Rationale: No measurements have been made on this effect. Conservative assumptions on such changes may allow sensitivity studies in this area.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Inner PyC Layer: Chemical attack by water	Release of graphite FP inventory
	Holdup reversal	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	6	Remedy:
Rationale: As the oxidation process continues, any fission products trapped at sites in the PyC may be released because of the thermal energy associated with the oxidation.	Rationale: This can be accounted for in a very simplistic yet conservative manner if details are not well known or more sophisticated models with detrapping can be used if the fundamental data needed for such models exist.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Inner PyC Layer: Chemical attack by water Temperature distribution	Impact of graphite oxidation on temperature distribution through material

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	8	Remedy:
Rationale: Very important in doing an oxidation calculation is to make sure the temperature response of the material as a result of the chemical reaction is properly calculated.	Rationale: This is well known and can be done in most of the safety codes used by NRC (e.g. MELCOR). The high conductivity of the PyC should make the gradient quite small in general. The degree of fine detail in the model may be an open question but can be handled with sensitivity studies.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Buffer Layer Gas-phase diffusion	Diffusion of gaseous fission products through layer (Knudsen and bulk diffusion through pore structure, and pressure driven permeation through structure)

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	7	Remedy:
Rationale: The transport is fairly rapid and thus oxidation is not expected to affect the transport in this layer significantly.	Rationale: Rapid diffusion through the porous structure of the buffer is assumed in both U.S. and German transport models. Knudsen diffusion calculations confirm rapid gas phase transport.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Buffer Layer Condensed-phase diffusion	Inter-granular diffusion and/or intra-grannular solid-state diffusion

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	7	Remedy:
Rationale: The transport is fairly rapid and thus oxidation is not expected to affect the transport in this layer significantly.	Rationale: Rapid transport of metallic fission products through the buffer has also been historically assumed in U.S. and German models. Key measurements needed to develop grain boundary diffusion models along the edges of the crystallite plans have never been obtained. Instead effective diffusion coefficients are used.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Buffer Layer Response to kernel swelling	Mechanical reaction of the layer to the growth of the kernel via swelling

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	4	Remedy:
Rationale: Not expected to be important in oxidation events	Rationale: Has been predicted by EU fuel modelers to be important at high burnup where swelling is large. Usually this is accommodated by appropriate changes in the buffer thickness to ensure that the kernel does not come in contact with the TRISO coated and cause large mechanical stresses. Has not been shown to be a problem in current irradiation database at relatively low burnup.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Buffer Layer Maximum fuel gaseous fission product uptake	Maximum loading of fission products that can deposit from the gas phase onto surfaces of materials surrounding the fuel kernel

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	2	Remedy:
Rationale: Not important in oxidation events; probably more important in reactivity related events	Rationale:	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Buffer Layer Layer oxidation	Reaction of buffer layer with oxide materials in the kernel

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	5	Remedy:
Rationale: Some oxide materials in the kernel become less stable resulting in additional oxygen that can react with the buffer causing additional CO formation.	Rationale: In UO_2 excess oxygen from fission reacts with fission products and then carbon from the buffer. This is well known and can be calculated and has been measured at low burnups. In UCO fuel no oxidation is expected.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Buffer Layer Thermal gradient	Change in temperature with distance

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	6	Remedy:
Rationale: In pebble cores, the temperature gradients are generally low because of the lower power per particle in the core. Thus, Soret effects are much less important. Thus, this effect is important as an initial condition for the accident. Under oxidation events the gradients are much smaller and thus much less important during the accident.	Rationale: Temperature gradients can drive thermal diffusion (Soret effect). Temperature gradients under normal operation are very high in prismatic cores (up to 10000 K/cm) which can cause Soret effects in fission product transport. Values of the heat of solution needed to model the fission product transport are sorely lacking.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Buffer Layer Irradiation and thermal shrinkage	Dimension changes in the buffer layer or changes in its porosity produced by irradiation or by exposure to elevated temperatures

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	7	Remedy:
Rationale: Rapid densification can occur in the buffer under exposure to neutrons. The state of the buffer is an important initial condition in fission product modeling. Thermal densification is not expected to be important at these temperatures.	Rationale: This is fairly well known and can be calculated.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Buffer Layer: Chemical attack by water Kinetics	Rate of reaction per unit surface area as a function of temperature and partial pressure of steam

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	7	Remedy:
Rationale: Overall considered to be of lower importance than the other layers in the particle	Rationale: Oxidation rates for PyC can be adjusted to estimate rates for the buffer.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Buffer Layer: Chemical attack by water	Modification of the reaction rate by fission products or impurities
	Catalysis	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	3	Remedy:
Rationale: In general, the effect is felt to be less important for this layer than other layers since rapid fission product transport through the layer is already assumed.	Rationale: Reaction rate testing of low-density carbon would implicitly include the effects of any impurities on the overall oxidation. No chemical reaction rate measurements have been performed using irradiated buffer material where fission products may be in the layer. In principle, sensitivity calculations can be performed with variations in the oxidation rate to bound this effect.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Buffer Layer: Chemical attack by water	Changes in chemical form resulting from oxidizing or reducing fission products
	Changes in chemical form of fission products	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: II	7	Remedy:
Rationale: This can be important because the transport behavior is dependent on the chemical form.	Rationale: This can also be calculated for a range of oxygen potentials to determine if any of the key fission products change in chemical form during the air or water ingress accident.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Buffer Layer: Chemical attack by water Changes in graphite properties	Changes in diffusivity, porosity, adsorptivity, etc.

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	3	Remedy:
Rationale: The oxidation can change the microstructure of the buffer by creating tunnels or pathways in the matrix. Thus, because the microstructure changes, the porosity, adsorptivity, etc., can also change. Given the high porosity in the buffer and the rapid fission product transport in this layer, these effects are not considered important.	Rationale: No measurements have been made on this effect.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Buffer Layer: Chemical attack by water	Release of graphite FP inventory
	Holdup reversal	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	3	Remedy:
Rationale: Given the rapid transport expected in the buffer, this effect is not expected to change the transport properties significantly.	Rationale: As the oxidation process continues, any fission products trapped at sites in the buffer may be released because of the thermal energy associated with the oxidation. This can be accounted for in a very simplistic yet conservative matter if details are not well known or more sophisticated models with detrapping can be used if the fundamental data needed for such models exist.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Buffer Layer: Chemical attack by water	Impact of graphite oxidation on temperature distribution through material
	Temperature distribution	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	8	Remedy:
Rationale: Very important in doing an oxidation calculation is to make sure the temperature response of the material as a result of the chemical reaction is properly calculated. It is rated medium because the reaction is endothermic.	Rationale: This is well known and can be done in most of the safety codes used by NRC (e.g. MELCOR). The degree of fine detail in the model may be any open question but can be handled with sensitivity studies.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Kernel Maximum fuel temperature	Maximum fuel temperature attained by the fuel kernel during the accident

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue *Closure Criteria*
Rank: H	7	Remedy:
Rationale: Temperature is the key parameter that drives fission product migration in the coated particle fuel.	Rationale: This can be calculated and sensitivity studies can determine its overall importance in any accident scenario.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Kernel Temperature vs. time transient conditions	The time-dependent variation of fuel temperature with time

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	7	Remedy:
Rationale: Similar to temperature and time at temperature, the thermal response of the particle is important to calculating fission product behavior in the particle.	Rationale: Sensitivity studies can be easily performed to determine the impact of this factor on the overall progression of the accident.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Kernel Energy Transport: Conduction within kernel	Flow of heat within a medium from a region of high temperature to a region of low temperature

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	6	Remedy:
Rationale: Needed to calculate thermal response of kernel	Rationale: Thermal conductivity of UO_2 is fairly high and reasonably well known. Conductivity of UCO is assumed to be that of UO_2. Can be varied easily in sensitivity studies to determine impact.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Kernel Thermodynamic state of fission products	Chemical and physical state of fission products

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	7	Remedy:
Rationale: Thermodynamic state of fission products can determine volatility and mobility of the species.	Rationale: Thermodynamic studies have been performed for UO_2, UCO and UC_2 systems and chemical states of major fission products have been identified as a function of burnup and temperature. The impact of air and/or water can be evaluated.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Kernel Oxygen flux	Mass transport of oxygen per unit surface area per unit time

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	6	Remedy:
Rationale: Less important in air and water ingress events than in traditional heatup events	Rationale:	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Kernel Grain growth	Enlargement of grains as a result of diffusion

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	4	Remedy:
Rationale: Not important for air or water ingress events	Rationale:	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Kernel Buffer carbon-kernel interaction	Chemical reaction between carbon and the fuel (UO_2) to form UC_2 and CO (gas)

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: II	6	Remedy:
Rationale: The reaction of the kernel and the buffer is known to form a "rind" of UC_2 at the interface between the two layers. Photomicrographs show a different phase that is easily distinguished optically. Such interaction can result in release of fission products.	Rationale:	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Kernel: Chemical attack by water Kinetics	Rate of reaction per unit surface area as a function of temperature and partial pressure of steam

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	7	Remedy:
Rationale: Kinetics determine changes in physio-chemical behavior of the kernel and associated fission product release. Especially important for exposed kernels assumed in this scenario.	Rationale: Data exist on the steam oxidation of UO_2 with lesser information available for UCO.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Kernel: Chemical attack by water	Modification of the reaction rate by fission products or impurities
	Catalysis	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	5	Remedy:
Rationale: Impurities can affect reaction rates, but influence of oxygen potential is more important.	Rationale: Implicitly built into the data on hydrolysis of irradiated UO_2 and UCO kernels.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Kernel: Chemical attack by water	Changes in chemical form resulting from oxidizing or reducing fission products
	Changes in chemical form of fission products	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	7	Remedy:
Rationale: The oxygen potential in the system (which is directly related to the oxygen partial pressure for air and the hydrogen to steam ratio of water) determines the chemical states of the fission products which affects their mobility.	Rationale: Can be calculated using thermodynamic tools	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Kernel: Chemical attack by water Changes in kernel properties	Changes in diffusivity, porosity, adsorptivity, etc.

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	5	Remedy:
Rationale: The oxidation can change the microstructure of the kernel and the resultant transport properties. Hyperstoichiometric uranium dioxide will behave differently than UO_2. In UCO, the oxygen will react with the carbide phase to produce more UO_2. The O/U ratio is a function of the hydrogen to steam pressure ratio. These are very important effects to determine fission product mobility in the kernel.	Rationale: Influence of water vapor on release from exposed kernels has been studied in in-pile tests.	Closure Criterion:

Additional Discussion

Appendix E.2

Detailed PIRT Submittal by the ORNL Panel Member

R. Morris

TRISO Fuel PIRT: Accident With Subsequent Water Intrusion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Fuel Element Irradiation history	The temperature, burnup and fast fluence history of the layer

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: II	≤ 1600 °C: 7	Remedy: None if the operating envelope remains the same, otherwise additional testing is necessary
	> 1600 °C: N/A	Remedy: N/A
Rationale: The fuel behavior is strongly related to its irradiation history. Increasing burnup and fluence beyond established limits generally degrades performance. The fraction of particles failed during normal operation is important as well as they will release first.	Rationale: (≤ 1600 °C) The Germans have collected a large database for their fuel under their specific operating conditions. Deviations from these conditions warrant additional testing. Note that the proven fuel envelope is less demanding than that required for the turbine concepts.	Closure Criterion: Verification that the fuel can meet any new operating condition.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

For a discussion of the best performing fuel see:

Performance Evaluation of Modern HTR TRISO Fuel, R. Gontard, H. Nabielek, HTA-IB-05/90, July 1990

Fuel Performance and Fission Product Behavior in Gas Cooled Reactors, IAEA-TECDOC-978 (1997)

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Fuel Element Condensed-phase diffusion	Inter-granular diffusion and/or intra-granular solid-state diffusion

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 4	Remedy: Defer to fission product transport area.
	> 1600 °C: N/A	Remedy: N/A
Rationale: The major barriers to fission product release are the particle coating layers. The diffusion through the fuel element matrix is considered to be relatively high, although it does sorb and trap some fission products. When this material is oxidized, these fission products can be released, so the inventory is important.	Rationale: (≤ 1600 °C) The fuel element matrix sorbs some of the released fission products (metals); data exist to estimate the inventory, however, chemical attack may alter things.	Closure Criterion: Diffusion and trapping coefficients for the material of interest as a function of temperature
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

Diffusion through the fuel element matrix is fairly rapid compared to the particle coating layers. Gases are not held up, but there is significant sorption of the released metals. Overall, the reactor core components can provide an attenuation factor of 10-1000 for the metallics; oxidation could release this inventory. The GT-MHR may change its matrix composition from the historical resins; if so, additional investigations may be necessary.
For examples of diffusion and sorption behavior in different HTGR materials see:

Fuel Performance and Fission Product Behavior in Gas Cooled Reactors, IAEA-TECDOC-978 (1997)

For general interest in the transport of volatile fission products through the reactor system see:

Plateout Phenomena in Direct-Cycle High Temperature Gas-Cooled Reactors, EPRI, Palo Alto, CA: 2002. 1003387.
An analytical Study of Volatile Metallic Fission Product Release From Very High Temperature Gas-Cooled Reactor Fuel and Core, S. Mitake, et. al., Nuclear Technology, 81 (1988), pages 7-12.
Fission Product Plateout and Liftoff in the MHTGR Primary System: A Review, NUREG/CR-5647

There are several codes for examining fission product transport in a HTGR core. The US, Germans, and Japanese all have models.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Fuel Element Gas phase diffusion	Diffusion of gaseous fission products through layer (Knudsen and bulk diffusion through pore structure, and pressure driven permeation through structure). Other factors include holdup, cracking, adsorption, site poisoning, permeability, sintering, and annealing.

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: II	≤ 1600 °C: 7	Remedy: None
	> 1600 °C: N/A	Remedy: N/A
Rationale: The fission gases migrate rapidly through the fuel element matrix after they escape from the particle. This fact is used to monitor fuel behavior via R/B. Any damaged particles will release fission gases. Water will react in these regions.	Rationale: (≤ 1600 °C) Data shows that the gases move rapidly through the matrix material and quickly enter the coolant and/or fuel element.	Closure Criterion: None
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

Fission gases move rapidly to the coolant once they exit the particle. In a reactor they are removed by the coolant purification system so the circulating inventory is low. Transport of volatile metallics is determined by the sorption isotherms and dust. Gases released by damaged particles will rapidly move through the reactor core system.

The actual reaction of water with the core materials is more complex. For a discussion of water ingress accidents and their effect on fuel see:

Fuel Performance and Fission Product Behavior in Gas Cooled Reactors, IAEA-TECDOC-978 (1997)
Source Term Estimation for Small-Sized HTRs: Status and Further Needs, Extracted From German Safety Analysis, R. Moormann, et. al., Nuclear Technology, 135, (2001), pages 183-193
Methods and Data for HTGR Fuel Performance and Radionuclide Release Modeling during Normal Operational and Accidents for Safety Analysis, K. Verfondern, et. al., Jul-2721

For examples of the type of modeling that has been done for transport see:

Fission Product Plateout and Liftoff in the MHTGR Primary System: A Review, NUREG/CR-5647
For fuel accident models see: *Compilation of Fuel Performance and Fission Product Transport Models and Database for MHTGR Design*, Martin, R.C., ORNL/NPR-91/6

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Fuel Element: Transport of metallic FPs through fuel element Chemical form	Chemical stoichiometry of the chemical species that includes the radioisotope of interest

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 5	Remedy: Determine the need for this detailed knowledge.
	> 1600 °C: N/A	Remedy: N/A
Rationale: The chemical form of the fission product will determine how it interacts with the reactor system materials. The chemical environment of the kernel and the reactor system can be quite different and depend on the kernel composition and the coolant impurities. The kernel is expected to be somewhat oxidizing and the normal reactor system quite reducing, thus the chemical form of the fission product may change as it leaves the fuel. Once the accident starts, the environment may become oxidizing again.	Rationale: (≤ 1600 °C) Thermochemical calculations can give plausible chemical forms, but this author is not aware of any measurements confirming the chemical states.	Closure Criterion: If necessary, collect or calculate the compounds.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

This issue of chemical forms probably should be covered under fission product transport since the reactor system has a difference chemical potential than the fuel. It will change again with the accident. Water will oxidize any carbides. See:

Fission Product Plateout and Liftoff in the MHTGR Primary System: A Review, NUREG/CR-5647
Chemical Behavior of Fission Products in Core Heatup Accidents in High-Temperature Gas-Cooled Reactors, R. Moormann, Nuclear Technology, 94 (1991), pages 56-67.
Source Term Estimation for Small-Sized HTRs: Status and Further Needs, Extracted From German Safety Analysis, R. Moormann, et. al., Nuclear Technology, 135, (2001), pages 183-193
Methods and Data for HTGR Fuel Performance and Radionuclide Release Modeling during Normal Operational and Accidents for Safety Analysis, K. Verfondern, et. al., Jul-2721

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Fuel Element: Chemical attack by water	Rate of reaction per unit surface area as a function of temperature and partial pressure of steam
	Kinetics	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: II	≤ 1600 °C: 4	Remedy: Review data and perform tests to fill in gaps.
	> 1600 °C: N/A	Remedy: N/A
Rationale: The kinetics are necessary in order to determine the reaction rates.	Rationale: (≤ 1600 °C) Some testing has been done on the reaction of steam with matrix material and graphite.	Closure Criterion: Sufficient data to resolve gaps.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

The reactor design should be accessed for the water ingress potential before proceeding with this testing, as it is expensive. Some testing has been done in this area. See:

Source Term Estimation for Small-Sized HTRs: Status and Further Needs, Extracted From German Safety Analysis, R. Moormann, et. al., Nuclear Technology, 135, (2001), pages 183-193

Fuel Performance and Fission Product Behavior in Gas Cooled Reactors, IAEA-TECDOC-978 (1997)

Compilation of Fuel Performance and Fission Product Transport Models and Database for MHTGR Design, R. Martin, ORNL/NPR-91/6

Methods and Data for HTGR Fuel Performance and Radionuclide Release Modeling during Normal Operational and Accidents for Safety Analysis, K. Verfondern, et. al., Jul-2721

The Reaction of Steam with Large Specimens of Graphite For The Experimental Gas-Cooled Reactor, R.E. Helms, R.E. MacPherson, ORNL-TM-984, March 1965

Reactivity of Graphite and Fueled Graphite Spheres with Oxidizing Gases, J.P. Blakely, ORNL-TM-751, February 1964

Oxidation of Unfueled and Fueled Graphite Spheres by Steam, J.L. Rutherford, J.P. Blakely, L.G. Overholser, ORNL-3947, May 1966

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Fuel Element: Chemical attack by water	Modification of the reaction rate by fission products or impurities
	Catalysis	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	≤ 1600 °C: 4	Remedy: Determine the need for this information and whether the issue is important.
	> 1600 °C: N/A	Remedy: N/A
Rationale: The presence of catalysis can greatly increase local reaction rates. However, this is an endothermic reaction, so the consequences are much less severe that for air.	Rationale: (≤ 1600 °C) Some work has been done in this area. This is the water-gas reaction and it has been investigated for similar materials.	Closure Criterion: Sufficient data to resolve the data need.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

<u>Additional Discussion</u>

The steam carbon reaction has some industrial importance and has been investigated. It remains to be seen how much of this work can be applied to nuclear grade materials.

An industrial report is: *Catalytic Gasification of Graphite or Carbon*, H. Heinemann, LBL-21702, April 1986
Also see chemical textbooks.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Fuel Element: Chemical attack by water	Changes in chemical form resulting from oxidizing or reducing fission products
	Changes in chemical form of fission products	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 4	Remedy: Determine the need for this knowledge, collect as necessary.
	> 1600 °C: N/A	Remedy: N/A
Rationale: Changes in the chemical form of the fission products can greatly change their transport properties.	Rationale: (≤ 1600 °C) Thermochemical codes can calculate the possible chemical compounds. Little confirmation work is available.	Closure Criterion: Collect data to resolve uncertainties
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

The forms and migration of the fission products can be complex. For some information on the chemical forms see:

Fission Product Plateout and Liftoff in the MHTGR Primary System: A Review, NUREG/CR-5647

Chemical Behavior of Fission Products in Core Heatup Accidents in High-Temperature Gas-Cooled Reactors, R. Moormann, Nuclear Technology, 94 (1991), pages 56-67.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Fuel Element: Chemical attack by water Changes in graphite properties	Changes in diffusivity, porosity, adsorptivity, etc.

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: II	≤ 1600 °C: 4	Remedy: Determine the data needs and new materials and see if the existing data base is useful
	> 1600 °C: N/A	Remedy: N/A
Rationale: Changes in graphite properties may changes the rate at which the graphite reacts.	Rationale: (≤ 1600 °C) Steam corrosion of graphite has been investigated for HTGRs	Closure Criterion: Sufficient information to resolve the issue.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

Some investigations are contained in:

The Reaction of Steam with Large Specimens of Graphite For The Experimental Gas-Cooled Reactor, R.E. Helms, R.E. MacPherson, ORNL-TM-984, March 1965

Reactivity of Graphite and Fueled Graphite Spheres with Oxidizing Gases, J.P. Blakely, ORNL-TM-751, February 1964

The particular material under relevant conditions needs to be examined, as there can be considerable variation in results.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Fuel Element: Chemical attack by water	Release of graphite FP inventory
	Holdup reversal	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 4	Remedy: Determine the fission product inventories likely to be released and their impact on the safety case. Collect data as necessary to resolve the issue.
	> 1600 °C: N/A	Remedy: N/A
Rationale: One concern of chemical attack is the release of fission products deposited on reactor core materials.	Rationale: (≤ 1600 °C) Some work has been done in this area.	Closure Criterion: Determination of the safety case and/or data to access the impact.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

The importance of this issue depends on the amount of fission products outside of sound particles. If the fuel quality is very high, then the amount of material available for release will be very low. If this is the case, then detailed analysis may be unnecessary. See:

Methods and Data for HTGR Fuel Performance and Radionuclide Release Modeling during Normal Operational and Accidents for Safety Analysis, K. Verfondern, et. al., Jul-2721

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Fuel Element: Chemical attack by water	Impact of graphite oxidation on temperature distribution through material
	Temperature distribution	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: II	≤ 1600 °C: 4	Remedy: Review the ability to calculate temperature distributions and determine if the situation warrants more work.
	> 1600 °C: N/A	Remedy: N/A
Rationale: Reaction rates are generally strong functions of temperature.	Rationale: (≤ 1600 °C) General modeling has been done for graphite and fuel oxidation. The specific case needs to be accessed.	Closure Criterion: Resolution of the calculational and data needs.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

Some investigations are contained in:

The Reaction of Steam with Large Specimens of Graphite For The Experimental Gas-Cooled Reactor, R.E. Helms, R.E. MacPherson, ORNL-TM-984, March 1965

Reactivity of Graphite and Fueled Graphite Spheres with Oxidizing Gases, J.P. Blakely, ORNL-TM-751, February 1964

The particular material under relevant conditions needs to be examined, as there can be considerable variation in results.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Outer PyC Layer Gas-phase diffusion	Diffusion of gaseous fission products through layer (Knudsen and bulk diffusion through pore structure, and pressure driven permeation through structure)

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	≤ 1600 °C: 5	Remedy: Insure that proper PyC is manufactured. Material properties are difficult to characterize.
	> 1600 °C: N/A	Remedy: N/A
Rationale: The PyC layers hold gases well. The diffusion coefficients are generally quite low. The biggest concern is the rupture of the layer and the release of gases. This layer may be attacked by air/steam.	Rationale: (≤ 1600 °C) A great deal of testing has been conduced on PyC at the temperatures of interest. The primary concern is fabricating the proper material and its loss during the accident.	Closure Criterion: Test fuel performs as expected
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

Extensive testing has been done of the PyC for BISO and TRISO fuels under helium conditions, less so under air/steam see:

Performance Evaluation of Modern HTR TRISO Fuel, R. Gontard, H. Nabielek, HTA-1B-05/90, July 1990

Fuel Performance and Fission Product Behavior in Gas Cooled Reactors, IAEA-TECDOC-978 (1997)

Nuclear Technology, 35, Number 2 (entire issue devoted to coated particle fuels)

If the OpyC is unbreached, the helium heatup issues generally apply. If the layer is damaged or burned away, then the loss of OPyC issues would apply.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Outer PyC Layer Condensed-phase diffusion	Inter-granular diffusion and/or intra-granular solid-state diffusion

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	≤ 1600 °C: 7	Remedy: None
	> 1600 °C: N/A	Remedy: N/A
Rationale: Metallic fission products generally diffuse through the layer rapidly at high temperatures. Its loss would make some difference, but the primary issue would be exposing the SiC to the steam.	Rationale: (≤ 1600 °C) The OpyC offers little holdup to metallics at accident temperatures.	Closure Criterion: None
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

Extensive testing has been done of the PyC for in helium BISO and TRISO fuels; less has been done for air/steam. See:

Performance Evaluation of Modern HTR TRISO Fuel, R. Gontard, H. Nabielek, HTA-IB-05/90, July 1990

Fuel Performance and Fission Product Behavior in Gas Cooled Reactors, IAEA-TECDOC-978 (1997)

Nuclear Technology, 35, Number 2 (entire issue devoted to coated particle fuels)

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Outer PyC Layer Layer oxidation	Uptake of oxygen by the layer through a chemical reaction

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: II	≤ 1600 °C: 4	Remedy: Determine the conditions of interest and collect the necessary data.
	> 1600 °C: N/A	Remedy: N/A
Rationale: The oxidation rate determines the life of this layer under steam ingress. Generally, a bulk rate is assumed rather than detailed behavior.	Rationale: (≤ 1600 °C) Testing has been done, but it is of a more integral nature.	Closure Criterion: Resolution of the data gaps.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

For information on fuel exposure in steam see:

Source Term Estimation for Small-Sized HTRs: Status and Further Needs, Extracted From German Safety Analysis, R. Moormann, et. al., Nuclear Technology, 135, (2001), pages 183-193

Fuel Performance and Fission Product Behavior in Gas Cooled Reactors, IAEA-TECDOC-978 (1997)

Compilation of Fuel Performance and Fission Product Transport Models and Database for MHTGR Design, R. Martin, ORNL/NPR-91/6

Methods and Data for HTGR Fuel Performance and Radionuclide Release Modeling during Normal Operational and Accidents for Safety Analysis, K. Verfondern, et. al., Jul-2721

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Outer PyC Layer Stress state (compression/tension)	The state of the forces induced by external forces that are acting across the layer to resist movement

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	≤ 1600 °C: 6	Remedy: Review and collect new data for the codes if necessary. Material properties are the major issue.
	> 1600 °C: N/A	Remedy: N/A
Rationale: The stress state of the OPyC helps keep a compression force on the SiC. Failure of the OpyC by oxidation increases the likelihood of SiC failure.	Rationale: (≤ 1600 °C) The fuel design codes include these calculations. (Assumes the PyC is irradiation stable)	Closure Criterion: Adequate test fuel performance.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

See the PIRT Design Table for references on fuel design. Also see the accident models. The most common accident model is pressure vessel failure. See:

Revised MHTGR High-Temperature Fuel Performance Models, R.C. Martin, ORNL/NPR-92/16

Methods and Data for HTGR Fuel Performance and Radionuclide Release Modeling during Normal Operational and Accidents for Safety Analysis, K. Verfondern, et. al., Jul-2721

Compilation of Fuel Performance and Fission Product Transport Models and Database for MHTGR Design, Martin, R.C., ORNL/NPR-91/6

Revised MHTGR High-Temperature Fuel Performance Models, R.C. Martin, ORNL/NPR-92/16

Fuel Performance and Fission Product Behavior in Gas Cooled Reactors, IAEA-TECDOC-978 (1997)

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Outer PyC Layer Intercalation	Trapping of species between sheets of the graphite structure

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	≤ 1600 °C: 2	Remedy: Review data to determine if it is important.
	> 1600 °C: N/A	Remedy: N/A
Rationale: Small amounts of material may be trapped in the layer, but the material sorbed in the matrix is expected to be much larger.	Rationale: (≤ 1600 °C) Some work has been done in this area, but it has not been an important driver.	Closure Criterion: None
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

With good SiC, the fission product transport to the OPyC is very low. Some new modeling efforts are determining if this is an important factor.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Outer PyC Layer Trapping	Adsorption of fission products on defects

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	≤ 1600 °C: 3	Remedy: Review data to determine if it is important.
	> 1600 °C: N/A	Remedy: N/A
Rationale: Some trapping is used in the modeling and it may play a role in the transport, but the FPs in the matrix appears to be the major concern.	Rationale: (≤ 1600 °C) Some modeling has looked at this	Closure Criterion: None
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

With good SiC, the fission product transport to the OPyC is very low. Current modeling efforts are investigating this effect. Even if it is a real effect, it may be consumed up by general data uncertainties.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Outer PyC Layer Cracking	Lengths, widths and numbers of cracks produced in layer during operation or an accident

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: II	≤ 1600 °C: 5 (models determine failure rather than cracks)	Remedy: Better data and model for fuel performance, especially PyC behavior.
	> 1600 °C: N/A	Remedy: N/A
Rationale: Failure of the OpyC affects the likelihood of SiC failure and exposes it to air/steam. Cracking of particle layers can result in particle failure. One intact PyC can retain gases, but metallic release will be high. Modeling often assumes that particles fail by overpressure rather than a small crack. A crack is assumed to equal failure.	Rationale: (≤ 1600 °C) Fuel models have been developed to model normal and accident behavior. Particles are assumed to fail when they meet some weakness criteria based on a layer stress. Details of cracks are not modeled (yet). Agreement has been good for high quality fuel	Closure Criterion: Models that predict fuel behavior under normal and accident conditions. Does one need cracks or just failure? This adds a lot of complexity.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

For some work on examining the effects of cracks on fuel performance and general models see:

Consideration of the Effects on Fuel Particle Behavior from Shrinkage Cracks in the Inner Pyrocarbon Layer, G.Miller, et. al., Journal of Nuclear Materials, 295 (2001), pages 205-212.

Key Differences in the Fabrication, Irradiation and Safety Testing of U.S. and German TRISO-coated Particle Fuel and Their Implications on Fuel Performance, D.A. Petti, et. al Nuclear Engineering and Design, 222 (2003) 281-297.

MHTGR TRISO-P Fuel Failure Evaluation Report, DOE-HTGR-90390*Compilation of Fuel Performance and Fission Product Transport Models and Database for MHTGR Design*, Martin, R.C., ORNL/NPR-91/6

Methods and Data for HTGR Fuel Performance and Radionuclide Release Modeling during Normal Operational and Accidents for Safety Analysis, K. Verfondern, et. al., Jul-2721

Compilation of Fuel Performance and Fission Product Transport Models and Database for MHTGR Design, Martin, R.C., ORNL/NPR-91/6

Revised MHTGR High-Temperature Fuel Performance Models, R.C. Martin, ORNL/NPR-92/16

Fuel Performance and Fission Product Behavior in Gas Cooled Reactors, IAEA-TECDOC-978 (1997)

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Outer PyC Layer: Chemical attack by water Kinetics	Rate of reaction per unit surface area as a function of temperature and partial pressure of steam

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: II	≤ 1600 °C: 3	Remedy: Determine the relevance of the event and collect the necessary data.
	> 1600 °C: N/A	Remedy: N/A
Rationale: The kinetics determine the reaction rate and duration of the accident.	Rationale: (≤ 1600 °C) Some work has been done in this area. The rate is sensitive to the specific material.	Closure Criterion: The need and the required data.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

See:

Compilation of Fuel Performance and Fission Product Transport Models and Database for MHTGR Design, Martin, R.C., ORNL/NPR-91/6

Fuel Performance and Fission Product Behavior in Gas Cooled Reactors, IAEA-TECDOC-978 (1997)

Oxidation of Unfueled and Fueled Graphite Spheres by Steam, J.L. Rutherford, J.P. Blakely, L.G. Overholser, ORNL-3947, May 1966

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Outer PyC Layer: Chemical attack by water Catalysis	Modification of the reaction rate by fission products or impurities

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	≤ 1600 °C: 4	Remedy: Review the literature and determine if it is relevant or important
	> 1600 °C: N/A	Remedy: N/A
Rationale: A catalysis can increase the reaction rate in the layer and hasten its failure.	Rationale: (≤ 1600 °C) The carbon steam reaction has been studied in some detail. It needs to be applied to the fuel.	Closure Criterion: Collect the effects of catalysis if necessary.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

If the fission product inventory in the PyC is low and its loss does not significantly increase the SiC failure probably, then this issue may be unimportant. The industrial literature needs to be consulted, as this is an important commercial reaction.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Outer PyC Layer: Chemical attack by water	Changes in chemical form resulting from oxidizing or reducing fission products
	Changes in chemical form of fission products	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 4	Remedy: Determine the need for this knowledge, collect as necessary.
	> 1600 °C: N/A	Remedy: N/A
Rationale: Changes in the chemical form of the fission products can greatly change their transport properties.	Rationale: (≤ 1600 °C) Thermochemical codes can calculate the possible chemical compounds. Little confirmation work is available.	Closure Criterion: Collect data to resolve uncertainties
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

If the inventory of the layer is low, this issue may be of little practical importance. The forms and migration of the fission products can be complex. For some information on the chemical forms see:

Fission Product Plateout and Liftoff in the MHTGR Primary System: A Review, NUREG/CR-5647

Chemical Behavior of Fission Products in Core Heatup Accidents in High-Temperature Gas-Cooled Reactors, R. Moormann, Nuclear Technology, 94 (1991), pages 56-67.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Outer PyC Layer: Chemical attack by water	Changes in diffusivity, porosity, adsorptivity, etc.
	Changes in graphite properties	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	≤ 1600 °C: 1	Remedy: Determine if this item is relevant.
	> 1600 °C: N/A	Remedy: N/A
Rationale: The modeling is not performed at this level; generally, the layer is assumed to disappear at some rate.	Rationale: (≤ 1600 °C) Not examined in this detail.	Closure Criterion: Collect relevant detail.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

This level of detail may not be necessary if all one needs is time to significant fuel releases as the failure of the SiC may dominate.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Outer PyC Layer: Chemical attack by water	Release of graphite FP inventory
	Holdup reversal	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	≤ 1600 °C: 3	Remedy: Determine the conditions of interest and collect the necessary data.
	> 1600 °C: N/A	Remedy: N/A
Rationale: As the OPyC is removed; any inventory of fission products will be released. The inventory of this layer is low for high quality fuel.	Rationale: (≤ 1600 °C) Some steam ingress experiments have been done.	Closure Criterion: Determine the relevance of this need and collect data.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

If the fuel performs as expected, the inventory of this layer will be very low. Thus, the actual details of its release may not be important. The greater problem will be that its loss exposes the SiC to water. See:

Compilation of Fuel Performance and Fission Product Transport Models and Database for MHTGR Design, Martin, R.C., ORNL/NPR-91/6

Fuel Performance and Fission Product Behavior in Gas Cooled Reactors, IAEA-TECDOC-978 (1997)

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Outer PyC Layer: Chemical attack by water	Impact of graphite oxidation on temperature distribution through material
	Temperature distribution	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 5	Remedy: Determine if the uncertainty in the temperatures is acceptable. Refine models and collect data as necessary.
	> 1600 °C: N/A	Remedy: N/A
Rationale: The temperature determines the reaction rates and thus how fast the layer is attacked.	Rationale: (≤ 1600 °C) Enough modeling has been done to reasonably estimate the temperatures.	Closure Criterion: Adequate data for calculations.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

<u>Additional Discussion</u>

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	SiC Layer Gas-phase diffusion	Diffusion of gaseous fission products through layer (Knudsen and bulk diffusion through pore structure, and pressure driven permeation through structure)

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 4	Remedy: Determine relevance of this issue and collect data if necessary.
	> 1600 °C: N/A	Remedy: N/A
Rationale: The SiC is an important barrier to fission products. Its damage will allow fission product to migrate. It is assumed that the OPyC has been destroyed so that air/steam can reach the layer. Also, note that the IPyC must also fail for gas release.	Rationale: (≤ 1600 °C) Germans have done extensive testing in this area with a helium atmosphere. The major problem is attack of the layer. Some work has been done in this area. Extensive work to collect diffusion coefficients has not been done.	Closure Criterion: Resolution of the uncertainties.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

Much work has been done in a helium atmosphere, but less has been done with steam. See:

Compilation of Fuel Performance and Fission Product Transport Models and Database for MHTGR Design, Martin, R.C., ORNL/NPR-91/6

Fuel Performance and Fission Product Behavior in Gas Cooled Reactors, IAEA-TECDOC-978 (1997)

Methods and Data for HTGR Fuel Performance and Radionuclide Release Modeling during Normal Operational and Accidents for Safety Analysis, K. Verfondern, et. al., Jul-2721

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	SiC Layer Condensed-phase diffusion	Inter-granular diffusion and/or intra-granular solid-state diffusion

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 4	Remedy: Outline the course of the accident and collect the relevant data.
	> 1600 °C: N/A	Remedy: N/A
Rationale: The SiC is the major barrier to the release of metallic fission products. It is assumed that the OPyC has been removed and team is attacking the SiC.	Rationale: (≤ 1600 °C) Integral experiments exposing a particle to air and steam have been done.	Closure Criterion: The course of the accident and the necessary data.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

Much work has been done in a helium atmosphere, but less has been done with steam. See:

Compilation of Fuel Performance and Fission Product Transport Models and Database for MHTGR Design, Martin, R.C., ORNL/NPR-91/6

Fuel Performance and Fission Product Behavior in Gas Cooled Reactors, IAEA-TECDOC-978 (1997)

Methods and Data for HTGR Fuel Performance and Radionuclide Release Modeling during Normal Operational and Accidents for Safety Analysis, K. Verfondern, et. al., Jul-2721

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	SiC Layer Thermal deterioration/decomposition	Decline in the quality of the layer due to thermal loading

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	≤ 1600 °C: 4	Remedy: If 1600°C and the irradiation envelope are adequate then okay; otherwise testing may be necessary, especially if air/steam contact layer.
	> 1600 °C: N/A	Remedy: N/A
Rationale: The loss of the SiC will result in the release of metallics even if the PyCs are in good shape. The loss of the OPyC will probably result in accelerated failure due to loss of strength.	Rationale: (≤ 1600 °C) Extensive testing at 1600°C has shown it to be a "safe" limit, but exposure to air/steam may accelerate the process.	Closure Criterion: Accident definition and the uncertainties with air/steam resolved.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

1600°C has been used as the maximum temperature; it is conservative and some researchers feel that 1650-1700°C may be allowable, but the steam exposure my greatly change the situation. The modeling approach to this situation needs to be resolved. This is a complex issue. Some references:

Compilation of Fuel Performance and Fission Product Transport Models and Database for MHTGR Design, Martin, R.C., ORNL/NPR-91/6

Fuel Performance and Fission Product Behavior in Gas Cooled Reactors, IAEA-TECDOC-978 (1997)

Methods and Data for HTGR Fuel Performance and Radionuclide Release Modeling during Normal Operational and Accidents for Safety Analysis, K. Verfondern, et. al., Jul-2721

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	SiC Layer Fission product corrosion	Attack of layer by fission products, e.g., Pd

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	≤ 1600 °C: 7	Remedy: None, if the particle operating temperature/time is below an acceptable damage limit.
	> 1600 °C: N/A	Remedy: N/A
Rationale: Some fission products may migrate to the SiC layer and damage it. This corrosion process is a function of temperature. The corrosion mostly occurs during normal operation at the higher temperatures and weakens the particle for the accident. At the higher accident temperatures, thermal decomposition effects dominate.	Rationale: (≤ 1600 °C) This effect has been studied both in-pile and out of pile. Controlling the maximum operating temperature is a major factor.	Closure Criterion: Insure that the operating conditions are acceptable
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

Palladium is one element that is of great concern for high temperature corrosion of SiC and temperature is an important driving factor. Corrosion rates are strong functions of temperature. See the other PIRT Tables and:

Fission Product Pd-SiC Interaction in Irradiated Coated-Particle Fuels, T.N. Tiegs, Nuclear Technology, 57, pages 389-398.

Silicon Carbide Corrosion in High-Temperature Gas-Cooled Reactor Fuel Particles, H. Grubmeier, et. al., Nuclear Technology, 35 (1977), pages 413-427

Out-of-Reactor Studies of Fission Product-Silicon Carbide Interactions in HTGR Fuel Particles, R. Lauf, et. al., Journal of Nuclear Materials, 120 (1984), pages 6-30

Carbon Monoxide-Silicon Carbide Interaction in HTGR Fuel Particles, K. Minato, et. al., Journal of Materials Science, 26 (1991), pages 2379-2388

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	SiC Layer Heavy metal diffusion	Diffusion of heavy metals through layer

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	≤ 1600 °C: 5	Remedy: None
	> 1600 °C: N/A	Remedy: N/A
Rationale: Diffusion of heavy metal through the particle could result is the redistribution of fissile material.	Rationale: (≤ 1600 °C) To this author's knowledge, heavy metal diffusion through the SiC is not a problem.	Closure Criterion: None
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

Significant migration of fissile material through SiC during an accident is not an issue at the temperatures of interest. See: *Compilation of Fuel Performance and Fission Product Transport Models and Database for MHTGR Design*, Martin, R.C., ORNL/NPR-91/6

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	SiC Layer Layer oxidation	Uptake of oxygen by the layer through a chemical reaction

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	≤ 1600 °C: 4	Remedy: Determine chemical conditions and release time for the relevant case.
	> 1600 °C: N/A	Remedy: N/A
Rationale: Oxidation of the SiC layer will destroy its fission product retention capability. A major issue is whether SiO or SiO_2 is produced. SiO_2 will produce a layer that impedes mass transfer while SiO is volatile. Also, if the IPyC breaks, the SiC layer may be exposed to CO that could slowly corrode it. This is less of a concern for UCO fuel.	Rationale: (≤ 1600 °C) Experiments have been done with particles and spheres.	Closure Criterion: Resolution of release rates.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

This is a complex issue. Some references:

Compilation of Fuel Performance and Fission Product Transport Models and Database for MHTGR Design, Martin, R.C., ORNL/NPR-91/6

Fuel Performance and Fission Product Behavior in Gas Cooled Reactors, IAEA-TECDOC-978 (1997)

Methods and Data for HTGR Fuel Performance and Radionuclide Release Modeling during Normal Operational and Accidents for Safety Analysis, K. Verfondern, et. al., Jul-2721

CO corrosion can be a problem at the higher pressures and temperatures if a crack in the IPyC allows access to the SiC. Controlling the IPyC properties and controlling the CO by using UCO or gettering the fuel can mitigate this problem. See other PIRT tables and:

Carbon Monoxide-Silicon Carbide Interaction in HTGR Fuel Particles, K. Minato, et. al., Journal of Materials Science, 26 (1991), pages 2379-2388

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	SiC Layer Fission product release through undetected defects	Passage of fission products from the buffer region through defects in the SiC layer

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	≤ 1600 °C: 7	Remedy: Defer to fuel fabrication
	> 1600 °C: N/A	Remedy: N/A
Rationale: Defective SiC will allow gas transport if the PyCs both fail. This is more of a manufacturing issue that shows up when the fuel is stressed.	Rationale: (≤ 1600 °C) This is a manufacturing issue that shows up during accident conditions.	Closure Criterion: None
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

The SiC layer can be damaged during compact fabrication by iron impurities. The particles will still retain gases as long as one of the PyCs is good. See the PIRT on Manufacturing Design. It is not known if the chemical attack will worsen the situation.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	SiC Layer Fission product release through failures, e.g. cracking	Passage of fission products from the buffer region through regions in the SiC layer that fail during operation or an accident

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: II	≤ 1600 °C: 4	Remedy: If the fuel is used outside of its tested region, more testing is needed.
	> 1600 °C: N/A	Remedy: N/A
Rationale: Failure of the SiC will allow fission gas to pass through it. If the PyC remains good, the gas will not be released, if not, the gas will be released. Metallics will be released in both cases. See previous SiC entries.	Rationale: (≤ 1600 °C) C Accident models have been compared to experiments to approximately model the situation. If material properties are consistent, useful predictions can be made, however chemical attack issues can change the results.	Closure Criterion: Resolution of identified concerns.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

Most SiC failure models are based on pressure vessel failure. More recent models are considering cracking. See the other PIRT Tables and:

Revised MHTGR High-Temperature Fuel Performance Models, R.C. Martin, ORNL/NPR-92/16

Methods and Data for HTGR Fuel Performance and Radionuclide Release Modeling during Normal Operational and Accidents for Safety Analysis, K. Verfondern, et. al., Jul-2721

MHTGR TRISO-P Fuel Failure Evaluation Report, DOE-HTGR-90390, 1993

Fuel Performance and Fission Product Behavior in Gas Cooled Reactors, IAEA-TECDOC-978 (1997)

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	SiC Layer Thermodynamics of the SiC-fission product system	Chemical form of fission products including the effects of solubility, intermetallics, and chemical activity

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 7	Remedy: None, if the particle operating temperature/time is below an acceptable damage limit.
	> 1600 °C: N/A	Remedy: N/A
Rationale: Some fission products may migrate to the SiC layer and damage it. This corrosion process is a function of temperature. See the entry on corrosion. If the SiC fails and steam enters, the oxidation state may increase, which may not be bad.	Rationale: (≤ 1600 °C) This effect has been studied both in-pile and out of pile. Controlling the maximum operating temperature is a major factor.	Closure Criterion: Acceptable performance.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

See entries on corrosion and the other PIRT Tables. Also see entries on UCO. One of the goals of kernel design is to stabilize the corrosive elements so they do not migrate to the SiC. Also, determine if steam attack kernel.

During normal or accident conditions, the SiC can crack or break due to over pressure or an interaction with cracked PyC. High temperatures increase the pressure in a particle. Above 1600 °C or so, decomposition begins to weaken the SiC and it can fail.

For some work on examining the effects of cracks on fuel performance and general models see the other PIRT tables and:

Consideration of the Effects on Fuel Particle Behavior from Shrinkage Cracks in the Inner Pyrocarbon Layer, G.Miller, et. al., Journal of Nuclear Materials, 295 (2001), pages 205-212.

Key Differences in the Fabrication, Irradiation and Safety Testing of U.S. and German TRISO-coated Particle Fuel and Their Implications on Fuel Performance, D.A. Petti, et. al., INEEL/EXT-02-00300

Revised MHTGR High-Temperature Fuel Performance Models, R.C. Martin, ORNL/NPR-92/16

Methods and Data for HTGR Fuel Performance and Radionuclide Release Modeling during Normal Operational and Accidents for Safety Analysis, K. Verfondern, et. al., Jul-2721

MHTGR TRISO-P Fuel Failure Evaluation Report, DOE-HTGR-90390, 1993

Fuel Performance and Fission Product Behavior in Gas Cooled Reactors, IAEA-TECDOC-978 (1997)

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	SiC Layer Sintering	Change of graphite microstructure as a function of temperature

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	≤ 1600 °C: 7	Remedy: None if temperatures are below 1600 °C, an steam environment may modify this.
	> 1600 °C: N/A	Remedy: N/A
Rationale: SiC doesn't appear to suffer any significant changes at normal operating conditions and survives at 1600 °C without large changes.	Rationale: (≤ 1600 °C) Extensive testing at 1600 °C for hundreds of hours has shown the good behavior of SiC.	Closure Criterion: None
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

The major challenge is to reproduce the SiC that performed so well in past testing. The exposure to steam is expected to lead to corrosion effects rather than sintering effects. The loss of the SiC integrity is the major issue.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	SiC Layer: Chemical attack by water	Rate of reaction per unit surface area as a function of temperature and partial pressure of steam
	Kinetics	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	≤ 1600 °C: 1	Remedy: Determine chemical conditions and release time for the relevant case.
	> 1600 °C: N/A	Remedy: N/A
Rationale: The rates determine how long the SiC will last. Also, oxidation of the SiC layer will destroy its fission product retention capability. A major issue is whether SiO or SiO_2 is produced. SiO_2 will produce a layer that impedes mass transfer while SiO is volatile. This is less important for steam.	Rationale: (≤ 1600 °C) Not much is known about this rate. It is assumed to be small and most experiments look at kernel oxidation rather than SiC. SiC work has been done at lower temperatures.	Closure Criterion: Resolution of reaction rates.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

Steam is less aggressive than air and this may not be a significant problem. Some references:

Compilation of Fuel Performance and Fission Product Transport Models and Database for MHTGR Design, Martin, R.C., ORNL/NPR-91/6

Fuel Performance and Fission Product Behavior in Gas Cooled Reactors, IAEA-TECDOC-978 (1997)

Methods and Data for HTGR Fuel Performance and Radionuclide Release Modeling during Normal Operational and Accidents for Safety Analysis, K. Verfondern, et. al., Jul-2721

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	SiC Layer: Chemical attack by water	Modification of the reaction rate by fission products or impurities
	Catalysis	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	≤ 1600 °C: 1	Remedy: Determine the relevance of this issue.
	> 1600 °C: N/A	Remedy: N/A
Rationale: A catalysis could increase the reaction rate and enhance the failure of the SiC.	Rationale: (≤ 1600 °C) Unknown	Closure Criterion: Resolution of issue.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

This area is less explored for fuel. Some industrial literature may exist. Since water is less aggressive than air, this issue may be less important.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	SiC Layer: Chemical attack by water	Changes in chemical form resulting from oxidizing or reducing fission products
	Changes in chemical form of fission products	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 4	Remedy: Determine the need for this knowledge, collect as necessary.
	> 1600 °C: N/A	Remedy: N/A
Rationale: Changes in the chemical form of the fission products can greatly change their transport properties. Once the SiC fails, the potential for significant particle releases increase. The greatest change may come from the reaction of UC and the change in kernel structure.	Rationale: (≤ 1600 °C) Thermochemical codes can calculate the possible chemical compounds. Little confirmation work is available.	Closure Criterion: Collect data to resolve uncertainties
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

The forms and migration of the fission products can be complex. For some information on the chemical forms see:

Fission Product Plateout and Liftoff in the MHTGR Primary System: A Review, NUREG/CR-5647

Chemical Behavior of Fission Products in Core Heatup Accidents in High-Temperature Gas-Cooled Reactors, R. Moormann, Nuclear Technology, 94 (1991), pages 56-67.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	SiC Layer: Chemical attack by water	Changes in diffusivity, porosity, adsorptivity, etc.
	Changes in SiC properties	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	≤ 1600 °C: 1	Remedy: Determine if this item is relevant.
	> 1600 °C: N/A	Remedy: N/A
Rationale: The modeling is not performed at this level; generally, the layer is assumed to disappear at some rate.	Rationale: (≤ 1600 °C) Not examined in this detail.	Closure Criterion: Collect relevant detail.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

<u>Additional Discussion</u>

This level of detail may not be necessary if all one needs is time to significant fuel releases as the SiC fails. An integral failure of the SiC may be sufficient without all this detail.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	SiC Layer: Chemical attack by water	Release of SiC FP inventory
	Holdup reversal	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	≤ 1600 °C: 3	Remedy: Determine the conditions of interest and collect the necessary data
	> 1600 °C: N/A	Remedy: N/A
Rationale: As the SiC is removed; any inventory of fission products will be released. The inventory of this layer is low for high quality fuel	Rationale: (≤ 1600 °C) Some air ingress work has been done.	Closure Criterion: Determine the relevance of this need and collect data
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

If the fuel performs as expected, the inventory of this layer will be very low. Thus, the actual details of its release may not be important. The greater problem is that its loss exposes the high inventory kernel. See:

Compilation of Fuel Performance and Fission Product Transport Models and Database for MHTGR Design, Martin, R.C., ORNL/NPR-91/6

Fuel Performance and Fission Product Behavior in Gas Cooled Reactors, IAEA-TECDOC-978 (1997)

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	SiC Layer: Chemical attack by water	Impact of SiC oxidation on temperature distribution through material
	Temperature distribution	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 5	Remedy: Determine if the uncertainty in the temperatures is acceptable. Refine models and collect data as necessary.
	> 1600 °C: N/A	Remedy: N/A
Rationale: The temperature determines the reaction rates and thus how fast the layer is attacked.	Rationale: (≤ 1600 °C) Enough modeling has been done to reasonably estimate the temperatures	Closure Criterion: Adequate data for calculations.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Inner PyC Layer Gas-phase diffusion	Diffusion of gaseous fission products through layer (Knudsen and bulk diffusion through pore structure, and pressure driven permeation through structure)

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 4	Remedy: None at present
	> 1600 °C: N/A	Remedy: N/A.
Rationale: Gas diffusion through the PyCs is generally quite low at the temperatures of interest. The SiC layer must be brecched for the gases to get out. If the SiC layer has been damaged, the failure likelihood of the IPyC is increased. If attack of the IPyC occurs, significant release will soon follow.	Rationale: (≤ 1600 °C) Gas diffusion through the PyCs has been shown to be quite low. The issue is the layer behavior after is has been attacked. Some integral testing has been done.	Closure Criterion: Acceptable test fuel behavior
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

Extensive testing has been done on various fuels over a range of temperatures. The challenge is to reproduce this good material. See:

Performance Evaluation of Modern HTR TRISO Fuel, R. Gontard, H. Nabielek, HTA-1B-05/90, July 1990
Fuel Performance and Fission Product Behavior in Gas Cooled Reactors, IAEA-TECDOC-978 (1997)
Fission-Product Release During Postirradiation Annealing of Several Types of Coated Fuel Particles, R.E. Bullock, Journal of Nuclear Materials, 125 (1984), pages 304-319

The concern is how the chemical attack affects the layer. For accident models see:

Compilation of Fuel Performance and Fission Product Transport Models and Database for MHTGR Design, Martin, R.C., ORNL/NPR-91/6
Revised MHTGR High-Temperature Fuel Performance Models, R.C. Martin, ORNL/NPR-92/16
Methods and Data for HTGR Fuel Performance and Radionuclide Release Modeling during Normal Operational and Accidents for Safety Analysis, K. Verfondern, et. al., Jul-2721

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Inner PyC Layer Condensed-phase diffusion	Inter-granular diffusion and/or intra-granular solid-state diffusion

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	≤ 1600 °C: 4	Remedy: None, nothing can be done
	> 1600 °C: N/A	Remedy: N/A
Rationale: The diffusion of metallic fission products through the PyCs is known to be fairly high. Only modest credit can be taken for PyC as a barrier or release delay for metallics. Any chemical attack will only enhance the diffusion.	Rationale: (≤ 1600 °C) The PyCs are generally assumed to provide limited retention to metallic fission products at accident temperatures. Chemical attack may make the situation worse.	Closure Criterion: None
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

For a discussion of PyC and metallics see:

Nuclear Technology, 35, Number 2, Fission Product Release Section, pages 457-526

For the higher accident temperatures, the PyCs are assumed to have essentially no resistance to metallic transport. The PyC offers some impedance to metallic transport, but is not a major barrier. Chemical attack will worsen the situation, but the SiC layer is the important one.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Inner PyC Layer Pressure loading (Fission products)	Stress loading of the layer by increased pressure from fission products

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: II	≤ 1600 °C: 7	Remedy: Proper design and fabrication
	> 1600 °C: N/A	Remedy: N/A
Rationale: Depending on the particular configuration, the PyC layers can help keep the SiC in compression. Loss of a PyC layer can increase the probability of SiC failure.	Rationale: (≤ 1600 °C) Pressure can be controlled by particle design, burnup, and kernel composition. Analysis and designs are available	Closure Criterion: Acceptable fuel performance
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

According to the fuel models, the PyC functions as an important load-bearing component of the fuel particle. See the PIRT Design Table for more information concerning the stresses. Loss of other layers due to chemical attack influences the structural stability of the entire particle.

A major concern is the proper material properties – see the Manufacturing Design PIRT

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Inner PyC Layer	Stress loading of the layer by carbon monoxide by increased pressure
	Pressure loading (Carbon monoxide)	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 7	Remedy: Control pressure by design
	> 1600 °C: N/A	Remedy: N/A
Rationale: High CO product will result in high particle pressures, especially at the higher accident temperatures. Changing the kernel composition can control CO production.	Rationale: (≤ 1600 °C) Pressure can be controlled by particle design, burnup, and kernel composition. Analysis and designs are available.	Closure Criterion: Proof testing of final fuel design
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

For a discussion on kernel design to minimize CO and immobilize key fission products see:

Stoichiometric Effects on Performance of High-Temperature Gas-Cooled Reactor Fuels from the U-C-O System, F.J. Homan, et. al., Nuclear Technology, 35, pages 428-441.
See the other PIRT Tables for fuel design issues.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Inner PyC Layer Layer oxidation	Reaction of pyrolytic graphic with oxygen released from the kernel.

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: II	≤ 1600 °C: 3	Remedy: Collect relevant data
	> 1600 °C: N/A	Remedy: N/A
Rationale: Defects or cracks in the OPyC and SiC can allow steam to enter the particle and oxidize the IPyC. This will release fission gases and provide a direct path to the kernel.	Rationale: (≤ 1600 °C) This behavior is similar to the burn leach tests used to determine fuel quality. The rates are assumed to be the same as for OPyC	Closure Criterion: Reasonable calculational basis.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

If both the OPyC and the SiC are breeched, then the particle is releasing.

Performance Evaluation of Modern HTR TRISO Fuel, R. Gontard, H. Nabielek, HTA-1B-05/90, July 1990
Fuel Performance and Fission Product Behavior in Gas Cooled Reactors, IAEA-TECDOC-978 (1997)
Fission-Product Release During Postirradiation Annealing of Several Types of Coated Fuel Particles, R.E. Bullock, Journal of Nuclear Materials, 125 (1984), pages 304-319

For accident models see:

Compilation of Fuel Performance and Fission Product Transport Models and Database for MHTGR Design, Martin, R.C., ORNL/NPR-91/6
Revised MHTGR High-Temperature Fuel Performance Models, R.C. Martin, ORNL/NPR-92/16
Methods and Data for HTGR Fuel Performance and Radionuclide Release Modeling during Normal Operational and Accidents for Safety Analysis, K. Verfondern, et. al., Jul-2721

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Inner PyC Layer Stress state (compression/tension)	The state of the forces induced by external forces that are acting across the layer to resist movement

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 7	Remedy: Control pressure by design
	> 1600 °C: N/A	Remedy: N/A
Rationale: Failure of the PyC can increase the likelihood of SiC failure. See the previous pressure loading entries.	Rationale: (≤ 1600 °C) Pressure can be controlled by particle design, burnup, and kernel composition. Analysis and designs are available	Closure Criterion: Proof testing of final fuel design
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

See the table entries about pressure loading and also the PIRT Design Tables.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Inner PyC Layer Cracking	Lengths, widths and numbers of cracks produced in layer during accident

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 4 (failure only, cracking is not calculated)	Remedy: Review and collect new data for the codes if necessary.
	> 1600 °C: N/A	Remedy: N/A
Rationale: Failure of the IPyC affects the likelihood of SiC failure. See the entry on stress state. The lengths, widths, and number of cracks don't really matter – the failure does. Many models assume the SiC layer will dominate the particle failure. Effects of chemical attack may not be included.	Rationale: (≤ 1600 °C) Fuel models have been developed to model normal and accident behavior. Particles are assumed to fail when they meet some weakness criteria rather based a layer stress.	Closure Criterion: Models that predict fuel behavior under normal and accident conditions. Does one need cracks or just failure? This adds a lot of complexity.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

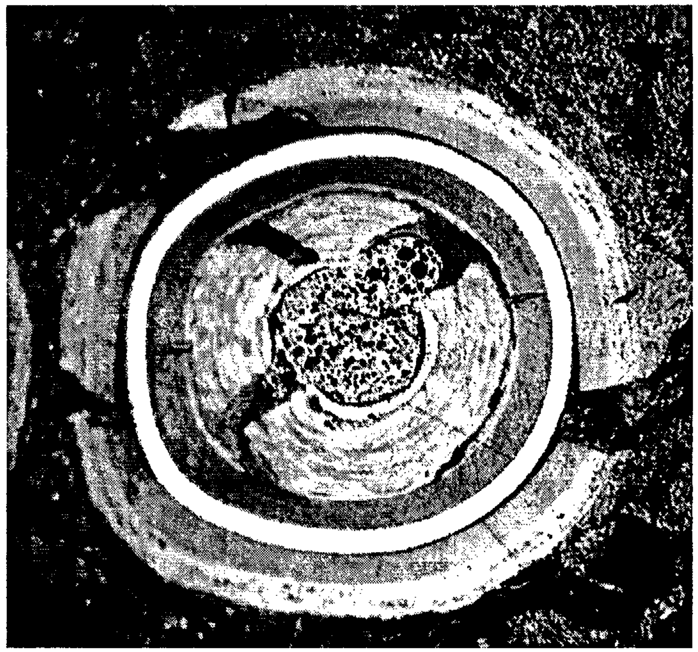
Under accident conditions, a pressure vessel type failure model has been used with the particle failing when the pressure exceeds a critical value. The accident models may not include all the chemical attack effects.

For some work on examining the effects of cracks on fuel performance and general models see:

Consideration of the Effects on Fuel Particle Behavior from Shrinkage Cracks in the Inner Pyrocarbon Layer, G.Miller, et. al., Journal of Nuclear Materials, 295 (2001), pages 205-212.
Key Differences in the Fabrication, Irradiation and Safety Testing of U.S. and German TRISO-coated Particle Fuel and Their Implications on Fuel Performance, D.A. Petti, et. al Nuclear Engineering and Design, 222 (2003) 281-297.

MHTGR TRISO-P Fuel Failure Evaluation Report, DOE-HTGR-90390

Compilation of Fuel Performance and Fission Product Transport Models and Database for MHTGR Design, Martin, R.C., ORNL/NPR-91/6
Revised MHTGR High-Temperature Fuel Performance Models, R.C. Martin, ORNL/NPR-92/16
Methods and Data for HTGR Fuel Performance and Radionuclide Release Modeling during Normal Operational and Accidents for Safety Analysis, K. Verfondern, et. al., Jul-2721



Massive pyrocarbon failure In HRB-21 due to a design flaw (seal coats) resulted in cracks that appear to have compromised the SiC and resulted in releases. (ORNL)

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Inner PyC Layer Intercalation	Trapping of species between sheets of the graphite structure

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	≤ 1600 °C: 2	Remedy: None
	> 1600 °C: N/A	Remedy: N/A
Rationale: This layer is likely to be saturated with fission products and this effect may only make a minor difference.	Rationale: (≤ 1600 °C) This situation has not caused problems	Closure Criterion: None
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

Some modeling is looking at this situation.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Inner PyC Layer: Chemical attack by water Kinetics	Rate of reaction per unit surface area as a function of temperature and partial pressure of steam

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 3	Remedy: Determine the relevance of the event and collect the necessary data.
	> 1600 °C: N/A	Remedy: N/A
Rationale: The kinetics determine the reaction rate and duration of the accident.	Rationale: (≤ 1600 °C) Some work has been done in this area. The rate is sensitive to the specific material.	Closure Criterion: The need and the required data.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

See:

Compilation of Fuel Performance and Fission Product Transport Models and Database for MHTGR Design, Martin, R.C., ORNL/NPR-91/6

Fuel Performance and Fission Product Behavior in Gas Cooled Reactors, IAEA-TECDOC-978 (1997)

Oxidation of Unfueled and Fueled Graphite Spheres by Steam, J.L. Rutherford, J.P. Blakely, L.G. Overholser, ORNL-3947, May 1966

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Inner PyC Layer: Chemical attack by water Catalysis	Modification of the reaction rate by fission products or impurities

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	≤ 1600 °C: 4	Remedy: Review the literature and determine if it is relevant or important
	> 1600 °C: N/A	Remedy: N/A
Rationale: A catalysis can increase the reaction rate in the layer and hasten its failure.	Rationale: (≤ 1600 °C) The carbon steam reaction has been studied in some detail. It needs to be applied to the fuel.	Closure Criterion: Collect the effects of catalysis if necessary.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

If the fission product inventory in the PyC is low and its loss does not significantly increase the SiC failure probably, then this issue may be unimportant. The industrial literature needs to be consulted, as this is an important commercial reaction.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Inner PyC Layer: Chemical attack by water	Changes in chemical form resulting from oxidizing or reducing fission products
	Changes in chemical form of fission products	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 4	Remedy: Determine the need for this knowledge, collect as necessary.
	> 1600 °C: N/A	Remedy: N/A
Rationale: Changes in the chemical form of the fission products can greatly change their transport properties. Once the SiC fails, the potential for significant particle releases increase. The greatest change may come from the reaction of UC and the change in kernel structure.	Rationale: (≤ 1600 °C) Thermochemical codes can calculate the possible chemical compounds. Little confirmation work is available.	Closure Criterion: Collect data to resolve uncertainties
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

The forms and migration of the fission products can be complex. For some information on the chemical forms see:

Fission Product Plateout and Liftoff in the MHTGR Primary System: A Review, NUREG/CR-5647

Chemical Behavior of Fission Products in Core Heatup Accidents in High-Temperature Gas-Cooled Reactors, R. Moormann, Nuclear Technology, 94 (1991), pages 56-67.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Inner PyC Layer: Chemical attack by water	Changes in diffusivity, porosity, adsorptivity, etc.
	Changes in graphite properties	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	≤ 1600 °C: 1	Remedy: Determine if this item is relevant.
	> 1600 °C: N/A	Remedy: N/A
Rationale: The modeling is not performed at this level; generally, the layer is assumed to disappear at some rate.	Rationale: (≤ 1600 °C) Not examined in this detail.	Closure Criterion: Collect relevant detail.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

This level of detail may not be necessary if all one needs is time to significant fuel releases as the failure of the SiC may dominate.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Inner PyC Layer: Chemical attack by water	Release of graphite FP inventory
	Holdup reversal	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	≤ 1600 °C: 3	Remedy: Nothing, as the kernel release will dominate.
	> 1600 °C: N/A	Remedy: N/A
Rationale: Once the SiC fails and the IPyC is exposed, releases begin to increase rapidly. The inventory of the IPyC is irrelevant compared to the kernel, which is exposed as soon as the IPyC is damaged.	Rationale: (≤ 1600 °C) The actual inventory of the IPyC at the time the SiC is breeched is only roughly known.	Closure Criterion: None
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

Once the IPyC is exposed to chemical attack, releases will increase, as the kernel will be exposed.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Inner PyC Layer: Chemical attack by water	Impact of graphite oxidation on temperature distribution through material
	Temperature distribution	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: II	≤ 1600 °C: 5	Remedy: Determine if the uncertainty in the temperatures is acceptable. Refine models and collect data as necessary.
	> 1600 °C: N/A	Remedy: N/A
Rationale: The temperature determines the reaction rates and thus how fast the layer is attacked.	Rationale: (≤ 1600 °C) Enough modeling has been done to reasonably estimate the temperatures.	Closure Criterion: Adequate data for calculations.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Buffer Layer Gas-phase diffusion	Diffusion of gaseous fission products through layer (Knudsen and bulk diffusion through pore structure, and pressure driven permeation through structure)

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 7	Remedy: None
	> 1600 °C: N/A	Remedy: N/A
Rationale: The buffer layer is designed to be a void to collect the gases released from the kernel. The problem would be if it weren't porous.	Rationale: (≤ 1600 °C) The buffer layer appears to work as planned. Gases are expected to diffusive through this layer.	Closure Criterion: None
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

Once this layer is exposed, the kernel is essentially exposed.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Buffer Layer Condensed-phase diffusion	Inter-granular diffusion and/or intra-granular solid-state diffusion

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 7	Remedy: None
	> 1600 °C: N/A	Remedy: N/A
Rationale: The buffer layer is essentially void volume and is not expected to offer resistance to transport. Some material may be sorbed on this layer.	Rationale: (≤ 1600 °C) The buffer layer appears to work as planned. Fission products are expected to diffusive through this layer.	Closure Criterion: None
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

Once this layer is exposed, the kernel is essentially exposed.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Buffer Layer Response to kernel swelling	Mechanical reaction of the layer to the growth of the kernel via swelling

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	≤ 1600 °C: 7	Remedy: None
	> 1600 °C: N/A	Remedy: N/A
Rationale: The buffer layer must be weak enough that it will deform or crush without transmitting high forces to the IPyC as the kernel distorts.	Rationale: (≤ 1600 °C) All evidence to date indicates that the buffer layer performs as expected.	Closure Criterion: None
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

In the accident fuel testing done to date, no evidence of adverse buffer reaction to kernel swelling was apparent.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Buffer Layer Maximum fuel gaseous fission product uptake	Maximum loading of fission products that can deposit from the gas phase onto surfaces of materials surrounding the fuel kernel

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: II	≤ 1600 °C: 7	Remedy: None
	> 1600 °C: N/A	Remedy: N/A
Rationale: The buffer layer must have sufficient void volume to control the pressure from released fission gases and CO.	Rationale: (≤ 1600 °C) All evidence to date indicates that the buffer layer performs as expected.	Closure Criterion: None
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

This is really a design issue. See the PIRT Design Table.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Buffer Layer Layer oxidation	Reaction of buffer layer with oxide materials in the kernel.

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	≤ 1600 °C: 7	Remedy: None
	> 1600 °C: N/A	Remedy: N/A
Rationale: A small portion of the layer is oxidized by the excess oxygen released form the kernel. This is of no consequence, as the layer has no structural function. It is of no consequence if the buffer is oxidized by air/steam as the particle is already failed.	Rationale: (≤ 1600 °C) No problem ahs been observed. The basic problem is CO production that has been outlined elsewhere.	Closure Criterion: None
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

See the discussions on the use of UCO to control CO pressure.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Buffer Layer Thermal gradient	Change in temperature with distance

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	≤ 1600 °C: 7	Remedy: None
	> 1600 °C: N/A	Remedy: N/A
Rationale: During accident conditions, the particle gradient is low because the power production is low relative to operating conditions and heat transfer is no longer driven by strong convection	Rationale: (≤ 1600 °C) The codes can compute these temperatures.	Closure Criterion: None
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

It is not likely that the chemical reactions will generate thermal gradients that are comparable with normal operation.

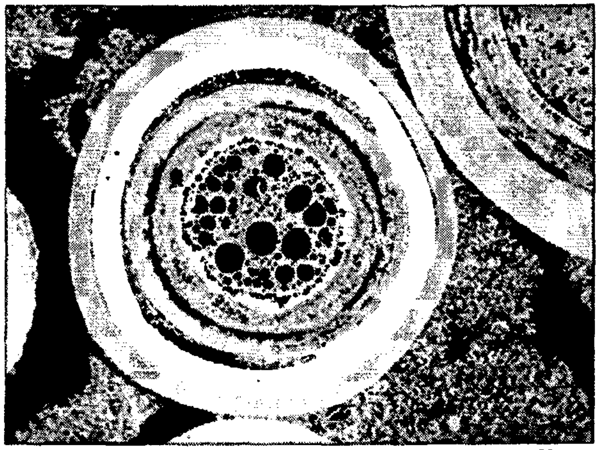
Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Buffer Layer Irradiation and thermal shrinkage	Dimension changes in the buffer layer or changes in its porosity produced by irradiation or by exposure to elevated temperatures

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	≤ 1600 °C: 6	Remedy: None
	> 1600 °C: N/A	Remedy: N/A
Rationale: Ideally, the buffer layer should isolate the kernel from the IPyC, but small cracks or limited shrinkage do not seem to cause trouble.	Rationale: (≤ 1600 °C) Modest buffer shrinkage and small cracks don't seem to result in problems	Closure Criterion: None
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

In this high burnup Pu kernel (ORNL), considerable shrinkage took place in the buffer layer and the IPyC separated from the SiC. While one would like to see less behavior of this sort, the particle performed well under irradiation.

One concern is that cracks could offer a direct path for corrosive fission products to the SiC if the IPyC also breaks. Some current modeling is looking at this.



R71558 (C93000318-03) 200x — 20 µm

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Buffer Layer: Chemical attack by water Kinetics	Rate of reaction per unit surface area as a function of temperature and partial pressure of steam

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	≤ 1600 °C: 4	Remedy: Review the literature and determine if it is relevant or important
	> 1600 °C: N/A	Remedy: N/A
Rationale: A catalysis can increase the reaction rate in the layer and hasten its failure.	Rationale: (≤ 1600 °C) The carbon steam reaction has been studied in some detail. It needs to be applied to the fuel.	Closure Criterion: Collect the effects of catalysis if necessary.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

The industrial literature needs to be consulted, as this is an important commercial reaction.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Buffer Layer: Chemical attack by water Catalysis	Modification of the reaction rate by fission products or impurities

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	≤ 1600 °C: 4	Remedy: Review the literature and determine if it is relevant or important
	> 1600 °C: N/A	Remedy: N/A
Rationale: This layer is already releasing and increasing the rate may not matter much.	Rationale: (≤ 1600 °C) The carbon steam reaction has been studied in some detail. It needs to be applied to the fuel.	Closure Criterion: Collect the effects of catalysis if necessary.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

Once the buffer is exposed, additional chemical attack may not matter much.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Buffer Layer: Chemical attack by water Changes in chemical form of fission products	Changes in chemical form resulting from oxidizing or reducing fission products

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: II	≤ 1600 °C: 4	Remedy: Determine the need for this knowledge, collect as necessary.
	> 1600 °C: N/A	Remedy: N/A
Rationale: Changes in the chemical form of the fission products can greatly change their transport properties. The greatest change may come from the reaction of UC and the change in kernel structure	Rationale: (≤ 1600 °C) Thermochemical codes can calculate the possible chemical compounds. Little confirmation work is available.	Closure Criterion: Collect data to resolve uncertainties
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

The forms and migration of the fission products can be complex. For some information on the chemical forms see:

Fission Product Plateout and Liftoff in the MHTGR Primary System: A Review, NUREG/CR-5647

Chemical Behavior of Fission Products in Core Heatup Accidents in High-Temperature Gas-Cooled Reactors, R. Moormann, Nuclear Technology, 94 (1991), pages 56-67.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Buffer Layer: Chemical attack by water Changes in graphite properties	Changes in diffusivity, porosity, adsorptivity, etc.

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	≤ 1600 °C: 1	Remedy: Determine if this item is relevant.
	> 1600 °C: N/A	Remedy: N/A
Rationale: The modeling is not performed at this level; generally, the layer is assumed to disappear at some rate.	Rationale: (≤ 1600 °C) Not examined in this detail.	Closure Criterion: Collect relevant detail.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

This level of detail may not be necessary if all one needs is time to significant fuel releases as the failure of the SiC may dominate.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Buffer Layer: Chemical attack by water	Release of graphite FP inventory
	Holdup reversal	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	≤ 1600 °C: 4	Remedy: None.
	> 1600 °C: N/A	Remedy: N/A
Rationale: By the time the buffer layer is attacked, the particle has failed and is releasing. The kernel is now the dominate factor.	Rationale: (≤ 1600 °C) The buffer inventory is not well known under accident conditions.	Closure Criterion: None.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

The kernel release is now the dominate mechanism.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Buffer Layer: Chemical attack by water	Impact of graphite oxidation on temperature distribution through material
	Temperature distribution	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	≤ 1600 °C: 5	Remedy: Determine if the uncertainty in the temperatures is acceptable. Refine models and collect data as necessary.
	> 1600 °C: N/A	Remedy: N/A
Rationale: The buffer temperature is the same as the kernel, which is dominating the releases at this point since all the other layers have failed.	Rationale: (≤ 1600 °C) Enough modeling has been done to reasonably estimate the temperatures	Closure Criterion: Adequate data for calculations
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

See the reactor core models for temperature distributions.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Kernel Maximum fuel temperature	Maximum fuel temperature attained by the fuel kernel during the accident

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 7	Remedy: Insure that core models are up to date.
	> 1600 °C: N/A	Remedy: N/A
Rationale: The SiC layer is the primary barrier, but diffusion through the kernel does delay the release somewhat. The kernel retains a considerable amount of material and release is a function of temperature.	Rationale: (≤ 1600 °C) The core codes should be good enough to calculate the temperatures.	Closure Criterion: Acceptable uncertainties.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

For a study comparing the relative contributions of core and fuel materials and fission product retention see: *An Analytical Study of Volatile Metallic Fission Product Release From Very High Temperature Gas-Cooled Reactor Fuel and Core*, S. Mitake, et. al., Nuclear Technology, 81, 7-12.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Kernel Temperature vs. time transient conditions	The time-dependent variation of fuel temperature with time

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 7	Remedy: None, expect to watch for hot spots
	> 1600 °C: N/A	Remedy: N/A
Rationale: The temperature history of the fuel is important. Higher temperature operation even if it is followed by lower temperature operation can result in greater corrosion problems. High temperatures also increase fission product diffusion.	Rationale: (≤ 1600 °C) Modern codes can computer the time history of the fuel. The greatest problem is material property uncertainties.	Closure Criterion: Calculations within the needed uncertainties.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

This is really a core design issue.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Kernel Energy Transport: Conduction within kernel	Flow of heat within a medium from a region of high temperature to a region of low temperature

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	≤ 1600 °C: 7	Remedy: None
	> 1600 °C: N/A	Remedy: N/A
Rationale: The kernel conductivity determines the kernel peak temperature. The kernel is fairly small, so modest changes in conductivity won't matter much. Higher temperatures could result in greater diffusion of fission products out of the kernel.	Rationale: (≤ 1600 °C) These numbers have been measured for the fuels of interest. No major issues are associated with them.	Closure Criterion: None
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

Kernel conductivity depends on the kernel composition and changes as the kernel burns up. The small size of the kernel limits these effects in coated particle fuel.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Kernel Thermodynamic state of fission products	Chemical and physical state of fission products

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 4	Remedy: If fuel kernels other than UO_2 are to be used, testing is required to assure that they work as expected.
	> 1600 °C: N/A	Remedy: N/A
Rationale: The chemical state of the fission products determines how they will migrate and the temperature dependence. It is desirable to oxidize some fission products without producing CO. Steam could cause additional changes by reacting with the UCO.	Rationale: (≤ 1600 °C) A considerable amount of work has been done kernel composition to limit the migration of fission products and control CO pressure. However, only UO_2 has been extensively tested in a high quality fuel. Also, the kernel will oxide with air and water.	Closure Criterion: Demonstrated performance under the conditions of interest
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

For a discussion on kernel design to minimize CO and immobilize key fission products see:

Stoichiometric Effects on Performance of High-Temperature Gas-Cooled Reactor Fuels from the U-C-O System, F.J. Homan, et. al., Nuclear Technology, 35, pages 428-441.

The effect of Water Vapor on the Release of Gaseous Fission Products from High-Temperature Gas-Cooled Reactor Fuel Compacts Containing Exposed Uranium Oxycarbide Fuel, B. Myers, DOE-HTGR-88486

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Kernel Oxygen flux	Mass transport of oxygen per unit surface area per unit time

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	≤ 1600 °C: 3	Remedy: Determine if this area is of any significance
	> 1600 °C: N/A	Remedy: N/A
Rationale: The mass of oxygen from the kernel will determine the rate at which CO is formed and particle pressure. Since the particles are designed assuming maximum pressure, the rate does not seem that important, but his area is somewhat unexplored. Water will oxidize the kernel. See previous entry.	Rationale: (≤ 1600 °C) Some work has been done in this area. The full implications are not clear.	Closure Criterion: Resolution of the issue.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

Tests have shown that the oxygen does not immediately leave the kernel, leading to a somewhat lower CO pressure than normally would occur. This effect is probably more important for low burnup fuel than high burnup fuel. Upcoming tests on German fuel at higher burnups should shed more light on the oxygen issue. See:

Production of Carbon Monoxide During Burn-up of UO_2 Kerneled HTR Fuel Particles, E. Proksch, et. al., Journal of Nuclear Materials, 107 (1982) pages 280-285.

Influence of Irradiation Temperature, Burnup, and Fuel Composition on Gas Pressure (Xe, Kr, CO, CO2) in Coated Particle Fuels, G.W. Horsley, et. al., Journal of the American Ceramic Society, 59, Number 1-2, pages 1-4.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Kernel Grain growth	Enlargement of grains as a result of diffusion

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	≤ 1600 °C: 3	Remedy: None at present
	> 1600 °C: N/A	Remedy: N/A
Rationale: Kernel grain growth has not been an issue. The higher burnups of coated particles fuels often results in the destruction of any structure. Gas release could be higher, but this issue hasn't come up.	Rationale: (≤ 1600 °C) The grain growth issue appears to be less important with coated particle fuel because the layers form the fission product boundary.	Closure Criterion: None at present
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

Unlike LWR fuel, the grain structure appears to be less important.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Kernel Buffer carbon-kernel interaction	Chemical reaction between carbon and the fuel (UO2) to form UC2 and CO (gas)

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	≤ 1600 °C: 5	Remedy: None
	> 1600 °C: N/A	Remedy: N/A
Rationale: A significant problem in this area has not been observed.	Rationale: (≤ 1600 °C) Reactions of this nature can be investigated using thermochemical codes. Nothing has come up to date.	Closure Criterion: None
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

This issue is discussed to some extent in: *Stoichiometric Effects on Performance of High-Temperature Gas-Cooled Reactor Fuels from the U-C-O System*, F.J. Homan, et. al., Nuclear Technology, 35, pages 428-441.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Kernel: Chemical attack by water	Rate of reaction per unit surface area as a function of temperature and partial pressure of steam
	Kinetics	

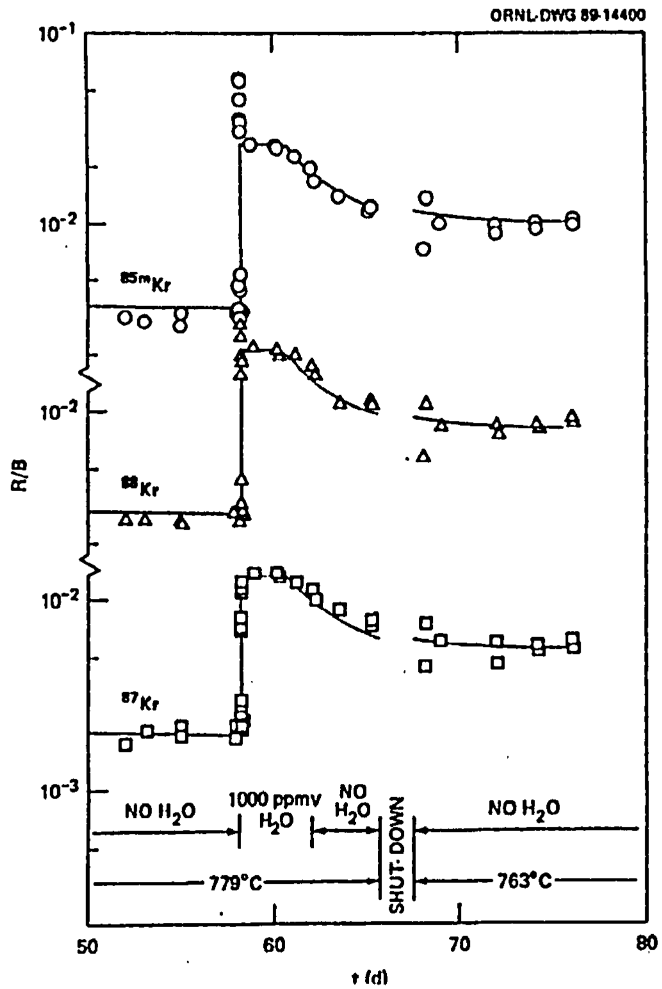
Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 4	Remedy: Determine if the existing data is good enough, collect more if necessary
	> 1600 °C: N/A	Remedy: N/A
Rationale: This determines the enhanced rate at which the fission products are released from the kernel.	Rationale: (≤ 1600 °C) Moisture ingress tests have been done on UO_2 and UCO fuel.	Closure Criterion: Enough data to bind the accident of interest.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

The amount of damaged fuel determines how significant this issue is. If the fuel performs as advertised, then it may not matter. See
Fuel Performance and Fission Product Behavior in Gas Cooled Reactors, IAEA-TECDOC-978 (1997)

The effect of Water Vapor on the Release of Gaseous Fission Products from High-Temperature Gas-Cooled Reactor Fuel Compacts Containing Exposed Uranium Oxycarbide Fuel, B. Myers, DOE-HTGR-88486

Water Increases Release From Exposed UCO Kernels
A pulse of water restructures the (bare) UCO kernel and releases the stored fission gas. After the release, the R/B gradually drops back to pre injection values. (ORNL)



Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Kernel: Chemical attack by water	Modification of the reaction rate by fission products or impurities
	Catalysis	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	≤ 1600 °C: 1	Remedy: Determine if relevant.
	> 1600 °C: N/A	Remedy: N/A
Rationale: A catalysis could increase the reaction rate and accelerate releases.	Rationale: (≤ 1600 °C) Unknown	Closure Criterion: Collection of relevant data.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

Accelerated releases from the kernel under accident conditions due to catalysis have not been explored.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Kernel: Chemical attack by water	Changes in chemical form resulting from oxidizing or reducing fission products
	Changes in chemical form of fission products	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 4	Remedy: Determine the need for this knowledge, collect as necessary.
	> 1600 °C: N/A	Remedy: N/A
Rationale: Changes in the chemical form of the fission products can greatly change their transport properties. The greatest change may come from the reaction of UC and the change in kernel structure	Rationale: (≤ 1600 °C) Thermochemical codes can calculate the possible chemical compounds. Little confirmation work is available	Closure Criterion: Collect data to resolve uncertainties
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

The forms and migration of the fission products can be complex. For some information on the chemical forms see:

Fission Product Plateout and Liftoff in the MHTGR Primary System: A Review, NUREG/CR-5647

Chemical Behavior of Fission Products in Core Heatup Accidents in High-Temperature Gas-Cooled Reactors, R. Moormann, Nuclear Technology, 94 (1991), pages 56-67.

Fuel Performance and Fission Product Behavior in Gas Cooled Reactors, IAEA-TECDOC-978 (1997)

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Kernel: Chemical attack by water	Changes in diffusivity, porosity, adsorptivity, etc.
	Changes graphite properties	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 5	Remedy: Determine the relevance of this situation
	> 1600 °C: N/A	Remedy: N/A
Rationale: As the kernel restructures because of oxidation, it releases some its stored inventory of fission products, mostly gases.	Rationale: (≤ 1600 °C) Moisture testing has been done and exposed kernels are the major issue, rather than good fuel.	Closure Criterion: Relevance of this situation and any data.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

The amount of damaged fuel determines how significant this issue is. If the fuel performs as advertised, then it may not matter. See *Fuel Performance and Fission Product Behavior in Gas Cooled Reactors*, IAEA-TECDOC-978 (1997)

The effect of Water Vapor on the Release of Gaseous Fission Products from High-Temperature Gas-Cooled Reactor Fuel Compacts Containing Exposed Uranium Oxycarbide Fuel, B. Myers, DOE-HTGR-88486

Appendix E.3

Detailed PIRT Submittal by the SNL Panel Member

E. A. Powers

TRISO Fuel PIRT: Accident With Subsequent Water Intrusion

This PIRT is based more on geometry than it is on phenomenology, despite the name. The PIRT seems to be attempting to identify the critical component of the coated particle fuel structure that deserves the most attention. This is done at the expense of identifying the critical phenomena that need to be understood to anticipate the behavior of the fuel in normal and off normal circumstances. As a result questions are asked repetitively about each of the major elements of the fuel perhaps to see if one or more of the elements are more vulnerable than others. The questions do not illuminate in any detail the type of information that must be derived for coated particle fuel or the types of testing that must be done to gather the information. For instance, lumped within the simple question of gas phase diffusion are bulk and Knudsen diffusion. Though the question is repeated for each layer even when the layers are very similar, such as inner and outer PyC, there is no request for details of the materials that would be essential to estimate Knudsen versus bulk diffusion such as porosity and tortuosity. There is no indication of whether tests of permeability need to be done for layers ***in situ*** or such data can be obtained from macroscopic samples of analog material. We do not know from the PIRT whether phenomena such as thermal diffusion require testing to be done in prototypic gradients or just known gradients. We do not know from the PIRT whether diffusion must be considered as approximately binary diffusion or has to be viewed as a multicomponent process. This focus on the structure at the expense of phenomena limits the utility of the PIRT for the design of fuel models and experimental studies. Perhaps, the PIRT is more useful in other respects because of its focus on structure.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Fuel Element Irradiation history	The temperature, burnup and fast fluence history of the layer

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: II	Level: 3	Remedy: There is a need for studies of the energetics of radiation damage to the materials making up the coated particle fuel layers. (Damage to the kernel is of lesser interest). The needed information can probably be obtained by thermal analysis of specimens irradiated under prototypic conditions for varying lengths of time. There is further need for information on the kinetics of oxidant reactions and reactions of nitrogen with the materials as functions of temperature.
Rationale: The fast fluence history of the layers will dictate how much radiation damage is built into the materials. This will affect the kinetics of reaction. Also as reaction proceeds, the radiation damage energy will be released augmenting the energy of chemical reactions with the layers	Rationale: We have some knowledge of the radiation damage that can develop in carbon materials at the operating temperatures of interest for this work. We don't have such information about the specific materials involved in the coated particle fuel. Furthermore, we don't have data or models on the effects of radiation damage on the kinetics of oxidant interactions with the materials	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Fuel Element Surface diffusion	Inter grannular diffusion and/or intra-grannular solid-state diffusion

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	Level: 1	Remedy: The essential remedy is to wait until a specific and reproducible material is specified. Then the material has to be characterized in terms of grain size and orientation as well as in terms of the surface and grain boundary diffusion coefficients of irradiated material. Diffusion studies will have to take into account the fact that the material will not be isothermal. Rather there will be necessarily a temperature gradient across the material from the fuel particles (which are the source of the decay heat) and the coolant. A major issue to confront here is whether the release modeling should be so complete that it considers release limitations by the matrix material surrounding the fuel particles. It would not be an unreasonable conservatism to neglect this barrier to release since it appear unlikely that there will soon be useful experimental data to validate models of the barrier
Rationale: Grain boundary and surface diffusion of fission products will be faster mechanisms of mass transport of fission products from the perimeter of the fuel particles to the surfaces of the matrix material and into the reactor coolant system from where they can escape into the plant environment. Surface diffusion and grain boundary diffusion are notoriously sensitive to impurity concentrations of the material. They are also sensitive to the grain sizes and the preferential orientation of grains. Presumably they are also sensitive to the irradiation of the material though I am not familiar with definitive studies of this issue. Diffusion in the systems will be complicated by the presence of a thermal gradient across the material.	Rationale: The bulk matrix material has not been specified and certainly has not been characterized sufficiently to estimate diffusion coefficients for the fission products. There are of course no measured data because the specification of the material has not yet been made. Studies of generic material may provide some guidance.	Closure Criterion:

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Fuel Element Gas diffusion	Diffusion of gaseous fission products through layer (Knudsen and bulk diffusion through pore structure, and pressure driven permeation through structure) Other factors include holdup craking adsorption, site poisoning, permeability, sintering and annealing

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: II	Level: 4	Remedy: The gas phase mass transport across elements rom multi-point sources is a sufficiently complicated process that it is probably useful to set up models now and test them against models used for catalysts and the like. Detailed analyses of the issue will have to wait until there are real data on the fuel matrix materials that will be used in the reactor. A major issue to confront here is whether the release modeling should be so complete that it considers release limitations by the matrix material surrounding the fuel particles. It would not be an unreasonable conservatism to neglect this barrier to release since it appear unlikely that there will soon be useful experimental data to validate models of the barrier
Rationale: Vapor transport through pores and voids in the matrix material will be the fastest mechanism of mass transport of fission products from the fuel particle surfaces to the boundary of the fuel elements, The transport may driven by pressure differences or it may be by diffusion (either chemical or Knudsen). The presence of a thermal gradient will affect the diffusion process. It may be necessary to develop the diffusion equations to include thermal diffusion. Certainly the mass transport will have to address multicomponent effects using something like the Stefan Maxwell equations rather than Fickian diffusion equations	Rationale: The physics of the process is relative well understood and, indeed, fairly sophisticated models of this kind of mass transport have been developed by the catalyst community. What we don't know with any detail is the speciation of the fission product vapors or the pore and void structure of the matrix material. Diffusion coefficients for the vapors can be estimated with surprisingly good reliability from simple first order Chapman Enskog theory. Second order theory must be used to estimate thermal diffusion coefficients which may not be negligible if the thermal gradients are large and if there are gases that have low molecular weights relative to the fission product vapors. Application of models of this type to the issue is not possible now because we do not have data on the material such as its void and porosity structure and its permeability	A major issue to confront here is whether the release modeling should be so complete that it considers release limitations by the matrix material surrounding the fuel particles. It would not be an unreasonable conservatism to neglect this barrier to release since it appear unlikely that there will soon be useful experimental data to validate models of the barrier

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Fuel Element: Transport of metallic FPs through fuel element Chemical form	Chemical stoichiometry of the chemical species that includes the radioisotope of interest

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 4	Remedy:There needs to be an agreed upon thermodynamic data base for the important species arising in the analysis of fission product release at these gas-cooled reactors. Much of the data in this base could be borrowed from existing data bases. There needs also to be a search for possible species many of which have been identified in the literature but not characterized sufficiently to include in data bases now available.
Rationale: metallic fission products are going to be transported through the matrix material primarily as vapors. The effective vapor pressures of the metallic fission products depend on their gas phase speciation. There have been fairly limited investigations of the speciation of the fission products in the strongly reducing environment of the fuel element. Certainly the elemental forms will be important. What is of interest is whether there are more exotic species such as carbonyls and carbides and even cyanides that can augment the vapor pressures significantly. A reliable database on the thermodynamics of fission product species appropriate for this kind of a reducing environment (At least prior to oxidant intrusion) has not been assembled. Existing databases treat primarily elements, oxides and in some cases hydroxides. Once the oxidant (water vapor) intrudes, these other possible vapor species as well as vapor phase hydrides need to be considered to know the vapor pressures of the fission products	Rationale: Elemental vapor pressures are rather well established for most of the fission products. Databases exist for most oxides and some hydroxides. Hydride, carbonyl, carbide data are scattered in the literature and have not been systematized nor has there been a systematic survey to identify more exotic vapor species. Polyatomic vapor species become less important as temperatures increase and pressures decrease.	Closure Criterion:

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Fuel Element: Chemical attack by water Kinetics	Rate of reaction per unit surface area as a function of temperature and partial pressure of steam

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 4	Remedy:Because water is so ubiquitous in the reactor situation it will be imperative that any model of fission product release and transport account for the effects of water.
Rationale: There is one essential difference between the attack of water on graphite and the attack of air. Water attack on graphite can be endothermic rather than exothermic. Otherwise many of the points raised in connection with the attack on graphite by air are applicable for water as well. The attack can be localized. The speciation of the fission products is affected locally. Transport pathways are affected. Kinetics must be evaluated to know if the fuel particles as well as the matrix will be attacked by the oxidant. Instead of the issues of cyanogens and its effects on vapor pressure the effects of hydrogen and the formation of gas phase hydrides needs to be considered. For example CsH becomes an important vapor phase species of cesium at moderately high temperatures in the presence of hydrogen.	Rationale The databases on steam attack on the specific types of graphite used for the fuel matrix are not rich. There are data for analogous reactions of similar materials	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Fuel Element: Chemical attack by water	Modification of the reaction rate by fission products or impurities
	Catalysis	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 4	Remedy: This will have to be included in any model of graphite reactions with steam.
Rationale: catalysis of the steam reactions with graphite are known and the catalytic agents are the same as those that catalyze the reactions of oxygen.	Rationale: some data available on analogous materials. A suitable model does not exist	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Fuel Element: Chemical attack by water	Changes in chemical form resulting from oxidizing or reducing fission products
	Changes in chemical form of fission products	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: II	Level: 5	Remedy: The speciation of the fission products ill be an essential part of any model of fission product release and transport. The model will probably have to speciation as a spatially dependent calculation
Rationale: Just as for air intrusion the presence of water can affect the speciation of the fission products and consequently the vapor pressures. The presence of water raises the possibilities of gas phase hydroxides of the fission products. The presence of hydrogen as a reaction product raises the possibility of vapor phase hydrides of fission products such as CsH and RuH contributing to the vapor pressure. See also the discussion of speciation during air intrusion.	Rationale: there is a technical basis for estimating the speciation for fission products though it is not as strong as the basis for doing the speciation of fission products in light water reactors	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Fuel Element: Chemical attack by water	Changes in diffusivity, porosity, adsorptivity, etc.
	Changes in graphite properties	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 2	Remedy: This modeling of the oxidation along pathways for mass transport could be a very challenging feature of a fission product release model. Whether the development of such a model needs to be done or not depends on whether credit is taken for the barrier to fission product release provided by the matrix material
Rationale: As noted above, especially at lower temperatures, oxidant attack on graphite is localized, not uniform and the localized attack is on the regions that will facilitate gas phase mass transport of fission product vapors through the fuel matrix like cracks and pore networks, the attack opens these pathways and makes transport easier	Rationale: The prediction of the effects of oxidant attack on the pathways is challenging. There has been some work in the chemical engineering field on analogous issues that could serve as a basis for modeling this phenomenon	Closure Criterion:
	The effects of oxidant attack on cracks and pore networks becomes less important as temperature become very high	

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Fuel Element: Chemical attack by water Holdup reversal	Release of graphite FP inventory

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 5	Remedy: It is not clear that this phenomenon needs to be included in a model. Certainly it does not need to be included if the barrier to release presented by the matrix is neglected as a conservative measure that considerably relieves the challenges in estimating releases for risk assessments
Rationale: It is known that energetic sites will adsorb fission product vapors and create some holdup of the release of radionuclides. It is not evident that there are enough of these sites to cause the holdup of a significant fraction of the radionuclide inventory. It is known that chemical reactions that destroy energetic sites or even the intrusion of polarizable gases that will compete for site occupancy can result in the release of the adsorbed fission products. But it the desorption does not involve a large fraction of the inventory of particular class of fission products the phenomenon is not significant	Rationale:) We probably do not have sufficient data on the holdup to make quantitatively defensible estimates of the holdup. We do know enough to make simple qualitative arguments about its significance Holdup on the matrix surfaces is less important at high temperatures because of the high vapor pressures of the fission product species of interest. Though we certainly know less about holdup on the surfaces at high temperature than we know at low temperatures, we probably know enough to say that if the importance of the phenomenon is questionable at low temperatures, it certainly is unimportant at very high temperatures	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Fuel Element: Chemical attack by water Temperature distribution	Impact of graphite oxidation on temperature distribution through material

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 5	Remedy: Any model of fission product transport will have to have a reliable description of the temperature distributions along the flow pathway.
Rationale: Because the reactions with graphite are not iosenergetic, they will affect the temperature distribution in the fuel element. Elsewhere it has been established that this temperature distribution can affect the transport of fission products through the fuel element to the surface	Rationale: It is in principle possible to calculate the distortion of the temperature distribution to an accuracy adequate for fission product release transport analysis. It is however not trivial even if we had good models of the thermal conductivity of the material and the effects of growing pores and voids on the thermal conductivity. The essential problem is that the oxidation process does come to be localized so simple geometries are not appropriate. The problem of calculating the temperature distribution actually becomes easier as reactions become more homogeneous and radiation across the pores and voids tends to even out their effects on the apparent thermal conductivity of the material.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Outer PyC Layer Gas Phase Diffusion	Diffusion of gaseous fission products through layer (Knudsen and bulk diffusion through pore structure, and pressure driven permeation through structure)

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 6	Remedy: Any model of fission product transport within the fuel particle will have to include a gas phase mass transport model recognizing bulk diffusion, pressure driven flow and Knudsen diffusion
Rationale: These gas phase mass transport processes are the fastest ways for fission products released from the kernel to cross the Outer PyC layer.	Rationale: Given the geometry and nature of the pore and crack network in the layer it is possible to calculate the gas phase mass transport across the layer. We can estimate most of the gas phase diffusion coefficients. The mass transport is probably not modeled well by Fickian diffusion and one will have to develop a multicomponent diffusion model much like the membrane models that have been developed in the chemical engineering literature. It may be necessary to include in these models the effects of thermal diffusion especially if the gas includes both low molecular weight species such as CO (MW=28) and fission product vapor species (MW>100) and temperature gradients are significant as they surely must be to get decay heat out of the particle. The most complicated part of the modeling will be to treat the geometries of the layer as a whole and	Closure Criterion: (continued from previous column) the pore, crack and void network in the layer. We know the layers will not by spherically symmetric. Does the deviation from symmetry have a significant effect on the rate of transport? Similarly the layers will not be uniformly thick and this may create short circuits or preferred pathways for mass transport. We do not have good data on the pore and void network. We are not likely to get adequate data from microscopic analysis. The cracks pores and voids that are of interest are too small to readily identify and detect and microscopic examinations will never yield anything but a biased estimate of the concentration and sizes of the networks. Transport data are needed, but it is not readily apparent how such data are obtained for the microscopic layers of the particles.
	The situation is much the same at elevated temperatures though gas phase mass transport becomes an even more dominant mechanism simply because the gas phase concentrations are higher. The ability to estimate diffusion coefficients and thermal diffusion coefficients for polyatomic vapor species begins to degrade because inelastic collision become more important	

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Outer PyC Layer Condensed phase diffusion	Intergrannular diffusion and'or intra-grannular solid-state diffusion

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	Level: 2	Remedy: Any model of fission product transport across the Outer PyC layer will have to include these processes, though it is likely that even with only modest vapor pressures the gas phase mass transport processes will be more important mechanisms. The diffusion process has the same problems discussed above. Spherical symmetry may be an overly crude approximation as may be the assumption that the layer is uniformly thick.
Rationale: Fission products that are not volatile will be transported across the barrier posed by the outer PyC layer by the condensed phase diffusion processes. Bulk diffusion is the slowest of these a low temperatures, but it has the highest activation energy so it does eventually become the dominant process. Even if the metals have only small vapor pressures, gas phase mass transport of fission products may still be the dominant mechanism for most fission products. There do appear to be some exceptions such as the transport of Ag.	Rationale: We do not have surface and grain boundary diffusion coefficients for the fission products and materials of interest here and surface and grain boundary diffusion are likely to be the dominant condensed phase transport processes. These coefficients cannot be estimated. They have to be measured and they are notoriously sensitive to impurities accumulated on the grain surfaces and at the grain boundaries	Closure Criterion:
	At sufficiently high temperatures (and it by no means established that 1600 is sufficiently high) bulk diffusion of fission products will be dominant transport processes for nonvolatile species. We do not have useful bulk diffusion coefficients for irradiated material. The need for irradiated material is to be emphasized since it is known that radiation defects can act as traps for diffusing species	

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Outer PyC Layer Layer oxidation	Reaction of pyrolytic graphite with oxygen released from the kernel

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 2	Remedy: Analysis of fission product release during air intrusion or water intrusion accidents will have to account for the effects of oxidant on the integrity of the outer PyC layer. It will have to be a kinetic analysis so that the analyst will know how much oxidant survives the interaction with the layer to attack other regions of the fuel particle.
Rationale: Oxidant can reach the Outer PyC layer either coming from oxygen evolved from the fuel kernel or oxidant intruding into the core (air or water). It is likely that the source of oxidant coming form the fuel will be sufficiently weak that most of this oxidant will be consumed by reactions with graphite etc. before it can reach the Outer PyC layer in any form other than CO. Oxidant from intrusive sources will have to survive reactions with graphitic materials along its transport path to the fuel particle. When it does survive this transport the results can be catastrophic with respect to fission product transport across the PyC layer. The oxidant will thin the layer, but more importantly localized attack on energetically preferred sites will result in widening and smoothing the cracks and pores through the layer thereby facilitating gas phase mass transport across the layer. The oxidation reactions can also heat the layer	Rationale: The oxidation reactions kinetics are enormously sensitive to impurities that can catalyze reactions. Fission products themselves may act as catalysts. Though we have some data on the oxidation reactions, we do not have data on the specific material. Without these data accurate quantitative analysis of the oxidation process at the Outer PyC layer is really not possible The situation becomes a little simpler at very high temperatures where the kinetics are less affected by the catalytic processes and proceed in a more uniform process. Still we donot have validated kinetic models.	Closure Criterion:

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Outer PyC Layer Stress state (compression/tension)	The state of the forces induced by external forces that are acting across the layer to resist movement

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 2	Remedy: it isn't clear that any remedy is needed
Rationale: This is a more important issue during normal operations since it can result in rupture of the layer prior to the accident . Thermal expansion may cause some stresses on the layer and it would be of interest to know if rupture can occur.	Rationale We really don' t know much about these forces	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Outer PyC Layer Intercalation	Trapping of species between sheets of the graphite structure

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 2	Remedy: no remedy needed
Rationale: It is known that energetic sites in the PyC layer will provide sites for fission product deposition and holdup. There can be a preference for fission products to migrate toward the basal planes of the graphite structure and be intercalated. It is not apparent that sufficient concentrations of sites will be formed to holdup a significant fraction of the radionuclide inventory of the fuel particle. Eventually oxidation or thermal annealing will eliminate these energetic sites and lead to the desorption of fission products that have been attracted to the sites. The elevated temperatures will eventually move fission products from the intercalation sites as well.	Rationale: We don't really know how much holdup can occur At sufficiently high temperatures there really will not be any holdup since the vapor pressures of the fission products will be so high	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Outer PyC Layer Trapping	Adsorption of fission products on defects

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 2	Remedy: no remedy needed
Rationale: It is known that energetic sites in the PyC layer will provide sites for fission product deposition and holdup. There can be a preference for fission products to migrate toward the basal planes of the graphite structure and be intercalated. It is not apparent that sufficient concentrations of sites will be formed to holdup a significant fraction of the radionuclide inventory of the fuel particle. Eventually oxidation or thermal annealing will eliminate these energetic sites and lead to the desorption of fission products that have been attracted to the sites. The elevated temperatures will eventually move fission products from the intercalation sites as well.	Rationale: We don't really know how much holdup can occur At sufficiently high temperatures there really will not be any holdup since the vapor pressures of the fission products will be so high	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Outer PyC Layer Cracking	Lengths, widths and numbers of cracks produced in layer during accident

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: II	Level: 1	Remedy: It is clear that any model of fission product transport through the fuel particles has to recognize the possibility of cracks in the material providing a short pathway for transport. Whether the cracking has to be modeled or cracking is input to the transport model is a decision that must be made. This decision may well rest on whether cracking occurs during the accident transient or is primarily a process that occurs during normal operations.
Rationale: Cracks through the layer facilitate gas phase mass transport of fission products across the layer	Rationale: It is not apparent that we are in any position to predict the cracking of the layers under any circumstances let alone under accident circumstances. It may not be practical to predict cracking and we will have to rely on empirical evidence for cracks. This is a challenge since cracks that can affect fission product release rates may be very difficult to detect microscopically	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Outer PyC Layer: Chemical attack by water Kinetics	Rate of reaction per unit surface area as a function of temperature and partial pressure of steam

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 6	Remedy: Any model of fission product transport treating intrusion accidents will have to consider water vapor reactions with the graphite and carbon.
Rationale Water attack, while not likely to be as dramatic as attack by air will still be of considerable influence both as it affects the volatility of the fission products and as it affects flow pathways and temperature distributions	Rationale: There is a lot of information about the rates of steam reactions with carbon – though perhaps not the specific carbon of the fuel particles.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Outer PyC Layer: Chemical attack by water Catalysis	Modification of the reaction rate by fission products or impurities

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: II	Level: 3	Remedy models of reactions will have to recognize that catalysis including catalysis by fission products will affect the kinetics:
Rationale: steam reactions with carbon are catalyzed especially in the lower temperature range	Rationale: see discussions of catalysis of air reactions	Closure Criterion:
	catalysis is of less importance at high temperatures where reaction rates are rapid and eventually are limited by mass transport	

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Outer PyC Layer: Chemical attack by water	Changes in chemical form resulting from oxidizing or reducing fission products
	Changes in chemical form of fission products	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 5	Remedy: The speciation of fission products will be an essential part of any model of fission product release and transport. This is especially the case here because of the dominant role that vapor phase mass transport is expected to play in the transport of fission products released from the kernel to the surface of the fuel particle. There will then have to be a significant model of the fission product thermochemistry in the fission product release model. In comparing predictions of release say to predictions by the applicant for certification, a key issue will be the thermodynamic data base used to make predictions of fission product speciation and vapor pressure.
Rationale: Just as for air intrusion the presence of water can affect the speciation fo the fission products and consequently their vapor pressures. The presence of water raises the possibilities of gas phase hydroxides of the fission products. The presence of hydrogen as a reaction product raises the possibility of vapor phase hydrides of fission products such CsH and RuH contributing to the vapor pressure. Se also the discussion of speciation during air intrusion	Rationale: There is a technical basis for estimating the speciation for fission products though it is not as strong as the basis for doing the speciation of fission products in light water reactors	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Outer PyC Layer: Chemical attack by water Changes in graphite properties	Changes in diffusivity, porosity, adsorptivity, etc.

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 3	Remedy:The modeling of oxidation along pathways for mass transport could be a very challenging feature of a fission product release model. It is important to include because gas phase mass transport of fission products is the most important mechanism to move materials from the surface of the kernel to the surface of the fuel particle. Some work has been done in the Chemical Engineering field to look at the ways chemical reactions open pathways in porous solids. This might be a useful starting point for the development of a model.
Rationale: The important effect of oxidation aside from changing the volatilities of the fission products is to facilitate the transport of fission products released from the kernel across the fuel particle by either thinning the barrier layers such as the outer PyC layer or, and more importantly, opening the void networks and cracks through the layer for gas phase mass transport.	Rationale: The calculation of the localized oxidation that leads to the opening of gas phase flow pathways is difficult to do. We don't now have the needed data on these pathways nor do we have the kinetic information on the reaction rates of steam with the particular material of interest. We do have data on some analogous materials so it might be possible now to formulate estimates whose quantitative reliability may be open to some question.	Closure Criterion:
	The situation is largely the same at the higher temperatures, however, the reactions become more rapid at elevated temperatures and consequently the material thinning becomes more important than the reactions to form more open pathways.	

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Outer PyC Layer: Chemical attack by water	Release of graphite FP inventory
	Holdup reversal	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 4	Remedy: no remedy needed
Rationale: Oxidation will destroy the energetic sites that have absorbed fission products and thus release the fission products. It is not apparent that adsorption of fission products on energetic sites produces holdup of sufficient fractions of the fission products for this reactive desorption process to be risk important	Rationale: we don't have the needed data on the fractional holdup in the layer by the adsorption process. One would suspect that for the outer layer of PyC this holdup is small if the fuel has operational integrity.	Closure Criterion:
	At elevated temperatures, the vapor pressures of the important, volatile radionuclides are so high that the adsorption fraction is low. Though we don't know any more at high temperatures than we do at low temperatures there is probably less need to know a great deal for high temperatures.	

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Outer PyC Layer: Chemical attack by water Temperature distribution	Impact of graphite oxidation on temperature distribution through material

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: II	Level: 3	Remedy: Any model of fission product release and transport will require quite a good model of the local temperature distributions in the fuel particle.
Rationale: The chemical reactions of oxidants with the carbon materials are not iso-enthalpic, so they will distort the temperature distributions in the particle. As noted elsewhere these temperature distributions can affect release both through the effect on the thermodynamic driving force for transport across the particle and from an effect on the transport processes themselves.	Rationale: We generally know the heats of reaction. We don't have as good an understanding of the rates of reaction especially of irradiated material where reaction will simultaneously involve the destruction of defects introduced by irradiation during operations.	Closure Criterion:
	The situation is largely the same at higher temperatures though the importance of irradiation defects will decrease as they are thermally annealed.	

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	SiC Layer Gas phase diffusion	Diffusion of gaseous fission products through layer (Knudsen and bulk diffusion through pore structure, and pressure driven permeation through structure)

Additional Discussion

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 6	Remedy: Any model of fission product transport within the fuel particles will have to include an gas phase mass transport model recognizing bulk diffusion, pressure driven flow and Knudsen diffusion The mechanistic detail with which a model could be constructed is probably not supported by adequate characterization of the irradiated layer. It may be necessary to adopt a more empirical modeling retaining perhaps the functional forms suggested by the theory of mass transport through porous materials.
Rationale: Gas phase mass transport across the SiC layer through cracks or through the pore and void network in the material will be by far the fastest mechanism for mass transport of fission products across this layer	Rationale: Given the geometry and nature of the pore and crack network in the layer it is possible to calculate the gas phase mass transport across the layer. We can estimate most of the gas phase diffusion coefficients about as accurately as they can be measured. The mass transport probably cannot be calculated using Fickian diffusion and neglecting temperature gradients in the material. A multicomponent model similar in nature to the models of mass transport across membranes used widely in the chemical engineering field will have to be used. It may be necessary to recognize the effects of thermal diffusion if the temperature gradients are large and there are significant differences in the molecular weights of gases. This may well be the case especially inside the SiC layer which will be pressurized with CO from the (continued next column)	Closure Criterion: (continued from previous column) reaction of carbon materials with the urania fuel kernel. Complication in the analysis come about if the deviations from spherical symmetry of the layer are significant and if the variations in the layer thickness is significant. Characterization of the pore, void or crack network in the layer is most important and quite challenging since the voids or cracks that can be effective for mass transport are not easily detected by microscopic examination. It is furthermore quite difficult to average sets of visual observations of cracks and voids to come up with a suitable 'average' description for the analysis of mass transport. What would really be desirable would be permeability measurements of the layer. It is of course not practical to make such measurements.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	SiC Layer Condensed phase diffusion	Inter-grannular diffusion and/or intra-grannular solid-state diffusion

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	Level: 2	Remedy: Modeling of fission product transport will have to include the modeling of condensed phase mass transport.
Rationale: Fission products that are not volatile will transport across the layer by diffusion. At low temperatures, grain boundary diffusion and surface diffusion will be the more rapid processes. Because the activation energy for bulk diffusion is highest, it will become, eventually the dominant mechanism of mass transport as the temperature is increased. Still, even if the fission product has only a very small vapor pressure, gas phase mass transport may outstrip condensed phase diffusion processes. There are some exceptions to this. Ag seems to be capable of fast transport across the layer and this fast transport has been ascribed to condensed phase diffusion although there are not the data necessary to conclusively demonstrate this.	Rationale: We really don't have good condensed phase diffusion coefficients for fission products during bulk, surface or grain boundary diffusion for the specific material that is of interest. Bulk diffusion coefficients from analogous materials may be adequate IF the defects in the crystal lattices produced by irradiation don't act as traps for diffusing species. Grain boundary and surface diffusion coefficients depend so much on the impurity levels at surfaces and grain boundaries where these impurities accumulate, that it would be difficult to ascribe significance to data sets for anything except the actual material of the layer including the correct crystallite orientation etc.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	SiC Layer Thermal deterioration/decomposition	Decline in the quality of the layer due to thermal loading

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	Level: 3	Remedy: no remedy may be needed.
Rationale: SiC is a most peculiar material. There have been reports of phase changes in the material from cubic to hexagonal at elevated temperatures. Modern phase diagrams do not reflect this phase change. It may be more important that the material is subject to polytypism based on the hexagonal structure. If the formation of the layer does not yield the thermodynamically stable product, thermal annealing during the temperature transient of an accident could cause some restructuring that will create pathways for gas phase mass transport. It might also be possible during a thermal transient for the heavily radiation damaged material to restructure to relieve the accumulation of strain energy of the irradiation defects (A sort of analogy to the formation of the rim in heavily irradiated fuel!). This restructuring could well lead to gas phase mass transport paths that will facilitate the transport of fission products released from the fuel kernel across the layer.	Rationale: To quantitatively examine this issue we would have to have considerable data on the product of the particle formation process to see if polytypism occurs and also to see if radiation restructuring can occur during an accident temperature transient. Then we would need data to see how annealing affected the permeability of the layer The situation is the same as above for lower temperatures	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	SiC Layer Fission product corrosion	Attack of layer by fission products, e.g., Pd

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 3	Remedy: AT this juncture it appears to me that holdup by chemical reaction with the SiC layer can be neglected until there is evidence that this important for more important radionuclides than Pd.
Rationale: Chemical attack on the layer by fission products will affect transport across the layer and certainly may affect the transport of the fission product doing the transporting since it will be converted to a more stable form which may be less volatile. It is however to become excessively concerned over this since the fission product inventory of the kernel is not large enough to produce massive damage to the layer that will affect the transport of all fission products. There is only one example of significant attack and that is with Pd which is not an especially important fission product from an accident consequences view point. The attack by Pd may suggest other noble metals such as Ru and Mo will produce similar attack. There would have to be substantial evidence of this to rate the process of higher significance.	RationaleWe don't have a comprehensive survey of the attack on SiC by fission products in part because SiC under reducing conditions is not an especially reactive material.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	SiC Layer Heavy metal diffusion	Diffusion of heavy metals through layer

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	Level: 2	Remedy: Modeling of fission product transport will have to include the modeling of condensed phase mass transport
Rationale: Fission products that are not volatile will transport across the layer by diffusion. At low temperatures, grain boundary diffusion and surface diffusion will be the more rapid processes. Because the activation energy for bulk diffusion is highest, it will become, eventually the dominant mechanism of mass transport as the temperature is increased. Still, even if the fission product has only a very small vapor pressure, gas phase mass transport may outstrip condensed phase diffusion processes. There are some exceptions to this. Ag seems to be capable of fast transport across the layer and this fast transport has been ascribed to condensed phase diffusion although there are not the data necessary to conclusively demonstrate this.	Rationale: We really don't have good condensed phase diffusion coefficients for fission products during bulk, surface or grain boundary diffusion for the specific material that is of interest. Bulk diffusion coefficients from analogous materials may be adequate IF the defects in the crystal lattices produced by irradiation don't act as traps for diffusing species. Grain boundary and surface diffusion coefficients depend so much on the impurity levels at surfaces and grain boundaries where these impurities accumulate, that it would be difficult to ascribe significance to data sets for anything except the actual material of the layer including the correct crystallite orientation etc.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	SiC Layer Layer oxidation	Uptake of oxygen by the layer through a chemical reaction

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 5	Remedy: No remedy needed.
Rationale: I distinguish here between the reaction of SiC with oxidant to form CO and SiO and the uptake to form nominally SiOC. This later uptake can only progress to the point of saturation. It will only be important if it causes swelling or decrepitation of the SiC layer and I can find no evidence that it does. All my experience is with higher oxygen potentials where SiO is not stable and SiO2 is the condensed product of reaction and this SiO2 does act to occlude surfaces which would interfere in gas phase mass transport at the highest temperatures. SiO, a vapor in the temperature ranges of interest could condense elsewhere in the particle and have some ramifications on the transport of fission products.	Rationale: There is a lot of information about the response of SiC to oxidizing conditions of various oxygen potentials. I don't' find information that indicates processes during uptake that would affect fission product transport (but see below when reaction is discussed)	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	SiC Layer Fission product release through defects	Passage of fission gas from the buffer region through defects in the SiC layer

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 1	Remedy: This mechanism probably cannot be modeled mechanistically. It will have to be treated by providing empirical evidence of the change in layer permeability as irradiation progresses.
Rationale: Defects introduced into the SiC lattice by manufacture or by irradiation will become mobile at elevated temperatures and accumulate to form dislocations that themselves will lead to the formation of porosity networks. These networks will provide a pathway for gas phase mass transport that will be the dominant mechanism for fission product transport across the layer.	Rationale: We don't have the information to assess this process now	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water intrusion	SiC Layer Fission product release through failures, e.g. craking	Passage of fission gas from the buffer region through regions in the SiC layer that fail during operations or an accident

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 4	Remedy: Mechanistic modeling of gas phase mass transport across a failed layer of SiC may not be undertaken though it can be done. A true failure of the layer may be taken somewhat but not greatly conservatively as meaning the layer no longer poses a barrier to fission product transport.
Rationale: SiC layer failure will permit the venting of accumulated fission product vapors and the ongoing releases of fission product vapors as they escape the fuel kernel and reach the SiC layer	Rationale: We don't have information that allows us to know when SiC layers fail or how massive the failures are. If we had this information it should not be difficult to model the gas phase mass transport across the layer through the failure locations.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	SiC Layer Thermodynamics of the SiC-fission product system	Include solubility, intermetallics, and chemical activity

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	Level: 2	Remedy: The remedy is some compatibility studies of fission products with SiC
Rationale: Fission products that dissolve in the SiC lattice will be stabilized and will be held from release at least temporarily. It does not appear, however, that this is major factor in the release of the more important, volatile fission products like I, Cs, Xe, Kr, Te etc. It may be more important for some of the transition metal fission products. Certainly Pd actually can react with SiC. Similarly Zr might react. It would also be of interest to know if other materials interacted badly with SiC, but even if we knew of some bad interactions involving materials other than fission products, we would have to have some idea of how these materials came into contact with the SiC within a fuel particle.	Rationale: There is amazingly little information about the phase relationships in the Si-C-FP systems of interest.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	SiC Layer Sintering	Change of graphite microstructure as a function of temperature

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 6	Remedy no remedy necessary:
Rationale: I do not find anything to suggest that changes in the microstructure of graphite will affect the SiC layer there may be some information suggesting that bonding of the graphite to the SiC affects the integrity of this layer, but it has nothing to do with microstructure issues	Rationale : there is really quite a lot of information about the sintering of SiC in the literature. It does not necessarily cover the entire region of interest nor does it address the effects of the fission product species on the sintering process. It should, however, be sufficient to estimate the magnitudes of any effects attributable to sintering on fission product transport. Far more important than simple, classic sintering will the thermal annealing of the radiation-induced defects in the SiC structure	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	SiC Layer: Chemical attack by water Kinetics	Rate of reaction per unit surface area as a function of temperature and partial pressure of steam

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 1	Remedy:Reaction kinetic information is required and the best information will involve dynamically prepared SiC reactions after material irradiation to produce representative defect concentrations. The data on reaction should also include data on the changes of permeability of the layer to gas phase mass transport.
Rationale: In this context water vapor is an oxidant much like air except the additional complexities of nitrogen reaction can be neglected IF one assumes pure water vapor can enter and no air can. An additional complexity that arises is the possibility that the products of reaction will include Si(OH)4 and Si(OH)2 rather than SiO. Still all these species are gases at the temperatures of real interest. The other product of reaction is hydrogen (as well as CO) and this leads to the possibility that hydrides may be formed to carry away material. Still the overall issue is whether the reaction of water vapor with SiC will facilitate fission product transport across the layer either by thinning the layer (a modest effect in light of the likely availability of oxidant) or my opening pathways for gas phase mass transport of fission products across the layer by preferential reaction with voids pores and cracks. These issues are of high importance only if the water vapor can survive transport to the SiC which is by no means established but clearly possible	Rationale: I have not been able to identify a suitable data base. I cannot find data for irradiated material of possible polytypism to address the question	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	SiC Layer: Chemical attack by water Catalysis	Modification of the reaction rate by fission products or impurities

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	Level: 1	Remedy see above:
Rationale: There is some evidence that impurities at the grain boundaries will accentuate the localized rate of attack on SiC. This might be of especial concern if it leads to more facile gas phase mass transport across the layer	Rationale: I can't identify suitable databases indicative of catalysis of water attack on SiC.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	SiC Layer: Chemical attack by water	Changes in chemical form resulting from oxidizing or reducing fission products
	Changes in chemical form of fission products	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 5	Remedy: Any effort to model the release and transport of fission products from coated particle fuel will have to track the fission product speciation and especially the vapor phase speciation as changes in local temperature and chemical potentials occur. To do this there will have to be a reliable thermochemical data base, again especially for the vapor species. Here mention is made of vapor phase oxides, hydroxides and hydrides.In the context of air intrusion vapor phase nitrides and cyanides are also of interest though the data bases for these are not at all well developed. Even without intrusion, vapor phase carbides and carbonyls need to be recognized and this will require development of data bases since these species have not been well explored.
Rationale: As with oxygen intrusion, the availability of water vapor can locally alter the speciation of fission products making some more volatile such as Ru, Pd, and Mo and others less volatile such as Ba, Sr, Ce, and La. Water vapor has the ancillary capability of creating vapor phase hydroxides of species such BaOH that can enhance the vapor pressure of fission products. Finally hydrogen produced by the reaction of water vapor with carbon can lead to the formation of vapor phase hydrides of fission products such as CsH and RuH that will enhance apparent fission product vapor pressures and consequently accentuate the release and transport of fission products.	Rationale We have some databases that can be used to estimate the effects of water vapor and reaction products on the vapor pressures of fission products. Best developed are the databases for elements and oxides. Bases for vapor phase hydroxides are mostly estimates obtained by considering the hydroxides to be pseudo halides somewhat intermediate in volatility between the fluorides and the chlorides of the fission product species. More spotty is the data base on hydrides of fission products	Closure Criterion:
	The situation is largely the same at higher temperatures except that vapor phase hydrides can become more important to the overall vapor pressure	

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	SiC Layer: Chemical attack by water	Changes in diffusivity, porosity, adsorptivity, etc.
	Changes in SiC properties	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: II	Level: 1	Remedy If it is concluded that there is a possibility of some water vapor reacting with the SiC layer and these reactions are to considered in the predictions of fission product transport, then there needs to be a data base on how water vapor reacting with dynamically prepared, irradiated SiC changes the permeability of the SiC:
Rationale: reaction of water vapor in the pores and networks of the SiC layer will facilitate the transport of fission products across the layer by gas phase mass transport	Rationale: I can identify no suitable data base on the reactions and the changes in the macrostructure of SiC layers with reaction	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	SiC Layer: Chemical attack by water	Release of SiC FP inventory
	Holdup reversal	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 1	Remedy no remedy needed:
Rationale: As discussed repeatedly above in connection with other layers, it is known that the reactions of energetic sites with adsorbed fission products will lead to the release of the fission products, but it is not clear that the layer will retain enough fission products to make this risk significant	Rationale: I can find no data on the adsorption in the layer	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	SiC Layer: Chemical attack by water Temperature distribution	Impact of SiC oxidation on temperature distribution through material

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 5	Remedy: modeling of fission product release and transport will require detailed temperatures locally.
Rationale: The chemical reactions are not iso-enthalpic so they will affect the temperature distributions in the layer and as noted elsewhere these temperatures affect both the volatilities of fission products and their transport.	Rationale We should be able to calculate the effects of reaction on the temperature distributions since we know the enthalpies of reaction. A complication arises because the reaction energies will also involve the energy release associated with the destruction of energetic radiation defects. We do need to know the kinetics of reaction well – which we do not now know.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Inner PyC Layer Gas Phase Diffusion	Diffusion of gaseous fission products through layer (Knudsen and bulk diffusion through pore structure, and pressure driven permeation through structure)

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 6	Remedy: Any model of fission product transport within the fuel particle will have to include a gas phase mass transport model recognizing bulk gaseous diffusion, pressure driven flow and Knudsen diffusion
Rationale: Gas phase mass transport is the fastest mechanism to move fission products release from the fuel kernel across the barrier posed by the inner PyC layer	Rationale: Given the geometry and nature of the pore and crack network through the layer it should be possible to calculate the gas phase mass transport across the layer. We can estimate the gas phase diffusion coefficients for most of the dominant gaseous species. The diffusion process itself probably cannot be modeled as strictly Fickian diffusion. One will have develop a multicomponent diffusionmodel much like the membrane modesl that have been developed in the chemical engineering literature. It may be necessary to include in these models the effects of thermal diffusion especially since we will have low molecular weight species (CO MW=28) migrating along the same paths as the high molecular weight (>100) fission product vapor species. The importance of this will depend on the magnitude of the thermal gradients across the layer which surely must be significant given the relatively high conductivity and the need to move (Continued next column)	Closure Criterion: (Continued from previous column) the decay heat away from the fuel kernel. The most complicated part of the modeling will be a realistic portrayal of the layer geometry and the pore and crack networks. It is tempting to model the layer as a spherical shell, but this is only justified if the deviations from spherical are not sufficient to provide a short circuit pathway in some regions. Similarly, it will be tempting to treat the layer as uniform in thickness though it never will really be. We do not have meaningful data on the pore and crack network. These networks may change if there is reaction with the intruding gases. We may not be able to derive useful descriptions of the pore and crack networks through the layer from microscopic examinations of these networks. Cracks and channels to small to be readily identified in microscopic analyses can be effective in the transport of material across the layer.

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Inner PyC Layer Condensed phase diffusion)	Inter-grannular and/or intra-grannular solid-state diffusion

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	Level: 2	Remedy: Any model of fission product transport across the inner PyC layer will have to include the condensed phase mass transport process to account for mass transport of fission products when the layer does not have pore and crack networks to facilitate gas phase mass transport across the layer
Rationale: Fission products that are not volatile will be transported across the inner PyC layer by the condensed phase diffusion processes. Bulk diffusion is the slowest of these at low temperatures but it has the highest activation energy so it does eventually become the dominant process. Even if the metals have only small vapor pressures, gas phase mass transport of fission products may still be the dominant mechanism for mass transport	Rationale We do not have surface and grain boundary diffusion coefficients to model the mass transport of fission products across the layer at lower temperatures. These cannot be estimated or transferred from studies of analogous materials since they are notoriously sensitive to the precise grain structure and the nature of impurities at the grain boundaries. We don't even have a data set of bulk diffusion coefficients for the PyC layer of demonstrated reliability.	Closure Criterion:
	At sufficiently high temperatures bulk diffusion will be the dominant condensed phase mass transport process This process is very sensitive to the presence of defects produced by irradiation acting as traps for diffusing species and we don't seem to have data on this.	

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Inner PyC Layer Pressure loading (Fission products)	Stress loading of the layer by fission products by increased pressure

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue *Closure Criteria*
Rank: L	Level: 2	Remedy to evaluate the pressure drop one would have to have some estimate of the permeability of the layer:
Rationale: Pressure loading will more likely be by CO pressure produced by the reaction of carbon with the fuel kernel. The loading will probably be on the SiC layer rather than the inner PyC layer though it is possible that there will be some pressure drop across the layer	Rationale: We need permeability data that seem not to exist to estimate the pressure drop across the layer. If this is significant then the layer can act at least temporarily as a barrier to fission product transport. But, if the pressure drop is significant then the layer is likely to rupture and completely lose its effectiveness as a barrier as the accident progresses and additional pressurization from both CO build up and fission product release occurs	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Inner PyC Layer Pressure loading (Carbon monoxide)	Stress loading of the layer by carbon monoxide by increased pressure

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: II	Level: 2	Remedy:no remedy needed
Rationale: The loading by CO should dominate that by fission products. Still it is not evident that the layer will have a substantial pressure retaining capability and the SiC layer is a more important layer for this.	Rationale: We need permeability data that seem not to exist to estimate the pressure drop across the layer. If this is significant then the layer can act at least temporarily as a barrier to fission product transport. But, if the pressure drop is significant then the layer is likely to rupture and completely lose its effectiveness as a barrier as the accident progresses and additional pressurization from both CO build up and fission product release occurs)	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Inner PyC Layer Layer oxidation	Reaction of pyrolytic graphite with oxygen released from the kernel

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 2	Remedy: Analysis of fission product transport will have to treat the effects of oxidants and ascertain if oxidants can reach the inner PyC layer. If so, the possibility of preferential and even catalyzed oxidation of the layer will have to be considered. Decent data sets on the reactions of the specific materials with oxidants are really needed.
Rationale: This high importance is assigned under the presumption that oxidant can reach the layer. The oxidant that comes is more likely to be from the fuel kernel than from the gases intruding in the accident scenario. Intruding gases will have to pass over an awful lot of reactive material before they can reach the inner PyC layer. On the other hand oxidant from the fuel will have to pass through a buffer layer of carbon to reach the inner PyC layer. If the oxidant reaches the material it can cause thinning of the layer (probably not especially important) or opening of the pathways for gas phase mass transport of fission products making the transport by gas phase processes even more rapid.	Rationale: The layer really does not take up oxidant. It reacts to form CO (and other equivalent species such as C2O and C2O3) that vaporizes. The reactions are enormously sensitive to catalysis and fission products can act as catalysts. We don't have a lot of data on which fission products will produce catalysis, We do know that Cs can catalyze the oxidation of C. We also know that irradiation makes the material more reactive. More than just rate of reaction data for the specific material, we need to know if the reaction takes place uniformly over the surface or if there is preferential reaction especially to open pathways for the gas phase transport of fission products across the layer	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Inner PyC Layer Stress state (compression/tension)	The state of the forces induced by external forces that are acting across the layer to resist movement

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 2	Remedy: Models or data to predict rupture of the layer are needed. These models may be nothing more than criteria identifying conditions for which layer integrity can no longer be assured.
Rationale: It is known that stress state can affect both condensed phase and gas phase diffusion across a layer, but this is a pretty subtle effect. More important is whether the layer stays in tact or is ruptured and allows essentially unimpeded gas phase mass transport across the layer, but this is treated in other questions	Rationale: We don't really know much about the forces and especially forces induced by the radiation caused growth of materials	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Inner PyC Layer Cracking	Lengths, widths and numbers of cracks produced in layer during accident

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 1	Remedy: Any model of the fission product transport across the inner PyC layer will have to admit to the possibility of cracks – perhaps quite narrow cracks – developing in the layer from radiation-induced growth or thermal expansion or mechanical forces on the layer including pressurization examined above.
Rationale: Any cracking of the layer will create effective pathways for gas phase mass transport across the layer	Rationale: We are not really in the position to predict cracking of the layer. Though there are data in abundance for PyC they are not for the specific material in the fuel particle and not for the material subjected to thermal transients and irradiation of the type that will be seen by the PyC layer	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Inner PyC Layer Intercalation	Trapping of species between sheets of the graphite structure

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	Level: 2	Remedy: WE need some sort of data or analyses to show whether intercalation will be an effective holdup mechanism for fission product release.
Rationale: Intercalation could act as a holdup mechanism for fission products. Intercalation usually occurs during the simultaneous condensation of vapors and graphitic material. Intercalation could occur because of the radiation displacements of materials. Intercalation is known to be an effective way to trap potassium in graphite and so it might be effective in trapping Cs in the graphite. Still, it is not evident that so much of the radionulcide inventory can be trapped in the layer that this is risk-significant issue	Rationale: I have no data on intercalation as a dynamic process either during an accident or during fuel operations Intercalation will reverse at very high temperatures and not be an issue	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Inner PyC Layer: Chemical attack by water Kinetics	Rate of reaction per unit surface area as a function of temperature and partial pressure of steam

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 6	Remedy: Any model of fission product transport treating intrusion accidents will have to consider water vapor reactions with graphite and carbon. The issues include both the quantitative kinetics and the homogeneity of the attack on carbon. Uniform attack only thins the layer. Though thinning the layer certainly facilitates mass transport across the layer the effect need not be dramatic. More important will be preferential reaction in pores and cracks that opens these pathways for gas phase mass transfer across the layer.
Rationale: As with air attack the rating for this issue is conditional on the ability of oxidant to get to the layer. Reaction of water with the inner PyC layer is not as dramatic as reaction of air. Still the reaction will affect the volatilities of fission products both because of the effect on ambient oxygen potential and because of the possible formation of vapor phase hydroxides and the transport of fission products either by thinning the layer or opening pathways for gas phase mass transport. If the steam is consumed the hydrogen gas could lead to the formation of vapor phase hydrides which are also pseudo-halides and could augment the vapor pressure of the fission products via formation of vapor species like CsH and RuH.	Rationale: There is a lot of information about the rates of steam reactions with carbon though perhaps not the specific, heavily irradiated carbon of the fuel particle. Irradiation is an important issue because it will affect the rates of reaction because the defects introduced by irradiation are quite reactive.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Inner PyC Layer: Chemical attack by water Catalysis	Modification of the reaction rate by fission products or impurities

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: II	Level: 3	Remedy:Models of the reactions of the inner PyC layer will have to recognize the possibility of catalysis especially at lower temperatures where it is more likely that oxidant will be available to penetrate to the inner PyC layer
Rationale: steam reactions with carbon are catalyzed and catalysis leads to preferential attack and even to penetrations through the layer to facilitate gas phase mass transport of fission products across the layer.	Rationale: see discussion s of catalysis of air reactions Catalysis is of less importance at high temperatures where reaction rates are high and eventually are limited by mass transport, Furthermore localized attack becomes less likely than uniform ablation of the layer material	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Inner PyC Layer: Chemical attack by water Changes in chemical form of fission products	Changes in chemical form resulting from oxidizing or reducing fission products

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 5	Remedy:The speciation of the fission products will be an essential part of any model of fission product release and transport. This is especially the case here because of the dominant role that vapor phase mass transport is expected to play in the transpor across the inner PyC layer. Significant model components will be the thermochemical data bases used to calculate speciation. It will be important to have reliable thermochemical data and estimates to compensate for the incompleteness of the experimental studies of species likely to contribute to the transport across the layer.
Rationale: Just as for air intrusion the presence of water vapor can affect the speciation of the fission products and consequently their vapor pressures. The effect is compounded by the possibility of formation of vapor phase hydroxides like BaOH and SrOH. If the steam is all reacted by the time it reaches the inner PyC layer the product hydrogen can affect fission product vaporization via the formation of vapor phase hydrides like CsH and RuH.	Rationale:There is a technical basis for estimating the oxygen potential effect on the vaporization of fission products. The database on vapor phase hydroxides consists mostly of estimated properties though some species such as CsOH, BaOH, SrOH are known well. The data base for vapor phase hydrides has not been systematically developed.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Inner PyC Layer: Chemical attack by water Changes in graphite properties	Changes in diffusivity, porosity, adsorptivity, etc.

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 3	Remedy:Preferential reactions of oxidant with the layer material to open pathways for mass transport will have to be considered in a model of fission product transport through coated particle fuels
Rationale: Again, IF water vapor can reach the inner PyC layer, its important effect aside from changing the volatilities of the fission products will be reaction to remove material from the layer. Thinning the layer is a modest effect. More important and more likely especially at lower temperatures is preferential reaction in pores and cracks to open pathways for gas phase mass transport of fission products across the layer.	Rationale: The calculation of the localized oxidation that leads to the opening of gas phase pathways across the layer is difficult to do. We don't now have the needed data on the pathways nor do we have the reaction kinetics information for the particular material of interest. If we had these data the calculation could be based on models of porous media reaction developed in other contexts in the chemical engineering literature) The situation is somewhat the same at higher temperatures though the reactions become more rapid at elevated temperatures and the propensity for localized or preferential attack on the carbon becomes less dominant.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Inner PyC Layer: Chemical attack by water	Release of graphite FP inventory
	Holdup reversal	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 4	Remedy:Not evident that a remedy is needed.
Rationale: Oxidation will destroy the energetic sites that have adsorbed fission products and thus release the fission products. It is not apparent, however, that the inventory of fission products absorbed on this layer will be so large that its release will be risk significant.	Rationale: We don't have the needed data on the fractional holdup in the layer fy the adsorption process. Nor do have the needed data on the concentrations of energetic sites available for adsorption	Closure Criterion:
	At elevated temperatures, the vapor pressures of the important volatile radionuclides are so high that adsorption fractions will be quite low. Though we don't know more about the adsorption/desorption processes at high temperatures than at low temperatures, we don't need to know as much to know that this will not be an important holdup process	

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Inner PyC Layer: Chemical attack by water Temperature distribution	Impact of graphite oxidation on temperature distribution through material

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 3	Remedy: Any model of fission product release and transport will require auite a good model of the local temperature distributions in the fuel particle. Good data on the thermal conductivity, reaction kinetics and defect energies will be needed.
Rationale: The chemical reactions of water vapor with PyC are not iso-entahlpic so they will distort the temperature distributions in the particle. As noted elsewhere these temperature distributions do affect release both through the effect on the thermodynamic driving force for transport across the particle and the effects on the transport processes themselves	Rationale: We generally know the heats of reaction with pristine material. These heats need to be modified for the effects of defect destruction by reaction. Then, if we understood the kinetics and the thermal conductivity of the material we could, in principle calculate the effects of reactions on the temperature distributions	Closure Criterion:
	The situation is largely the same as at lower temperatures except radiation heat transfer becomes a more important factor to consider .	

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Buffer Layer Gas phase diffusion	Diffusion of gaseous fission products through layer (Knudsen and bulk diffusion through pore structure, and pressure driven permeation through structure)

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 4	Remedy a fairly sophisticated model of the layer porosity will be needed as will a very sophisticated model of mass transport across the layer:
Rationale: Gas phase mass transport across this layer will be the dominant transport mechanism for volatile fission products because the temperatures are high and because the material is quite porous.	Rationale Given the nature of the porosity in the layer it should be possible to calculate the gas phase mass transport quite well. We can estimate the diffusion coefficients for most vapor species. The analysis probably cannot treat the diffusion as Fickian. A multicomponent model will have to be considered because there will be a flow of CO across the layer that may be, in fact, pressure driven rather than diffusion. Diffusion may have to be augmented by consideration of thermal diffusion because of the large temperature gradient and the mixture of molecular weights of the gaseous species. Other complexities in the analysis include lack of spherical symmetry of the layer and the variations in the layer thickness	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Buffer Layer Condensed phase diffusion	Inter-grannular diffusion and/or intra-grannular solid-state diffusion

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 1	Remedy:no remedy needed
Rationale: Fission products that reach the interface between the buffer carbon and the fuel kernel will have all escaped the kernel as some sort of a vapor species through the interconnected pore network in the urania. (The flux of fission products from the fuel via intragrannular diffusion is really quite small at temperatures that are well below the urania melting point) It does not seem likely that significant transport of even species with very modest vapor pressures would switch to a condensed phase process upon encountering the highly porous buffer region.	Rationale: Don't have definitive condensed phase diffusion coefficients for the material Condensed phase mass transport rather than vapor phase mass transport is even less likely to be dominant at higher temperatures and the condensed phase diffusion coefficients are even less known at elevated temperatures	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Buffer Layer Response to kernel swelling	Mechanical reaction of the layer to the growth of the kernel via swelling

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	Level: 4	Remedy:Because integrity of the layer is not critical, it may not be necessary to develop a very detailed understanding of the mechanical properties of the buffer layer. It may not even be present in future incarnations of coated particle fuel pellets
Rationale: cracking and otherwise opening pathways for gas phase mass transport as a result of mechanical interactions could facilitate fission product transport across the buffer region, but the region is already quite porous so the incremental effects of cracking on gas phase mass transport are not likely to be as dramatic as cracking of the more compact structural barriers in the coated particle fuel.	Rationale We have been shown some evidence that in the current inadequate fuels that mechanical interactions can rupture the buffer layer. We have not been shown any indication that this process can be predicted in a quantitative way. There are data on the mechanical properties of materials analogous to materials in the buffer region, but these data may not be applicable to the thin layer that can bond to either the kernel or to the bounding PyC layer	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Buffer Layer Maximum fuel gaseous fission product uptake	Maximum loading of fission products that can deposit from the gas phase onto surfaces of materials surrounding the fuel kernel

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 3	Remedy no remedy needed:
Rationale: It is likely that some fission products will deposit in the buffer region at least temporarily and this effect has to be considered in developing the modeling of the fission product transport. But it does not appear likely that the fraction of the released fission product inventory that can deposit in this region will be sufficiently large to be of risk significance	Rationale We know deposition can take place. We don't have quantitative information on the density of active sites for deposition or adsorption/desorption isotherms for the fission products	Closure Criterion:
	Adsorption on active sites become even less important at elevated temperatures first because the vapor pressures at such elevated temperatures are so high and second because at elevated temperatures active adsorption sites are being thermally annealed. So it is not that we know more about the situation at high temperatures, it is that relatively we need to know less.	

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Buffer Layer Layer oxidation	Reaction of pyrolytic graphite with oxygen released from the kernel

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 2	Remedy Easily one of the most important characteristics to understand for coated particle fuels is the reaction of carbon with the urania fuel. This may well be a heterogeneous reaction of gas phase oxidant with carbon. It may also involve a homogeneous direct reaction of two solid materials especially under conditions of irradiation. The reaction will be dependent on the ambient CO pressure. In fact leakage of the CO from the coated particle fuel may well dictate the extent of reaction
Rationale: The 'uptake' is really the reaction of oxygen from the fuel reacting with carbon in the buffer layer to form CO that pressurizes and possibly ruptures the compact barriers with the fuel particle such as the PyC layer and the SiC layer. Rupture of these layers will allow the venting of the vapor phase fission products within the particle and provide a facile pathway for the gas phase mass transport of fission products out of the fuel particle as the accident progresses. The reaction could also damage the crystal structure of urania at the surface of the kernel – converting it into UCO and eventually UCx. The crystallographic changes are sufficiently large that fission products within grains of the surface fuel will be expelled and ready to vaporize without mass transport limitations that affect release of fission products from grain surfaces within the fuel kernel.	Rationale Reactions of carbon with urania are thermodynamically possible at sufficiently low CO partial pressures even at low temperatures. They do appear to be slow. Irradiation of the carbon may create energetic sites that are more reactive than might be expected based on tests with unirradiated materials. Still the empirical evidence is that the reactions are slow in absence of some sort of catalyst. Always a concern is that the fission product species may act as catalysts under circumstances not so far encountered in the studies of coated particle fuels Reactions of carbon with urania definitely occur at more elevated temperatures. I am not aware of definitive rate data for the reactions	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Buffer Layer Thermal gradient	Change in temperature with distance

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: II	Level: 4	Remedy: Modeling of fission product transport in the coated particle fuels will require that there be a detailed model of the local temperatures and temperature gradients. To do this for the buffer layer will first require that the porosity of the layer be characterized and then some heat transfer modeling be done to develop expressions for the thermal conductivity of the material.
Rationale: Thermal gradients across the buffer layer – which could be substantial in magnitude – will affect the fission product release both by chemical diffusion of vapors and by thermal diffusion of vapors	Rationale: In principle we can calculate the mass transport across the layers given the temperature distributions. Calculations of the thermal distributions are made complicated by the poor knowledge of the material thermal conductivity and the effects of radiation defects and pores or cracks on the thermal conductivity. It is unlikely that simple corrections of material thermal conductivity using things like the Loeb correction will be adequate since the layer is so thin the bulk averaging inherent in the Loeb correction and similar corrections simply will underestimate the effects of porosity. Something much more sophisticated will have to be done.	Closure Criterion:
	The situation is largely the same at elevated temperatures except that radiation heat transfer within the layer becomes more of an issue. It is not simple to calculate because the ambient CO cannot be taken as transparent to the radiation.	

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Buffer Layer Irradiation and thermal shrinkage of buffer	Dimension changes in the buffer layer or changes in its porosity produced by irradiation or by exposure to elevated temperatures

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 5	Remedy: The only real issue that must be borne in mind is whether the dimensional changes are sufficient to cause rupture and then this is of concern only if holdup of fission products in the buffer layer is actually credited in the transport process.
Rationale: The effects are small enough that they will probably be safely neglected in the modeling of fission product transport. Of course, if the changes open pathways for gas phase mass transport of fission products they facilitate this transport as discussed above.	Rationale: We know that the buffer layer material will grow as a result of radiation-induced defects in the material. Thermal expansion during accident transients will affect the material. While w e don't have data for the specific material, we do have data for analogous materials	Closure Criterion:

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Buffer Layer: Chemical attack by water Kinetics	Rate of reaction per unit surface area as a function of temperature and partial pressure of steam

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L – but see additional discussion below	Level: 6	Remedy: no remedy needed
Rationale: for conventional intrusion scenarios it is difficult to believe that oxidant will penetrate to the buffer layer without having reacted with other carbon materials along the way. Far more important will be the oxidation of the buffer layer by oxygen coming from the hot fuel kernel.	Rationale There is quite a lot of data on the kinetics of steam reactions with carbon but none specific to the material of interest here. The information does suggest that at low temperatures attack can be localized and the reactions can be catalyzed. Reaction rates will be very sensitive to impurity levels and the specifics of porosity and microstructure at low temperatures	Closure Criterion:
	Attack of steam on carbon is much more uniform at very high temperatures. Still information specific to the material of interest here seems not to be available.	

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Buffer Layer: Chemical attack by water Catalysis	Modification of the reaction rate by fission products or impurities

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 4	Remedy:no remedy needed
Rationale: Catalysis of the reactions of water vapor may not be important if water vapor cannot reach the buffer layer prior to reacting with other carbon materials along the way.	Rationale We know the reactions can be catalyzed and that some fission products can act as catalysts including Cs.	Closure Criterion:
	Catalysis is less important at high temperature where heterogeneous reaction rates are intrinsically rapid.	

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Buffer Layer: Chemical attack by water Changes in chemical form of fission products	Changes in chemical form resulting from oxidizing or reducing fission products

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	Level: 3	Remedy: Thermodynamic analyses essential in the modeling of fission product release and transport depend crucially on the identification of all the important vapor species. Not all the species that will contribute to the processes have been identified and characterized in the literature in a way that lets these species be included in the codes. NRC was advised by a panel of the National Academy of Science to estimate properties of species and include them in their fission product release models to assess possible importance and need for experimental investigations to prove the species exist and determine accurately their properties. This needs desperately to be done for the hydrides of fission product elements.
Rationale: Though the water vapor may not penetrate to the buffer layer the gaseous product of water vapor reactions with carbon – hydrogen- can penetrate to this layer and in fact will penetrate to this layer. The oxygen potential will not be affected, but there is the potential that hydrogen partial pressures will be high enough that the vapor pressures of some of the fission products will be augmented by the formation of vapor phase hydrides which are typically as volatile as the corresponding halides.	Rationale: There has not been a systematic examination of how vapor phase hydrides will affect the vapor pressures of the important fission products. We do know that CsH can be an important vapor phase form of cesium and species like RuH, BaH and the like can form. We don't really have agreed-upon thermodynamic data to assess the importance of these species. Furthermore, there has not been a systematic search for hydride species of all the fission products of interest.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or *Phenomenon*	Definition
Accident With Subsequent Water Intrusion	Buffer Layer: Chemical attack by water	Changes in diffusivity, porosity, adsorptivity, etc.
	Changes in graphite properties	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 3	Remedy:no rememdy is needed
Rationale: Again, if the oxidant cannot reach this buffer layer, the effects of preferential oxidation of the buffer layer cannot be important (but note the caveat about alternative accident scenarios above)	Rationale Without a better characterization of both reaction kinetics and the nature of pore and crack structures of the buffer layer it would not be possible to calculate the effects of reaction on porosity even if it could occur	Closure Criterion:
	localized attack is less likely at higher temperatures	

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Buffer Layer: Chemical attack by water Holdup reversal	Release of graphite FP inventory

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 4	Remedy: no remedy is needed
Rationale: It is not evident that intruding water vapor can reach the buffer layer to cause this release nor is it evident that holdup in the layer is so large that quantitative release of adsorbed fission products would be risk significant.	Rationale: We know reactions will release adsorbed fission products. We don't have the information on site density and isotherms to quantitatively calculate the holdup or the subsequent release in the event of reactions	Closure Criterion:
	Holdup becomes less important at elevated temperatures as active sites anneal and vapor pressures are so high that the adsorption is very small. So though we don't know more about the phenomenon at elevated temperatures than we do at low temperatures, we don't need to know as much for high temperature situations	

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Buffer Layer: Chemical attack by water Temperature distribution	Impact of graphite oxidation on temperature distribution through material

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	Level: 3	Remedy: Any model of fission product transport in the fuel particle will require a detailed model of the temperature distributions in the layer. To do this for the buffer layer requires some characterization of the porosity and a way to treat it in the thermal conduction modeling.
Rationale: As discussed in the case of reaction of air, water vapor attack on the buffer layer is not going to affect temperature distributions significantly. But water vapor attack on other layers will affect the temperature distributions in the buffer layer	Rationale: The pertinent knowledge bases are those associated with water vapor reactions with other layers and the calculations of temperature distributions throughout the particle. Most pertinent to the temperature distributions in the buffer layer is the thermal conductivity of the material. The material thermal conductivity is not so much of a problem since this can be estimated with adequate accuracy from data for analogous materials. The problem is the effects of porosity on the thermal conductivity of the small layer. Usual corrections for the effects of porosity on the thermal conductivity are not applicable. The layer is just too thin to get the necessary averaging of orientations implicit in the usual correction factors. A more sophisticated treatment is needed. A roadmap for such a more sophisticated treatment exists in the literature. Input to the treatment is a better characterization of the porosity of the layer	Closure Criterion:
	The situation at very high temperatures is about the same as above but radiation heat transfer becomes an additional issue complicated by the fact that the ambient CO will not be transparent to the thermal radiation.	

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Kernel Maximum fuel temperature	Maximum fuel temperature attained by the fuel kernel during the accident

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 6	Remedy:
Rationale: Temperature is well known to be one of the dominant variables controlling the release of fission products form urania kernels	Rationale: In principle, it should be possible to calculate the maximum kernel temperature fairly accurately. Even so, errors on the order of 50 degrees are possible. Definitive, defensible calculations for credible accidents have not yet appeared.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Kernel Temperature vs. time transient conditions	The time-dependent variation of fuel temperature with time

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 4	Remedy:
Rationale: Fission product release is a strong function of both time and temperature	Rationale: Though fairly reliable temperature histories are in principle possible to predict defensible calculations have not yet been produced. Most existing calculations are hopelessly optimistic about heat loss pathways.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Kernel Energy Transport: Conduction within kernel	Flow of heat within a medium from a region of high temperature to a region of low temperature

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	Level: 3	Remedy:
Rationale: Conduction as well as decay heat generation determine the temperature history of the kernel during the event	Rationale: Conduction in moderately porous urania is known with some accuracy. But, the porosity of the urania kernels can become heroic during extended operations and the events of the accident could easily produce porosities and configurations of the kernels that are quite intractable for conduction calculations.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Kernel Thermodynamic state of fission products	Chemical and physical state of fission products

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 5	Remedy:
Rationale: Fission product release depends on the chemical activity of the fission products. Completely diluted in the urania matrix, the fission product activities could be quite low. But, when the segregate into separate phases such as uranate phases or metallic nodules, chemical activities can be driven up substantially – orders of magnitude.	Rationale: We have a useful understanding of chemical activities of fission products in urania fuel at moderate burnups. At the higher burnups expected for some gas reactor fuels, our knowledge and predictive capabilities begin to fail us	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air and Water Intrusion	Kernel Oxygen flux	Mass transport of oxygen per unit surface area per unit time

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	Level: 3	Remedy:
Rationale: Diffusion of fission products will occur simultaneously with the diffusion of oxygen from the kernels to the reactive graphite at the buffer-kernel interface. The release is far more a multicomponent process than we have encountered in the case of fission product release from conventional fuels. The gettering of oxygen by reaction with the carbon is not passivating as is the case with gettering of oxygen by reaction with zirconium in the case of conventional fuels. It is not evident, then, that the usual Fickian diffusion approximation can be made incaustiously to predict release from the kernels	Rationale: Release analysis recognizing the multicomponent nature of the transport within fuel grains have not been published. In multicomponent systems, remarkable things can be predicted that appear counter-intuitive when viewed within the context of binary diffusion.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Kernel Grain growth	Enlargement of grains as a result of diffusion

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 8	Remedy:
Rationale: Grain growth is largely unimportant because of the grain boundary pinning effects of fission products and especially separated phases of fission products	Rationale: It has not been essential to consider grain growth in models of fission product release from conventional reactor fuels, though some codes include such models.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Kernel Buffer carbon-kernel interaction	Chemical reaction between carbon and the fuel (UO2 or UOC) to form UC2 and CO (gas)

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 3	Remedy:
Rationale: The reaction of the buffer with the kernel can be responsible for the pressurization perhaps to failure of the SiC layer. The reaction can also lead to fission product release as the reactive refinement of the urania progresses	Rationale: Details of the reaction process and even the phase relations in these systems are not known well.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Kernel: Chemical attack by water	Rate of reaction per unit surface area as a function of temperature and partial pressure of steam
	Kinetics	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 8	Remedy:
Rationale: The hypothesized scenario involves an atmosphere with only 1% water vapor. It is just not possible to imagine how such a low concentration of water vapor would persist in contact with the kernel despite opportunities to react with graphite.	Rationale: There is a wealth of information on the kinetics of low concentrations of steam reacting with urania. There is also good information on how this reaction of low concentration of steam will change the properties of the urania.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Kernel: Chemical attack by water Catalysis	Modification of the reaction rate by fission products or impurities

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 8	Remedy:
Rationale: The hypothesized scenario involves an atmosphere with only 1% water vapor. It is just not possible to imagine how such a low concentration of water vapor would persist in contact with the kernel despite opportunities to react with graphite.	There is a wealth of information on the kinetics of low concentrations of steam reacting with urania. There is also good information on how this reaction of low concentration of steam will change the properties of the urania	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Water Intrusion	Kernel: Chemical attack by water	Changes in chemical form resulting from oxidizing or reducing fission products
	Changes in chemical form of fission products	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 8	Remedy:
Rationale: The hypothesized scenario involves an atmosphere with only 1% water vapor. It is just not possible to imagine how such a low concentration of water vapor would persist in contact with the kernel despite opportunities to react with graphite.	There is a wealth of information on the kinetics of low concentrations of steam reacting with urania. There is also good information on how this reaction of low concentration of steam will change the properties of the urania	Closure Criterion:

Additional Discussion

APPENDIX F

PANEL MEMBER DETAILED PIRT SUBMITTALS FOR TRISO FUEL DEPRESSURIZATION ACCIDENT WITH AIR INGRESS

The INEEL submittal is provided in Appendix F.1 (pages F-2 through F-79).

The ORNL submittal is provided in Appendix F.2 (pages F-80 through F-160).

The SNL submittal is provided in Appendix F.3 (pages F-161 through F-239).

Appendix F.1

Detailed PIRT Submittal by the INEEL Panel Member

F. A. Petti

TRISO Fuel PIRT: Accident With Subsequent Air Intrusion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Fuel Element Irradiation history	The temperature, burnup and fast fluence history of the layer

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	7	Remedy:
Rationale: Irradiation history determines inventory at risk and initial conditions in particle relative to internal pressure in the particle and stress state.	Rationale:	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Fuel Element Condensed phase diffusion	Inter granular diffusion and/or intra-grannular solid-state diffusion

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	6	Remedy:
Rationale: Mechanism describing the transport of fission products in matrix of the fuel element. Important to understanding source term for the reactor.	Rationale: Air or water ingress can change the microstructure of the matrix, which can influence the surface diffusion of fission products by making transport easier. At very low partial pressures, air and water oxidation rates can be determined by the number of active sites in the matrix at which the oxidation can occur. In some cases oxidation can be catalyzed by impurity elements that are trapped at adsorption sites in the graphitic matrix. Thus there can be competition between fission product adsorption and the reaction between the air or steam and the matrix. The isotherms are fairly well known. The key issue is whether the internal surface area of the matrix has been changed by the air or water oxidation event and thus the amount of material available for release. Dislocations and/or defects can act as trapping sites for fission products as they transport through the matrix. If the number of dislocations is about the same as the number of fission products then the effect may be important. If the fission product concentration is much greater than the dislocation density then the effect is probably second order. Exact values have not been measured nor has any transport behavior been directly correlated with these parameters. The influence of the oxidation event may be to provide enough energy to the matrix to release fission products from the traps. Sensitivity analysis can be performed to scope this out.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Fuel Element Gas phase diffusion	Diffusion of gaseous fission products through layer (Knudsen and bulk diffusion through pore structure, and pressure driven permeation through structure). Other factors include holdup, cracking, adsorption, site poisoning, permeability, sintering and annealing.

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: II	5	Remedy:
Rationale: Gas phase diffusion is thought to be the mechanism for gaseous fission product transport in the matrix.	Rationale: Air or water ingress can change the microstructure and porosity of the matrix, which can influence the gas diffusion of fission products by making transport easier. The interconnected porosity can be a transport path for the air or water intrusion. The reaction of air or water with the matrix can change the microstructure, porosity, tortuosity, and permeability, and hence affect gaseous fission product transport in the matrix.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Fuel Element: Transport of metallic FPs through fuel element Chemical form	Chemical stoichiometry of the chemical species that includes the radioisotope of interest

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	7	Remedy:
Rationale: Transport has been assumed to be elemental for the major fission products (Cs, Ag, I, Xe, Sr). Potential changes in chemical form due to the presence of air or water can be calculated.	Rationale:	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Fuel Element: Chemical attack by air Kinetics	Rate of reaction per unit surface area as a function of temperature and partial pressure of air

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	7	Remedy:
Rationale: Key parameter to describe thermal response and subsequent fission product release during the event.	Rationale: Kinetics are fairly well known for both air and steam as a function of temperature and partial pressure and flowrate.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Fuel Element: Chemical attack by air Catalysis	Modification of the reaction rate by fission products or impurities

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	5	Remedy:
Rationale: Impurities can affect reaction rate and thus impact overall behavior during the intrusion event.	Rationale: Oxidation rate data have been determined for actual pebbles and compacts and thus implicitly include the effects of impurities. The effects of fission products have not been included because oxidation testing has not been performed on irradiated material. In principle, sensitivity calculations can be performed with variations in the oxidation rate to bound this effect.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Fuel Element: Chemical attack by air Changes in chemical form of fission products	Changes in chemical form resulting from oxidizing or reducing fission products

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	6	Remedy:
Rationale: This can be important because the transport behavior is dependent on the chemical form.	Rationale: This can also be calculated for a range of oxygen potentials to determine if any of the key fission products change in chemical form during the air or water ingress accident.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Fuel Element: Chemical attack by air Changes in graphite properties	Changes in diffusivity, porosity, adsorptivity, etc.

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	6	Remedy:
Rationale: The oxidation can change the microstructure of the graphite by creating tunnels or pathways in the matrix. Thus, because the microstructure changes, the porosity, adsorptivity, etc., can also change.	Rationale: No measurements have been made on this effect. Conservative assumptions on such changes may allow sensitivity studies in this area.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Fuel Element: Chemical attack by air Holdup reversals	Release of graphite FP inventory

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	6	Remedy:
Rationale: As the oxidation process continues any fission products trapped at sites in the matrix may be released because of the thermal energy associated with the oxidation.	Rationale: This can be accounted for in a very simplistic yet conservative manner if details are not well known or more sophisticated models with detrapping can be used if the fundamental data needed for such models exist.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Fuel Element: Chemical attack by air	Impact of graphite oxidation on temperature distribution through material
	Temperature distributions	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	8	Remedy:
Rationale: Very important in doing an oxidation calculation is to make sure the temperature response of the material as a result of the energy generation is properly calculated.	Rationale: This is well known and can be done in most of the safety codes used by NRC (e.g. MELCOR). The high conductivity of the PyC should make the gradient quite small in general. The degree of fine detail in the model may be an open question but can be handled with sensitivity studies.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Outer PyC Layer Gas-phase diffusion	Diffusion of gaseous fission products through layer (Knudsen and bulk diffusion through pore structure, and pressure driven permeation through structure)

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: II	6	Remedy:
Rationale: OPyC can hold up gaseous fission products.	Rationale: Effective diffusion coefficients for noble gases through PyC exist for both German and U.S. PyC. The Knudsen diffusion formalism has not been historically used in the modeling. The effect of oxidation on changes in the transport behavior has not been studied. Sensitivity studies can be performed to bound potential changes to determine the impact on the overall source term.	Closure Criterion:

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Outer PyC Layer Condensed-phase diffusion	Inter-granular diffusion an/or intra-grannular solid state diffusion

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	6	Remedy:
Rationale: PyC layers provide for some transport delay of metallic fission products.	Rationale: Data exist on the effective diffusivity of Cs, Ag, and Sr through the PyC layer. The mechanism responsible for the transport has not been definitively identified. The effect of oxidation on transport properties has not been studied. Sensitivity studies can be performed to bound potential changes to determine the impact on the overall source term.	Closure Criterion:

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Outer PyC Layer Layer oxidation	Uptake of oxygen by the layer through a chemical reaction

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: II	7	Remedy:
Rationale: Oxidation of OPyC is needed to understand thermal response of the particles in the fuel element.	Rationale: Reaction rates for PyC are known at these temperatures.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Outer PyC Layer Stress state (compression/tension)	The state of the forces induced by external forces that are acting across the layer to resist movement

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	8	Remedy:
Rationale: The stress state is judged to be of low importance for a chemical oxidation event.	Rationale: Stress state is easily calculated using current finite element models for coated particles.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Outer PyC Layer Intercalation	Trapping of species between crystallite planes of the graphite structure

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	4	Remedy:
Rationale: In an intact particle, little diffusion of fission products is expected. If the level of adsorption or defect sites is high in the OPyC due to neutron irradiation for example, then these sites may be effective in holding up fission products if they are not annealed out during the oxidation event. In a failed particle, the number of fission product atoms is so large that such a mechanism is very small. This is based on diffusion and trapping modeling performed for tritium under the NPR program in the early 1990s. The oxidation event if severe enough could probably liberate any adsorbed or trapped fission products. Sensitivity studies with a diffusion and trapping model can study this in more detail to determine overall significance in the core for the oxidation event.	Rationale:	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Outer PyC Layer Trapping	Adsorption of fission products on defects

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	4	Remedy:
Rationale: In an intact particle, little diffusion of fission products is expected. If the level of adsorption or defect sites is high in the OPyC due to neutron irradiation for example, then these sites may be effective in holding up fission products if they are not annealed out during the oxidation event. In a failed particle the number of fission product atoms is so large that such a mechanism is very small. This is based on diffusion and trapping modeling performed for tritium under the NPR program in the early 1990s. The oxidation event if severe enough could probably liberate any adsorbed or trapped fission products. Sensitivity studies with a diffusion and trapping model can study this in more detail to determine overall significance in the core for the oxidation event.	Rationale:	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Outer PyC Layer Cracking	Lengths, widths and numbers of cracks produced in layer during operation or an accident

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	6	Remedy:
Rationale: A cracked OPyC will not retain fission gases and would act as a fast transport path for oxidation of the SiC.	Rationale: Models can be used to calculate the stress state in the OPyC layer.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Outer PyC Layer: Chemical attack by air Kinetics	Rate of reaction per unit surface area as a function of temperature and partial pressure of air

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	7	Remedy:
Rationale: Oxidation of OPyC is needed to understand thermal response of the particles in the fuel element.	Rationale: Reaction rates for PyC are known at these temperatures.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Outer PyC Layer: Chemical attack by air Catalysis	Modification of the reaction rate by fission products or impurities

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	4	Remedy:
Rationale: Impurities can alter reaction rates and change nature of the event.	Rationale: Reaction rate testing of PyC would implicitly include the effects of any impurities on the overall oxidation. No chemical reaction rate measurements have been performed using irradiated PyC where fission products may be in the layer. In principle sensitivity calculations can be performed with variations in the oxidation rate to bound this effect.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Outer PyC Layer: Chemical attack by air	Changes in chemical form resulting from oxidizing or reducing fission products
	Changes in chemical form of fission products	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	7	Remedy:
Rationale: This can be important because the transport behavior is dependent on the chemical form.	Rationale: This can also be calculated for a range of oxygen potentials to determine if any of the key fission products change in chemical form during the air or water ingress accident.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Outer PyC Layer: Chemical attack by air Changes in graphite properties	Changes in diffusivity, porosity, adsorptivity, etc.

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	6	Remedy:
Rationale: The oxidation can change the microstructure of the PyC by creating tunnels or pathways in the matrix. Thus, because the microstructure changes, the porosity, adsorptivity, etc. can also change.	Rationale: No measurements have been made on this effect. Conservative assumptions on such changes may allow sensitivity studies in this area.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Outer PyC Layer: Chemical attack by air	Release of graphite FP inventory
	Holdup reversal	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	6	Remedy:
Rationale: As the oxidation process continues, any fission products trapped at sites in the PyC may be released because of the thermal energy associated with the oxidation and thus increase the source term.	Rationale: This can be accounted for in a very simplistic, yet conservative manner if details are not well known or more sophisticated models with detrapping can be used if the fundamental data needed for such models exist.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Outer PyC Layer: Chemical attack by air	Impact of graphite oxidation on temperature distribution through material
	Temperature distribution	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: II	8	Remedy:
Rationale: Very important in doing an oxidation calculation is to make sure the temperature response of the material as a result of the energy generation is properly calculated.	Rationale: This is well known and can be done in most of the safety codes used by NRC (e.g. MELCOR). The high conductivity of the PyC should make the gradient quite small in general. The degree of fine detail in the model may be an open question but can be handled with sensitivity studies.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer Gas-phase diffusion	Diffusion of gaseous fission products through layer (Knudsen and bulk diffusion through pore structure, and pressure driven permeation through structure)

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	7	Remedy:
Rationale: As the primary fission product barrier, understanding the transport is very important.	Rationale: Effective diffusion coefficients exist in both the U.S. and Germany for the fission gases through the SiC. They are probably a combination of bulk diffusion and Knudsen diffusion at these high temperatures but the two mechanisms have never been individually sorted out in any experiment. The parameters needed for such detailed models and the changes in microstructure of the SiC particle to particle and/or across the layer and/or as a result of the oxidation make such an effort very expensive and time consuming. The use of effective diffusion coefficients although less scientifically satisfying is more pragmatic and may be completely acceptable in system safety analysis when accompanied by proper sensitivity studies.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer Condensed-phase diffusion	Inter-granular diffusion and/or intra-grannular solid-state diffusion

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	7	Remedy:
Rationale: As the primary fission product barrier, understanding the transport is very important.	Rationale: Effective diffusion coefficients exist in both the U.S. and Germany for the metallic fission products through the SiC. They are probably a combination of bulk diffusion and grain boundary diffusion at these high temperatures but the two mechanisms have never been individually sorted out in any experiment. The parameters needed for such detailed models and the changes in microstructure of the SiC particle to particle and/or across the layer and/or as a result of the oxidation process make such an effort very expensive and time consuming. The use of effective diffusion coefficients although less scientifically satisfying is more pragmatic and may be completely acceptable in system safety analysis when accompanied by proper sensitivity studies.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer Thermal deterioration/decomposition	Decline in the quality of the layer due to thermal loading

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	8	Remedy:
Rationale: Less important in oxidation events than in the longer term traditional heatup event. (See similar factor in heatup PIRT table for more information).	Rationale:	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer Fission product corrosion	Attack of layer by fission products, e.g., Pd

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	7	Remedy:
Rationale: The deterioration of the SiC layer via Pd attack has been postulated as a key failure mechanism because Pd forms silicides based on phase diagram and experimental measurements. This is very important for the high burnup fuel being proposed in new reactor designs since the Pd yield from Pu fission is much greater (~ 25 x) that from U fission. Overall, it is judged to be of less importance in the oxidation event since it is assumed that the chemical energy associated with the oxidation event would dominate the subsequent fission product behavior in the particle.	Rationale: Various research institutions have performed many measurements. The kinetics of this mechanism is not known with enough certainty since extrapolations from the database are required. More testing would help develop a better understanding of the phenomena and its impact above 1600°C. Synergistic effects between oxidation and Pd attack (e.g., increase in temperature due to oxidation and its impact on greater Pd corrosion) have never been studied experimentally but can be examined use computer models with appropriate sensitivity studies.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer Heavy metal diffusion	Diffusion of heavy metals through the intact layer

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	3	Remedy:
Rationale: Although higher oxides of uranium (UO_{2+x}) can be volatile, this factor is judged to be of low importance in air or water ingress events since the ability of air or water to get to the kernel to mobilize the uranium is quite small given the large amount of carbon in the system available to react with air or steam.	Rationale: Heavy metal diffusion has never been observed in German accident heating tests.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer Layer oxidation	Uptake of oxygen by the layer through a chemical reaction

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	5	Remedy:
Rationale: Oxidation by air or water is important to understand the response of the fuel.	Rationale: At high partial pressures of air a protective layer of SiO_2 is expected. But at lower partial pressures of air, volatile SiO is predicted to form.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer Fission product release through undetected defects	Passage of fission products from the buffer region through defects in the SiC layer

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	5	Remedy:
Rationale: As the primary fission product barrier, understanding the transport is very important.	Rationale: Effective diffusion coefficients exist in both the U.S. and Germany for the fission gases through the SiC. Release via defects has never been individually sorted out from the other transport mechanisms in any experiment. The parameters needed to model release via defects and the presence or absence of defects in the SiC layer particle to particle, and/or across the layer, and/or changes in the defect structure as a result of oxidation makes such an effort very expensive and time consuming. The use of effective diffusion coefficients although less scientifically satisfying is more pragmatic and may be completely acceptable in system safety analysis when accompanied by proper sensitivity studies that assume some percentage of defective SiC layers present in the core.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer Fission product release through failures, e.g., cracking	Passage of fission products from the buffer region through regions in the SiC layer that fail during operation or an accident

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	7	Remedy:
Rationale: A particle with a failed SiC layer but intact PyC layers will not release fission gas. The PyC layers must fail in order to have fission gas release. A failed layer sometimes is modeled as having no fission product retention characteristics in fuel performance models. This conservative assumption is reasonable assuming that the code can adequately calculate when an SiC layer can fail. The oxidation event may cause failure of the layer, which would then result in fission product release.	Rationale: Such a causal relationship can be modeled and sensitivity studies performed to determine the overall impact in an oxidation event.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer Thermodynamics of the SiC-fission product system	Chemical form of fission products including the effects of solubility, intermetallics, and chemical activity

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	7	Remedy:
Rationale: Critical to understanding transport behavior of fission products	Rationale: Thermodynamic calculations have been performed for both the UO_2 and UCO systems over a broad temperature, burnup and enrichment range to establish the chemical forms of the fission products. Similar calculations can be performed in the presence of steam or air to determine the changes in chemical form of the fission products.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer Sintering	Change of SiC microstructure as a function of temperature

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	2	Remedy:
Rationale: The CVD SiC is very high density,almost theoretical, so it is difficult to see that there would be much of a role for sintering to change the microstructure. Chemical effects from the oxidation event are much more important.	Rationale:	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer: Chemical attack by air Kinetics	Rate of reaction per unit surface area as a function of temperature and partial pressure of air

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	5	Remedy:
Rationale: Oxidation by air or water is important to understand the response of the fuel.	Rationale: At high partial pressures of air a protective layer of SiO_2 is expected. But at lower partial pressures of air, volatile SiO is predicted to form.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer: Chemical attack by air Catalysis	Modification of the reaction rate by fission products or impurities

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	5	Remedy:
Rationale: Impurities can change the reaction rate	Rationale: Some air oxidation rate data have been determined for SiC and thus implicitly include the effects of impurities. The effects of fission products have not been included because oxidation testing has not been performed on irradiated SiC material with fission products. In principle, sensitivity calculations can be performed with variations in the oxidation rate to bound this effect.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer: Chemical attack by air Changes in chemical form of fission products	Changes in chemical form resulting from oxidizing or reducing fission products

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	7	Remedy:
Rationale: This can be important because the transport behavior is dependent on the chemical form.	Rationale: This can also be calculated for a range of oxygen potentials to determine if any of the key fission products change in chemical form during the air or water ingress accident.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer: Chemical attack by air Changes in SiC properties	Changes in diffusivity, porosity, adsorptivity, etc.

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	4	Remedy:
Rationale: The oxidation can change the microstructure of the SiC by creating tunnels or pathways in the matrix. Thus, because the microstructure changes, the porosity, adsorptivity, etc. can also change.	Rationale: No measurements have been made on this effect. Conservative assumptions on such changes may allow sensitivity studies in this area.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer: Chemical attack by air	Release of SiC FP inventory
	Holdup reversal	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	4	Remedy:
Rationale: As the oxidation process continues any fission products trapped at sites in the SiC may be released because of the thermal energy associated with the oxidation.	Rationale: This can be accounted for in a very simplistic, yet conservative manner if details are not well known or more sophisticated models with detrapping can be used if the fundamental data needed for such models exist.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer: Chemical attack by air Temperature distribution	Impact of SiC oxidation on temperature distribution through material

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	8	Remedy:
Rationale: Very important in doing an oxidation calculation is to make sure the temperature response of the material as a result of the chemical reaction is properly calculated.	Rationale: This is well known and can be done in most of the safety codes used by NRC (e.g. MELCOR). The degree of fine detail in the model may be an open question but can be handled with sensitivity studies.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Inner PyC Layer Gas-phase diffusion	Diffusion of gaseous fission products through layer (Knudsen and bulk diffusion through pore structure, and pressure driven permeation through structure)

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	6	Remedy:
Rationale: PyC can hold up gaseous fission products.	Rationale: PyC effectively retain fission gases. Effective diffusion coefficients for noble gases through PyC exist for both German and U.S. PyC. The Knudsen diffusion formalism has not been historically used in the modeling. The effect of oxidation on changes in the transport behavior has not been studied. Sensitivity studies can be performed to bound potential changes to determine the impact on the overall source term.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Inner PyC Layer Condensed phase diffusion	Inter-granular diffusion and/or intra-grannular solid-state diffusion

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	6	Remedy:
Rationale: Transport through intact particles is less important than those with exposed kernels in ingress events	Rationale: Data exist on the effective diffusivity of Cs, Ag, and Sr through the PyC layer. The mechanism responsible for the transport has not been definitively identified. The effect of oxidation on transport properties has not been studied. Sensitivity studies can be performed to bound potential changes to determine the impact on the overall source term.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Inner PyC Layer Pressure loading (Fission products)	Stress loading of the layer by increased pressure from fission products

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	8	Remedy:
Rationale: A key parameter to determine stress in coating layer.	Rationale: Noble gases contribute to the pressure loading in the particle. The effect of temperature due to the oxidation event on the pressure is easily calculated.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Inner PyC Layer Pressure loading (Carbon monoxide)	Stress loading of the layer by carbon monoxide by increased pressure

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H for UO_2 and L for UCO	8	Remedy:
Rationale: A key parameter to determine stress in coating layer.	Rationale: Co (for UO_2 only) contributes to the pressure loading in the particle. The effect of temperature due to the oxidation event on the pressure is easily calculated.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Inner PyC Layer Layer oxidation	Reaction of pyrolytic graphite with oxygen released from the kernel

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	3	Remedy:
Rationale: At high temperatures, oxygen release from kernel increases over that in normal operations because of instability of some oxidic fission products at high temperatures.	Rationale: Known at these temperatures	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Inner PyC Layer Stress state (compression/tension)	The state of the forces induced by external forces that are acting across the layer to resist movement

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	8	Remedy:
Rationale: The stress state is judged to be of low importance for a chemical oxidation event.	Rationale: Stress state is easily calculated using current finite element models for coated particles.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Inner PyC Layer Cracking	Lengths, widths and numbers of cracks produced in layer during accident

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	5	Remedy:
Rationale: A cracked IPyC will not retain fission gases and would act as a fast transport path for metallic fission products to the SiC layer. Furthermore, a cracked IPyC will allow CO to attack the SiC layer.	Rationale:	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Inner PyC Layer Intercalation	Trapping of species between sheets of the graphite structure

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	6	Remedy:
Rationale: Surface and bulk diffusion with intercalation of Cs and Sr (trapping) is probably the underlying mechanism of transport through the PyC. Given the large number of Cs atoms, the trapping may be somewhat less important in the IPyC than in the OPyC where fewer Cs atoms are expected and their concentration may be more on the order of the number of trapping sites.	Rationale: Transport models do not consider intercalation. Effective diffusion coefficients exist in both the U.S. and Germany for the Cs and Sr through IPyC. The data are probably a combination of diffusion and trapping via intercalation at these high temperatures but the two mechanisms have never been individually sorted out in any experiment. Furthermore, the models do not consider effects that oxidation could have on changing the microstucture and the intercalation behavior. The parameters needed for such detailed models and the changes in microstructure of the IPyC particle to particle and/or sometimes across the layer and/or as a result of oxidation make such an effort very expensive and time consuming. The use of effective diffusion coefficients although less scientifically satisfying is more pragmatic and may be completely acceptable in system safety analysis when accompanied by proper sensitivity studies.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Inner PyC Layer: Chemical attack by air Kinetics	Rate of reaction per unit surface area as a function of temperature and partial pressure of air

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	7	Remedy:
Rationale: Oxidation of IPyC is needed to understand thermal response of the particles in the fuel element.	Rationale: Reaction rates for PyC are known at these temperatures.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Inner PyC Layer: Chemical attack by air Catalysis	Modification of the reaction rate by fission products or impurities

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	4	Remedy:
Rationale: Impurities can affect the reaction rate and thus the cause of the ingress event.	Rationale: Reaction rate testing of PyC would implicitly include the effects of any impurities on the overall oxidation. No chemical reaction rate measurements have been performed using irradiated PyC where fission products may be in the layer. In principle sensitivity calculations can be performed with variations in the oxidation rate to bound this effect.	*Closure Criterion:*

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Inner PyC Layer: Chemical attack by air	Changes in chemical form resulting from oxidizing or reducing fission products
	Changes in chemical form of fission products	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	7	Remedy:
Rationale: This can be important because the transport behavior is dependent on the chemical form.	Rationale: This can also be calculated for a range of oxygen potentials to determine if any of the key fission products change in chemical form during the air or water ingress accident.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Inner PyC Layer: Chemical attack by air	Changes in diffusivity, porosity, adsorptivity, etc.
	Changes in graphite properties	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	6	Remedy:
Rationale: The oxidation can change the microstructure of the PyC by creating tunnels or pathways in the matrix. Thus, because the microstructure changes, the porosity, adsorptivity, etc. can also change.	Rationale: No measurements have been made on this effect. Conservative assumptions on such changes may allow sensitivity studies in this area.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Inner PyC Layer: Chemical attack by air	Release of graphite FP inventory
	Holdup reversal	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	6	Remedy:
Rationale: As the oxidation process continues, any fission products trapped at sites in the PyC may be released because of the thermal energy associated with the oxidation.	Rationale: This can be accounted for in a very simplistic, yet conservative manner if details are not well known or more sophisticated models with detrapping can be used if the fundamental data needed for such models exist.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Inner PyC Layer: Chemical attack by air Temperature distribution	Impact of graphite oxidation on temperature distribution through material

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	8	Remedy:
Rationale: Very important in doing an oxidation calculation is to make sure the temperature response of the material as a result of the energy generation is properly calculated.	Rationale: This is well known and can be done in most of the safety codes used by NRC (e.g. MELCOR). The high conductivity of the PyC should make the gradient quite small in general. The degree of fine detail in the model may be an open question but can be handled with sensitivity studies.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Buffer Layer Gas-phase diffusion	Diffusion of gaseous fission products through layer (Knudsen and bulk diffusion through pore structure, and pressure driven permeation through structure)

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	7	Remedy:
Rationale: The transport is fairly rapid and thus oxidation is not expected to affect the transport in this layer significantly.	Rationale: Rapid diffusion through the porous structure of the buffer is assumed in both U.S. and German transport models. Knudsen diffusion calculations confirm rapid gas phase transport.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Buffer Layer Condensed-phase diffusion	Inter-granular diffusion and/or intra-grannular solid-state diffusion

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	7	Remedy:
Rationale: The transport is fairly rapid and thus oxidation is not expected to affect the transport in this layer significantly.	Rationale: Rapid transport of metallic fission products through the buffer has also been historically assumed in U.S. and German models. Key measurements needed to develop grain boundary diffusion models along the edges of the crystallite plans have never been obtained. Instead, effective diffusion coefficients are used.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Buffer Layer Response to kernel swelling	Mechanical reaction of the layer to the growth of the kernel via swelling

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	4	Remedy:
Rationale: Not expected to be important in oxidation events	Rationale: Has been predicted by EU fuel modelers to be important at high burnup where swelling is large. Usually this is accommodated by appropriate changes in the buffer thickness to ensure that the kernel does not come in contact with the TRISO coated and cause large mechanical stresses. Has not been shown to be a problem in current irradiation database at relatively low burnup.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Buffer Layer Maximum fuel gaseous fission product uptake	Maximum loading of fission products that can deposit from the gas phase onto surfaces of materials surrounding the fuel kernel

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	2	Remedy:
Rationale: Not important in oxidation events; probably more important in reactivity related events.	Rationale:	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Buffer Layer Layer oxidation	Reaction of buffer layer with oxide materials in the kernel

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	5	Remedy:
Rationale: Some oxide materials in the kernel become less stable resulting in additional oxygen that can react with the buffer causing additional CO formation.	Rationale: In UO_2 excess oxygen from fission reacts with fission products and then carbon from the buffer. This is well known and can be calculated and has been measured at low burnups. In UCO fuel no oxidation is expected.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Buffer Layer Thermal gradient	Change in temperature with distance

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	6	Remedy:
Rationale: In pebble cores, the temperature gradients are generally low because of the lower power per particle in the core. Thus, Soret effects are much less important. Thus, this effect is important as an initial condition for the accident. Under oxidation events the gradients are much smaller and thus much less important during the accident.	Rationale: Temperature gradients can drive thermal diffusion (Soret effect). Temperature gradients under normal operation are very high in prismatic cores (up to 10000 K/cm) which can cause Soret effects in fission product transport. Values of the heat of solution needed to model the fission product transport are sorely lacking.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Buffer Layer Irradiation and thermal shrinkage	Dimension changes in the buffer layer or changes in its porosity produced by irradiation or by exposure to elevated temperatures

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	7	Remedy:
Rationale: Rapid densification can occur in the buffer under exposure to neutrons. The state of the buffer is an important initial condition in fission product modeling. Thermal densification is not expected to be important at these temperatures.	Rationale: This is fairly well known and can be calculated.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Buffer Layer: Chemical attack by air Kinetics	Rate of reaction per unit surface area as a function of temperature and partial pressure of air

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	7	Remedy:
Rationale: Overall considered to be of lower importance than the other layers in the particle.	Rationale: Oxidation rates for PyC can be adjusted to estimate rates for the buffer.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Buffer Layer: Chemical attack by air Catalysis	Modification of the reaction rate by fission products or impurities

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	3	Remedy:
Rationale: In general, the effect is felt to be less important for this layer than other layers since rapid fission product transport through the layer is already assumed.	Rationale: Reaction rate testing of low-density carbon would implicitly include the effects of any impurities on the overall oxidation. No chemical reaction rate measurements have been performed using irradiated buffer material where fission products may be in the layer. In principle sensitivity calculations can be performed with variations in the oxidation rate to bound this effect.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Buffer Layer: Chemical attack by air Changes in chemical form of fission products	Changes in chemical form resulting from oxidizing or reducing fission products

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	7	Remedy:
Rationale: This can be important because the transport behavior is dependent on the chemical form.	Rationale: This can also be calculated for a range of oxygen potentials to determine if any of the key fission products change in chemical form during the air or water ingress accident.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Buffer Layer: Chemical attack by air	Changes in diffusivity, porosity, adsorptivity, etc.
	Changes in graphite properties	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	3	Remedy:
Rationale: The oxidation can change the microstructure of the buffer by creating tunnels or pathways in the matrix. Thus, because the microstructure changes, the porosity, adsorptivity, etc. can also change. Given the high porosity in the buffer and the rapid fission product transport in this layer, these effects are not considered important.	Rationale: No measurements have been made on this effect.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Buffer Layer: Chemical attack by air Holdup reversal	Release of graphite FP inventory

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	3	Remedy:
Rationale: Given the rapid transport expected in the buffer, this effect is not expected to change the transport properties significantly.	Rationale: As the oxidation process continues any fission products trapped at sites in the buffer may be released because of the thermal energy associated with the oxidation. This can be accounted for in a very simplistic yet conservative manner if details are not well known or more sophisticated models with detrapping can be used if the fundamental data needed for such models exist.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Buffer Layer: Chemical attack by air Temperature distribution	Impact of graphite oxidation on temperature distribution through material

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	8	Remedy:
Rationale: Very important in doing an oxidation calculation is to make sure the temperature response of the material as a result of the chemical reaction is properly calculated.	Rationale: This is well known and can be done in most of the safety codes used by NRC (e.g. MELCOR). The degree of fine detail in the model may be an open question but can be handled with sensitivity studies.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Kernel Maximum fuel temperature	Maximum fuel temperature attained by the fuel kernel during the accident

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: II	7	Remedy:
Rationale: Temperature is the key parameter that drives fission product migration in the coated particle fuel.	Rationale: This can be calculated and sensitivity studies can determine its overall importance in any accident scenario.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Kernel Temperature vs. time transient conditions	The time-dependent variation of fuel temperature with time

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	7	Remedy:
Rationale: Similar to temperature and time at temperature, the thermal response of the particle is important to calculating fission product behavior in the particle.	Rationale: Sensitivity studies can be easily performed to determine the impact of this factor on the overall progression of the accident.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Kernel Energy Transport: Conduction within kernel	Flow of heat within a medium from a region of high temperature to a region of low temperature

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	6	Remedy:
Rationale: Needed to calculate thermal response of kernel	Rationale: Thermal conductivity of UO_2 is fairly high and reasonably well known. Conductivity of UCO is assumed to be that of UO_2. Can be varied easily in sensitivity studies to determine impact.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Kernel Thermodynamic state of fission products	Chemical and physical state of fission products

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	7	Remedy:
Rationale: Thermodynamic state of fission products can determine volatility and mobility of the species.	Rationale: Thermodynamic studies have been performed for UO_2, UCO and UC_2 systems and chemical states of major fission products have been identified as a function of burnup and temperature. The impact of air and/or water can be evaluated.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Kernel Oxygen flux	Mass transport of oxygen per unit surface area per unit time

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	6	Remedy:
Rationale: Less important in air and water ingress events than in traditional heatup events.	Rationale:	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Kernel Grain growth	Enlargement of grains as a result of diffusion

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	4	Remedy:
Rationale: Not important for air or water ingress events.	Rationale:	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Kernel Buffer carbon-kernel interaction	Chemical reaction between carbon and the fuel (UO_2) to form UC_2 and CO (gas)

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	6	Remedy:
Rationale: The reaction of the kernel and the buffer is known to form a "rind" of UC_2 at the interface between the two layers. Photomicrographs show a different phase that is easily distinguished optically. Such interaction can result in release of fission products.	Rationale:	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Kernel: Chemical attack by air Kinetics	Rate of reaction per unit surface area as a function of temperature and partial pressure of air

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	7 for UO_2/ 6 for UCO	Remedy:
Rationale: Oxidation kinetics are needed to understand physio-chemical changes in the kernel and effect on fission product release.	Rationale: Air oxidation of UO_2 has been studied and data are available in the literature. Less information is available on UCO.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Kernel: Chemical attack by air Catalysis	Modification of the reaction rate by fission products or impurities

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	3	Remedy:
Rationale: Impurities can influence reaction rates.	Rationale: Reaction rate testing of UO_2/ UCO would implicitly include the effects of any impurities on the overall oxidation. Reaction rate testing of irradiated kernel material would include the effect of fission products. In principle, sensitivity calculations can be performed with variations in the oxidation rate to bound this effect.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Kernel: Chemical attack by air Changes in chemical form of fission products	Changes in chemical form resulting from oxidizing or reducing fission products

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	7	Remedy:
Rationale: This can be important because the transport behavior is dependent on the chemical form.	Rationale: This can also be calculated for a range of oxygen potentials to determine if any of the key fission products change in chemical form during the air or water ingress accident.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Kernel: Chemical attack by air Changes in kernel properties	Change in diffusivity, porosity, adsorptivity, etc.

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	5	Remedy:
Rationale: The oxidation can change the microstructure of the kernel and the resultant transport properties. Hyperstoichiometric uranium dioxide will behave differently than UO_2. In UCO, the oxygen will react with the carbide phase to produce more UO_2. These are important effects to determine fission product mobility in the kernel. This is rated Medium because it is difficult to see how a lot of air can get all the way to the kernel.	Rationale: Little data exist on changes in transport properties. Some data exist on integral effect of fission production.	Closure Criterion:

Additional Discussion

Appendix F.2

Detailed PIRT Submittal by the ORNL Panel Member

R. Morris

TRISO Fuel PIRT: Accident With Subsequent Air Intrusion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Fuel Element Irradiation history	The temperature, burnup and fast fluence history of the layer

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: II	≤ 1600 °C: 7	Remedy: None if the operating envelope remains the same, otherwise additional testing is necessary
	> 1600 °C: N/A	Remedy: N/A
Rationale: The fuel behavior is strongly related to its irradiation history. Increasing burnup and fluence beyond established limits generally degrades performance. The fraction of particles failed during normal operation is important as well as the fact that they will release first.	Rationale: (≤ 1600 °C) The Germans have collected a large database for their fuel under their specific operating conditions. Deviations from these conditions warrant additional testing. Note that the proven fuel envelope may be less demanding than that required for the turbine concepts.	Closure Criterion: Verification that the fuel can meet any new operating condition.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

For a discussion of the best performing fuel see:

Performance Evaluation of Modern HTR TRISO Fuel, R. Gontard, H. Nabielek, HTA-IB-05/90, July 1990

Fuel Performance and Fission Product Behavior in Gas Cooled Reactors, IAEA-TECDOC-978 (1997)

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Fuel Element Condensed-phase diffusion	Inter-granular diffusion and/or intra-granular solid-state diffusion

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 4	Remedy: Defer to fission product transport area.
	> 1600 °C: N/A	Remedy: N/A
Rationale: The major barriers to fission product release are the particle coating layers. The diffusion through the fuel element matrix is considered to be relatively high, although it does sorb and trap some fission products. When this material is oxidized, these fission products can be released, so the inventory is important.	Rationale: (≤ 1600 °C) The fuel element matrix sorbs some of the released fission products (metals); data exist to estimate the inventory, however, chemical attack may alter things.	Closure Criterion: Diffusion and trapping coefficients for the material of interest as a function of temperature
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

Diffusion through the fuel element matrix is fairly rapid compared to the particle coating layers. Gases are not held up, but there is significant sorption of the released metals. Overall, the reactor core components can provide an attenuation factor of 10-1000 for the metallics; oxidation could release this inventory. The GT-MHR may change its matrix composition from the historical resins; if so, additional investigations may be necessary.
For examples of diffusion and sorption behavior in different HTGR materials see:

Fuel Performance and Fission Product Behavior in Gas Cooled Reactors, IAEA-TECDOC-978 (1997)

For general interest in the transport of volatile fission products through the reactor system see:

An analytical Study of Volatile Metallic Fission Product Release From Very High Temperature Gas-Cooled Reactor Fuel and Core, S. Mitake, et. al., Nuclear Technology, 81 (1988), pages 7-12.
Fission Product Plateout and Liftoff in the MHTGR Primary System: A Review, NUREG/CR-5647

This sorbed or plated out material could be released in the event of an accident.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Fuel Element Gas phase diffusion	Diffusion of gaseous fission products through layer (Knudsen and bulk diffusion through pore structure, and pressure driven permeation through structure). Other factors include holdup, cracking, adsorption, site poisoning, permeability, sintering, and annealing.

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 7	Remedy: None
	> 1600 °C: N/A	Remedy: N/A
Rationale: The fission gases migrate rapidly through the fuel element matrix after they escape from the particle. This fact is used to monitor fuel behavior via R/B. Any damaged particles will release fission gases. Air will react in these regions.	Rationale: (≤ 1600 °C) Data shows that the gases move rapidly through the matrix material and quickly enter the coolant and/or fuel element.	Closure Criterion: None
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

Fuel Performance and Fission Product Behavior in Gas Cooled Reactors, IAEA-TECDOC-978 (1997)
Source Term Estimation for Small-Sized HTRs: Status and Further Needs, Extracted From German Safety Analysis, R. Moormann, et. al., Nuclear Technology, 135, (2001), pages 183-193
Methods and Data for HTGR Fuel Performance and Radionuclide Release Modeling during Normal Operational and Accidents for Safety Analysis, K.

Fission gases move rapidly to the coolant once they exit the particle. In a reactor they are removed by the coolant purification system so the circulating inventory is low. Transport of volatile metallics is determined by the sorption isotherms and dust. Gases released by damaged particles will rapidly move through the reactor core system.

The actual reaction of air with the core materials is more complex. For a discussion of air ingress accidents and its effect on fuel see:
Verfondern, et. al., Jul-2721

For examples of the type of modeling that has been done for transport see:

Fission Product Plateout and Liftoff in the MHTGR Primary System: A Review, NUREG/CR-5647

For fuel accident models see: *Compilation of Fuel Performance and Fission Product Transport Models and Database for MHTGR Design*, Martin, R.C., ORNL/NPR-91/6

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Fuel Element: Transport of metallic FPs through fuel element Chemical form	Chemical stoichiometry of the chemical species that includes the radioisotope of interest

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 5	Remedy: Determine the need for this detailed knowledge.
	> 1600 °C: N/A	Remedy: N/A
Rationale: The chemical form of the fission product will determine how it interacts with the reactor system materials. The chemical environment of the kernel and the reactor system can be quite different and depend on the kernel composition and the coolant impurities. The kernel is expected to be somewhat oxidizing and the normal reactor system quite reducing, thus the chemical form of the fission product may change as it leaves the fuel. Once the accident starts, the environment may become oxidizing again.	Rationale: (≤ 1600 °C) Thermochemical calculations can give plausible chemical forms, but this author is not aware of any measurements confirming the chemical states.	Closure Criterion: If necessary, collect or calculate the compounds.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

This issue of chemical forms probably should be covered under fission product transport since the reactor system has a difference chemical potential than the fuel. It will change again with the accident. Carbides may oxidize. See:

Fission Product Plateout and Liftoff in the MHTGR Primary System: A Review, NUREG/CR-5647
Chemical Behavior of Fission Products in Core Heatup Accidents in High-Temperature Gas-Cooled Reactors, R. Moormann, Nuclear Technology, 94 (1991), pages 56-67.
Source Term Estimation for Small-Sized HTRs: Status and Further Needs, Extracted From German Safety Analysis, R. Moormann, et. al., Nuclear Technology, 135, (2001), pages 183-193
Methods and Data for HTGR Fuel Performance and Radionuclide Release Modeling during Normal Operational and Accidents for Safety Analysis, K. Verfondern, et. al., Jul-2721

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Fuel Element: Chemical attack by air Kinetics	Rate of reaction per unit surface area as a function of temperature and partial pressure of air

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 5	Remedy: Collect the relevant data.
	> 1600 °C: N/A	Remedy: N/A
Rationale: Kinetics data is necessary to determine the reaction rate for both the matrix material and the fuel materials.	Rationale: (≤ 1600 °C) Some reaction data is available, but more specific information may be required.	Closure Criterion: Adequate data for the calculations.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

For different reactor types a considerable amount graphite oxidation work has been done. The kinetics depend a lot on the type of material. Some results are discussed in:

Fuel Performance and Fission Product Behavior in Gas Cooled Reactors, IAEA-TECDOC-978 (1997)

Also, for graphite materials:

Corrosion of Nuclear-Grade Graphites: Air Oxidation of H-451, E.L. Fuller, et. al., ORNL/NPR-91/27, October 1992

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Fuel Element: Chemical attack by air Catalysis	Modification of the reaction rate by fission products or impurities

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 4	Remedy: Determine the sensitivity of the situation to rates. Collect the relevant data if necessary.
	> 1600 °C: N/A	Remedy: N/A
Rationale: The reactions rate can have great local variations due to catalysis from impurities or fission products.	Rationale: (≤ 1600 °C) Local rates can be quite different than global rates.	Closure Criterion: Resolution of the modeling needs or the collection of the relevant data.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

For the effects of trace elements on graphite H-451 see:

The Effect of Trace Elements on the Surface Oxidation of H-451 Graphite, O.C. Kopp, et. al., ORNL/NPR-92/56, December 1992

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Fuel Element: Chemical attack by air	Changes in chemical form resulting from oxidizing or reducing fission products
	Changes in chemical form of fission products	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 4	Remedy: Determine the need for this knowledge, collect as necessary.
	> 1600 °C: N/A	Remedy: N/A
Rationale: Changes in the chemical form of the fission products can greatly change their transport properties.	Rationale: (≤ 1600 °C) Thermochemical codes can calculate the possible chemical compounds. Little confirmation work is available.	Closure Criterion: Data to resolve uncertainties.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

The forms and migration of the fission products can be complex. For some information on the chemical forms see:

Fission Product Plateout and Liftoff in the MHTGR Primary System: A Review, NUREG/CR-5647

Chemical Behavior of Fission Products in Core Heatup Accidents in High-Temperature Gas-Cooled Reactors, R. Moormann, Nuclear Technology, 94 (1991), pages 56-67.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Fuel Element: Chemical attack by air Changes in graphite properties	Changes in diffusivity, porosity, adsorptivity, etc.

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: II	≤ 1600 °C: 4	Remedy: Determine the need for this data and collect the necessary information.
	> 1600 °C: N/A	Remedy: N/A
Rationale: Changes in graphite properties may change reaction rates and transport properties.	Rationale: (≤ 1600 °C) Some data is available for this from other reactor types.	Closure Criterion: Data and models to support the needs.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

This issue depends on the particular graphite and matrix materials involved.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Fuel Element: Chemical attack by air	Release of graphite FP inventory
	Holdup reversal	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 4	Remedy: Determine what is in the graphite and how it moves as the graphite oxidizes.
	> 1600 °C: N/A	Remedy: N/A
Rationale: As the matrix material and graphite are consumed during the reaction, the inventory of fission products may be released or converted to a form that migrates at a higher rate.	Rationale: (≤ 1600 °C) Air ingress experiments have been conducted and the releases examined. Also, modeling has been done for this and other reactor types.	Closure Criterion: Sufficient information to model or bound the situation.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

If the fuel is high quality and the operational temperatures below about 1300°C, only the in-service failed fuel will contribute to the release inventory. Thus, the actual material to be released may be quite small. See:

Source Term Estimation for Small-Sized HTRs: Status and Further Needs, Extracted From German Safety Analysis, R. Moormann, et. al., Nuclear Technology, 135, (2001), pages 183-193

Fuel Performance and Fission Product Behavior in Gas Cooled Reactors, IAEA-TECDOC-978 (1997)

Compilation of Fuel Performance and Fission Product Transport Models and Database for MHTGR Design, R. Martin, ORNL/NPR-91/6

Methods and Data for HTGR Fuel Performance and Radionuclide Release Modeling during Normal Operational and Accidents for Safety Analysis, K. Verfondern, et. al., Jul-2721

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Fuel Element: Chemical attack by air	Impact of graphite oxidation on temperature distribution through material
	Temperature distribution	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: II	≤ 1600 °C: 4	Remedy: Determine the data needed to be collected.
	> 1600 °C: N/A	Remedy: N/A
Rationale: The temperature distribution needs to be known to predict fuel performance and the course of the accident. Both afterheat and heat of combustion need to be known.	Rationale: (≤ 1600 °C) Graphite oxidation codes have been developed and similar cases run.	Closure Criterion: Sufficient information to resolve the issue.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Outer PyC Layer Gas-phase diffusion	Diffusion of gaseous fission products through layer (Knudsen and bulk diffusion through pore structure, and pressure driven permeation through structure)

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 5	Remedy: Insure that proper PyC is manufactured. Material properties are difficult to characterize.
	> 1600 °C: N/A	Remedy: N/A
Rationale: The PyC layers hold fission gases well. The diffusion coefficients are generally quite low. The biggest concern is the rupture of the layer and the release of gases (if other layers are bad). This layer may be attacked by air.	Rationale: (≤ 1600 °C) A great deal of testing has been conduced on PyC at the temperatures of interest. The primary concern is fabricating the proper material and its loss during the accident.	Closure Criterion: Test fuel performs as expected
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

Extensive testing has been done of the PyC for BISO and TRISO fuels under helium conditions, less so under air/steam see:

Performance Evaluation of Modern HTR TRISO Fuel, R. Gontard, H. Nabielek, HTA-1B-05/90, July 1990

Fuel Performance and Fission Product Behavior in Gas Cooled Reactors, IAEA-TECDOC-978 (1997)

Nuclear Technology, 35, Number 2 (entire issue devoted to coated particle fuels)

If the OpyC is unbreached, the helium heatup issues generally apply. If the layer is damaged or burned away, then the loss of OPyC issues would apply.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Outer PyC Layer Condensed-phase diffusion	Inter-granular diffusion and/or intra-granular solid-state diffusion

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: II	≤ 1600 °C: 7	Remedy: None
	> 1600 °C: N/A	Remedy: N/A
Rationale: Metallic fission products generally diffuse through the layer rapidly at high temperatures. Its loss would make some difference, but the primary issue would be exposing the SiC to the air.	Rationale: (≤ 1600 °C) The OPyC offers little holdup to metallics at accident temperatures.	Closure Criterion: None
	Rationale (> 1600 °C) N/A.	Closure Criterion: N/A

Additional Discussion

Extensive testing has been done of the PyC for in helium BISO and TRISO fuels; less has been done for air/steam. See:

Performance Evaluation of Modern HTR TRISO Fuel, R. Gontard, H. Nabielek, HTA-1B-05/90, July 1990

Fuel Performance and Fission Product Behavior in Gas Cooled Reactors, IAEA-TECDOC-978 (1997)

Nuclear Technology, 35, Number 2 (entire issue devoted to coated particle fuels)

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Outer PyC Layer Layer oxidation	Uptake of oxygen by the layer through a chemical reaction

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 4	Remedy: Determine the conditions of interest and collect the necessary data.
	> 1600 °C: N/A	Remedy: N/A
Rationale: The oxidation rate determines the life of this layer under air ingress. Generally, a bulk rate is assumed rather than detailed behavior.	Rationale: (≤ 1600 °C) Testing has been done, but it is of a more integral nature.	Closure Criterion: Resolution of the data gaps.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

For information on fuel exposure in steam/air see:

Source Term Estimation for Small-Sized HTRs: Status and Further Needs, Extracted From German Safety Analysis, R. Moormann, et. al., Nuclear Technology, 135, (2001), pages 183-193

Fuel Performance and Fission Product Behavior in Gas Cooled Reactors, IAEA-TECDOC-978 (1997)

Compilation of Fuel Performance and Fission Product Transport Models and Database for MHTGR Design, R. Martin, ORNL/NPR-91/6

Methods and Data for HTGR Fuel Performance and Radionuclide Release Modeling during Normal Operational and Accidents for Safety Analysis, K. Verfondern, et. al., Jul-2721

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Outer PyC Layer Stress state (compression/tension)	The state of the forces induced by external forces that are acting across the layer to resist movement

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	≤ 1600 °C: 6	Remedy: Review and collect new data for the codes if necessary. Material properties are the major issue.
	> 1600 °C: N/A	Remedy: N/A
Rationale: The stress state of the OPyC helps keep a compression force on the SiC. Failure of the OPyC by oxidation increases the likelihood of SiC failure.	Rationale: (≤ 1600 °C) The fuel design codes include these calculations. (Assumes the PyC is irradiation stable)	Closure Criterion: Adequate test fuel performance.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

Revised MHTGR High-Temperature Fuel Performance Models, R.C. Martin, ORNL/NPR-92/16

Methods and Data for HTGR Fuel Performance and Radionuclide Release Modeling during Normal Operational and Accidents for Safety Analysis, K.

See the PIRT Design Table for references on fuel design. Also see the accident models. The most common accident model is pressure vessel failure. See: Verfondern, et. al., Jul-2721

Compilation of Fuel Performance and Fission Product Transport Models and Database for MHTGR Design, Martin, R.C., ORNL/NPR-91/6

Revised MHTGR High-Temperature Fuel Performance Models, R.C. Martin, ORNL/NPR-92/16

Fuel Performance and Fission Product Behavior in Gas Cooled Reactors, IAEA-TECDOC-978 (1997)

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Outer PyC Layer Intercalation	Trapping of species between sheets of the graphite structure

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	≤ 1600 °C: 2	Remedy: Review data to determine if it is important.
	> 1600 °C: N/A	Remedy: N/A
Rationale: Small amounts of material may be trapped in the layer, but the material sorbed in the matrix is expected to be much larger.	Rationale: (≤ 1600 °C) Some work has been done in this area, but it has not been an important driver.	Closure Criterion: None
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

With good SiC, the fission product transport to the OPyC is very low. Some new modeling efforts are determining if this is an important factor.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Outer PyC Layer Trapping	Adsorption of fission products on defects

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	≤ 1600 °C: 3	Remedy: Review data to determine if it is important.
	> 1600 °C: N/A	Remedy: N/A
Rationale: Some trapping is used in the modeling and it may play a role in the transport, but the FPs in the matrix appears to be the major concern.	Rationale: (≤ 1600 °C) Some modeling has looked at this	Closure Criterion: None
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

With good SiC, the fission product transport to the OPyC is very low. Current modeling efforts are investigating this effect. Even if it is a real effect, it may be consumed by general data uncertainties.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Outer PyC Layer Cracking	Lengths, widths and numbers of cracks produced in layer during operation or an accident

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 5 (models determine failure rather than cracks)	Remedy: Better data and model for fuel performance, especially PyC behavior.
	> 1600 °C: N/A	Remedy: N/A
Rationale: Failure of the OPyC affects the likelihood of SiC failure and exposes it to air/steam. Cracking of particle layers can result in particle failure. One intact PyC can retain gases, but metallic release will be high. Modeling often assumes that particles fail by overpressure rather than a small crack. A crack is assumed to equal failure.	Rationale: (≤ 1600 °C) Fuel models have been developed to model normal and accident behavior. Particles are assumed to fail when they meet some weakness criteria based on a layer stress. Details of cracks are not modeled (yet). Agreement has been good for high quality fuel	Closure Criterion: Models that predict fuel behavior under normal and accident conditions. Does one need cracks or just failure? This adds a lot of complexity.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

For some work on examining the effects of cracks on fuel performance and general models see:

Consideration of the Effects on Fuel Particle Behavior from Shrinkage Cracks in the Inner Pyrocarbon Layer, G.Miller, et. al., Journal of Nuclear Materials, 295 (2001), pages 205-212.

Key Differences in the Fabrication, Irradiation and Safety Testing of U.S. and German TRISO-coated Particle Fuel and Their Implications on Fuel Performance, D.A. Petti, et. al Nuclear Engineering and Design, 222 (2003) 281-297.
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MHTGR TRISO-P Fuel Failure Evaluation Report, DOE-HTGR-90390*Compilation of Fuel Performance and Fission Product Transport Models and Database for MHTGR Design*, Martin, R.C., ORNL/NPR-91/6

Methods and Data for HTGR Fuel Performance and Radionuclide Release Modeling during Normal Operational and Accidents for Safety Analysis, K. Verfondern, et. al., Jul-2721

Compilation of Fuel Performance and Fission Product Transport Models and Database for MHTGR Design, Martin, R.C., ORNL/NPR-91/6

Revised MHTGR High-Temperature Fuel Performance Models, R.C. Martin, ORNL/NPR-92/16

Fuel Performance and Fission Product Behavior in Gas Cooled Reactors, IAEA-TECDOC-978 (1997)

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Outer PyC Layer: Chemical attack by air Kinetics	Rate of reaction per unit surface area as a function of temperature and partial pressure of air

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 4	Remedy: Determine conditions and perform testing.
	> 1600 °C: N/A	Remedy: N/A
Rationale: The reaction rate determines how long the layer will last and support or protect the SiC.	Rationale: (≤ 1600 °C) Much work has been done, but the results are sensitive to materials.	Closure Criterion: Collect the required data.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

Some work has been done in this area, but specific rates and mechanisms have not been isolated: *Methods and Data for HTGR Fuel Performance and Radionuclide Release Modeling during Normal Operational and Accidents for Safety Analysis*, K. Verfondern, et. al., Jul-2721

Compilation of Fuel Performance and Fission Product Transport Models and Database for MHTGR Design, Martin, R.C., ORNL/NPR-91/6

Fuel Performance and Fission Product Behavior in Gas Cooled Reactors, IAEA-TECDOC-978 (1997)

Reactivity of Graphite and Fueled Graphite Spheres with Oxidizing Gases, J.P. Blakely, ORNL-TM-751, February 1964

The particular material under relevant conditions needs to be examined, as there can be considerable variation in results.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Outer PyC Layer: Chemical attack by air	Modification of the reaction rate by fission products or impurities
	Catalysis	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	≤ 1600 °C: 3	Remedy: Determine if it is relevant or important
	> 1600 °C: N/A	Remedy: N/A
Rationale: A catalysis can increase the reaction rate in the layer and hasten its failure.	Rationale: (≤ 1600 °C) This is an unexplored area for fuel, but the graphite air reaction has seen much work.	Closure Criterion: Collect the effects of catalysis if necessary.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

If the fission product inventory in the PyC is low and its loss does not significantly increase the SiC failure probably, then this issue may be unimportant.

For the effects of trace elements on graphite H-451 see:

The Effect of Trace Elements on the Surface Oxidation of H-451 Graphite, O.C. Kopp, et. al., ORNL/NPR-92/56, December 1992
A literature search should come up with some material on catalysis for PyC. It is likely to be sensitive to the exact nature of the materials.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Outer PyC Layer: Chemical attack by air	Changes in chemical form resulting from oxidizing or reducing fission products
	Changes in chemical form of fission products	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 4	Remedy: Determine the need for this knowledge, collect as necessary.
	> 1600 °C: N/A	Remedy: N/A
Rationale: Changes in the chemical form of the fission products can greatly change their transport properties.	Rationale: (≤ 1600 °C) Thermochemical codes can calculate the possible chemical compounds. Little confirmation work is available.	Closure Criterion: Collect data to resolve uncertainties
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

If the inventory of the layer is low, this issue may be of little practical importance. The forms and migration of the fission products can be complex. For some information on the chemical forms see:

Fission Product Plateout and Liftoff in the MHTGR Primary System: A Review, NUREG/CR-5647

Chemical Behavior of Fission Products in Core Heatup Accidents in High-Temperature Gas-Cooled Reactors, R. Moormann, Nuclear Technology, 94 (1991), pages 56-67.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Outer PyC Layer: Chemical attack by air	Changes in diffusivity, porosity, adsorptivity, etc.
	Changes in graphite properties	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	≤ 1600 °C: 1	Remedy: Determine if this item is relevant.
	> 1600 °C: N/A	Remedy: N/A
Rationale: The modeling is not performed at this level; generally, the layer is assumed to disappear at some rate.	Rationale: (≤ 1600 °C) Not examined in this detail.	Closure Criterion: Collect relevant detail.
	Rationale (> 1600 °C) N/A.	Closure Criterion: N/A

Additional Discussion

This level of detail may not be necessary if all one needs is time to significant fuel releases as the failure of the SiC may dominate.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Outer PyC Layer: Chemical attack by air	Release of graphite FP inventory
	Holdup reversal	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	≤ 1600 °C: 3	Remedy: Determine the conditions of interest and collect the necessary data.
	> 1600 °C: N/A	Remedy: N/A
Rationale: As the OPyC is burned away; any inventory of fission products will be released. The inventory of this layer is low for high quality fuel.	Rationale: (≤ 1600 °C) Some air ingress experiments have been done.	Closure Criterion: Determine the relevance of this need and collect data.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

If the fuel performs as expected, the inventory of this layer will be very low. Thus, the actual details of its release may not be important. The greater problem will be that its loss exposes the SiC to air. For a summary of burning data see:

Compilation of Fuel Performance and Fission Product Transport Models and Database for MHTGR Design, Martin, R.C., ORNL/NPR-91/6

Fuel Performance and Fission Product Behavior in Gas Cooled Reactors, IAEA-TECDOC-978 (1997)

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Outer PyC Layer: Chemical attack by air	Impact of graphite oxidation on temperature distribution through material
	Temperature distribution	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 5	Remedy: Determine if the uncertainty in the temperatures is acceptable. Refine models and collect data as necessary.
	> 1600 °C: N/A	Remedy: N/A
Rationale: The temperature determines the reaction rates and thus how fast the layer is attacked.	Rationale: (≤ 1600 °C) Enough modeling has been done to reasonably estimate the temperatures.	Closure Criterion: Adequate data for calculations.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer Gas-phase diffusion	Diffusion of gaseous fission products through layer (Knudsen and bulk diffusion through pore structure, and pressure driven permeation through structure)

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 4	Remedy: Determine relevance of this issue and collect data if necessary.
	> 1600 °C: N/A	Remedy: N/A
Rationale: The SiC is an important barrier to fission products. Its damage will allow fission product to migrate. It is assumed that the OPyC has been destroyed so that air can reach the layer. Also, note that the IPyC must also fail for gas release.	Rationale: (≤ 1600 °C) Germans have done extensive testing in this area with a helium atmosphere. The major problem is attack of the layer. Some work has been done in this area. Extensive work to collect diffusion coefficients has not been done.	Closure Criterion: Resolution of the uncertainties.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

Much work has been done in a helium atmosphere, but less has been done with air. See:

Compilation of Fuel Performance and Fission Product Transport Models and Database for MHTGR Design, Martin, R.C., ORNL/NPR-91/6

Fuel Performance and Fission Product Behavior in Gas Cooled Reactors, IAEA-TECDOC-978 (1997)

Methods and Data for HTGR Fuel Performance and Radionuclide Release Modeling during Normal Operational and Accidents for Safety Analysis, K. Verfondern, et. al., Jul-2721

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer Condensed-phase diffusion	Inter-granular diffusion and/or intra-granular solid-state diffusion

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 4	Remedy: Outline the course of the accident and collect the relevant data.
	> 1600 °C: N/A	Remedy: N/A
Rationale: The SiC is the major barrier to the release of metallic fission products. It is assumed that the OPyC has been removed and air/steam is attacking the SiC.	Rationale: (≤ 1600 °C) Integral experiments exposing a particle to air and steam have been done.	Closure Criterion: The course of the accident and the necessary data.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

Much work has been done in a helium atmosphere, but less has been done with air. See:

Compilation of Fuel Performance and Fission Product Transport Models and Database for MHTGR Design, Martin, R.C., ORNL/NPR-91/6

Fuel Performance and Fission Product Behavior in Gas Cooled Reactors, IAEA-TECDOC-978 (1997)

Methods and Data for HTGR Fuel Performance and Radionuclide Release Modeling during Normal Operational and Accidents for Safety Analysis, K. Verfondern, et. al., Jul-2721

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer Thermal deterioration/decomposition	Decline in the quality of the layer due to thermal loading

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 4	Remedy: If 1600°C and the irradiation envelope are adequate then okay; otherwise testing may be necessary, especially if air/steam contact layer.
	> 1600 °C: N/A	Remedy: N/A
Rationale: The loss of the SiC will result in the release of metallics even if the PyCs are in good shape. The loss of the OPyC will probably result in accelerated failure due to loss of strength.	Rationale: (≤ 1600 °C) Extensive testing at 1600°C has shown it to be a "safe" limit, but exposure to air/steam may accelerate the process.	Closure Criterion: Accident definition and the uncertainties with air/steam resolved.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

1600°C has been used as the maximum temperature; it is conservative and some researchers feel that 1650-1700°C may be allowable, but the air exposure my greatly change the situation. The modeling approach to this situation needs to be resolved. This is a complex issue. Some references:

Compilation of Fuel Performance and Fission Product Transport Models and Database for MHTGR Design, Martin, R.C., ORNL/NPR-91/6

Fuel Performance and Fission Product Behavior in Gas Cooled Reactors, IAEA-TECDOC-978 (1997)

Methods and Data for HTGR Fuel Performance and Radionuclide Release Modeling during Normal Operational and Accidents for Safety Analysis, K. Verfondern, et. al., Jul-2721

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer Fission product corrosion	Attack of layer by fission products, e.g., Pd

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 7	Remedy: None, if the particle operating temperature/time is below an acceptable damage limit.
	> 1600 °C: N/A	Remedy: N/A
Rationale: Some fission products may migrate to the SiC layer and damage it. This corrosion process is a function of temperature. The corrosion mostly occurs during normal operation at the higher temperatures and weakens the particle for the accident. At the higher accident temperatures, thermal decomposition effects dominate.	Rationale: (≤ 1600 °C) This effect has been studied both in-pile and out of pile. Controlling the maximum operating temperature is a major factor.	Closure Criterion: Insure that the operating conditions are acceptable
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

Palladium is one element that is of great concern for high temperature corrosion of SiC and temperature is an important driving factor. Corrosion rates are strong functions of temperature. See the other PIRT Tables and:

Fission Product Pd-SiC Interaction in Irradiated Coated-Particle Fuels, T.N. Tiegs, Nuclear Technology, 57, pages 389-398.

Silicon Carbide Corrosion in High-Temperature Gas-Cooled Reactor Fuel Particles, H. Grubmeier, et. al., Nuclear Technology, 35 (1977), pages 413-427

Out-of-Reactor Studies of Fission Product-Silicon Carbide Interactions in HTGR Fuel Particles, R. Lauf, et. al., Journal of Nuclear Materials, 120 (1984), pages 6-30

Carbon Monoxide-Silicon Carbide Interaction in HTGR Fuel Particles, K. Minato, et. al., Journal of Materials Science, 26 (1991), pages 2379-2388

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer Heavy metal diffusion	Diffusion of heavy metals through layer

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	≤ 1600 °C: 5	Remedy: None
	> 1600 °C: N/A	Remedy: N/A
Rationale: Diffusion of heavy metal through the particle could result is the redistribution of fissile material.	Rationale: (≤ 1600 °C) To this author's knowledge, heavy metal diffusion through the SiC is not a problem.	Closure Criterion: None
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

Significant migration of fissile material through SiC during an accident is not an issue at the temperatures of interest. See: *Compilation of Fuel Performance and Fission Product Transport Models and Database for MHTGR Design*, Martin, R.C., ORNL/NPR-91/6

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer Layer oxidation	Uptake of oxygen by the layer through a chemical reaction

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 4	Remedy: Determine chemical conditions and release time for the relevant case.
	> 1600 °C: N/A	Remedy: N/A
Rationale: Oxidation of the SiC layer will destroy its fission product retention capability. A major issue is whether SiO or SiO_2 is produced. SiO_2 will produce a layer that impedes mass transfer while SiO is volatile. Also, if the IPyC breaks, the SiC layer may be exposed to CO that could slowly corrode it. This is less of a concern for UCO fuel.	Rationale: (≤ 1600 °C) Experiments have been done with particles and spheres.	Closure Criterion: Resolution of release rates.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

This is a complex issue. Some references:

Compilation of Fuel Performance and Fission Product Transport Models and Database for MHTGR Design, Martin, R.C., ORNL/NPR-91/6

Fuel Performance and Fission Product Behavior in Gas Cooled Reactors, IAEA-TECDOC-978 (1997)

Methods and Data for HTGR Fuel Performance and Radionuclide Release Modeling during Normal Operational and Accidents for Safety Analysis, K. Verfondern, et. al., Jul-2721

CO corrosion can be a problem at the higher pressures and temperatures if a crack in the IPyC allows access to the SiC. Controlling the IPyC properties and controlling the CO by using UCO or gettering the fuel can mitigate this problem. See other PIRT tables and:

Carbon Monoxide-Silicon Carbide Interaction in HTGR Fuel Particles, K. Minato, et. al., Journal of Materials Science, 26 (1991), pages 2379-2388

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer Fission product release through undetected defects	Passage of fission products from the buffer region through defects in the SiC layer

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	≤ 1600 °C: 7	Remedy: Defer to fuel fabrication
	> 1600 °C: N/A	Remedy: N/A
Rationale: Defective SiC will allow gas transport if the PyCs both fail. This is more of a manufacturing issue that shows up when the fuel is stressed.	Rationale: (≤ 1600 °C) This is a manufacturing issue that shows up during accident conditions.	Closure Criterion: None
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

The SiC layer can be damaged during compact fabrication by iron impurities. The particles will still retain gases as long as one of the PyCs is good. See the PIRT on Manufacturing Design. It is not known if the chemical attack will worsen the situation.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer Fission product release through failures, e.g. cracking	Passage of fission products from the buffer region through regions in the SiC layer that fail during operation or an accident

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 4	Remedy: If the fuel is used outside of its tested region, more testing is needed.
	> 1600 °C: N/A	Remedy: N/A
Rationale: Failure of the SiC will allow fission gas to pass through it. If the PyC remains good, the gas will not be released, if not, the gas will be released. Metallics will be released in both cases. See previous SiC entries.	Rationale: (≤ 1600 °C) C Accident models have been compared to experiments to approximately model the situation. If material properties are consistent, useful predictions can be made, however chemical attack issues can change the results.	Closure Criterion: Resolution of identified concerns.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

Most SiC failure models are based on pressure vessel failure. More recent models are considering cracking. See the other PIRT Tables and:

Revised MHTGR High-Temperature Fuel Performance Models, R.C. Martin, ORNL/NPR-92/16
Methods and Data for HTGR Fuel Performance and Radionuclide Release Modeling during Normal Operational and Accidents for Safety Analysis, K. Verfondern, et. al., Jul-2721
MHTGR TRISO-P Fuel Failure Evaluation Report, DOE-HTGR-90390, 1993
Fuel Performance and Fission Product Behavior in Gas Cooled Reactors, IAEA-TECDOC-978 (1997)

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer Thermodynamics of the SiC-fission product system	Chemical form of fission products including the effects of solubility, intermetallics, and chemical activity

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 7	Remedy: None, if the particle operating temperature/time is below an acceptable damage limit.
	> 1600 °C: N/A	Remedy: N/A
Rationale: Some fission products may migrate to the SiC layer and damage it. This corrosion process is a function of temperature. See the entry on corrosion. If the SiC fails and air/steam enters, the oxidation state may increase, which may not be bad.	Rationale: (≤ 1600 °C) This effect has been studied both in-pile and out of pile. Controlling the maximum operating temperature is a major factor.	Closure Criterion: Acceptable performance.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

See entries on corrosion and the other PIRT Tables. Also see entries on UCO. One of the goals of kernel design is to stabilize the corrosive elements so they do not migrate to the SiC. Also, determine if air attack kernel.
During normal or accident conditions, the SiC can crack or break due to over pressure or an interaction with cracked PyC. High temperatures increase the pressure in a particle. Above 1600 °C or so, decomposition begins to weaken the SiC and it can fail.

For some work on examining the effects of cracks on fuel performance and general models see the other PIRT tables and:

Consideration of the Effects on Fuel Particle Behavior from Shrinkage Cracks in the Inner Pyrocarbon Layer, G.Miller, et. al., Journal of Nuclear Materials, 295 (2001), pages 205-212.

Key Differences in the Fabrication, Irradiation and Safety Testing of U.S. and German TRISO-coated Particle Fuel and Their Implications on Fuel Performance, D.A. Petti, et. al., INEEL/EXT-02-00300

Revised MHTGR High-Temperature Fuel Performance Models, R.C. Martin, ORNL/NPR-92/16

Methods and Data for HTGR Fuel Performance and Radionuclide Release Modeling during Normal Operational and Accidents for Safety Analysis, K. Verfondern, et. al., Jul-2721

MHTGR TRISO-P Fuel Failure Evaluation Report, DOE-HTGR-90390, 1993

Fuel Performance and Fission Product Behavior in Gas Cooled Reactors, IAEA-TECDOC-978 (1997)

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer Sintering	Change of graphite microstructure as a function of temperature

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	≤ 1600 °C: 7	Remedy: None if temperatures are below 1600 °C, an air environment may modify this.
	> 1600 °C: N/A	Remedy: N/A
Rationale: SiC doesn't appear to suffer any significant changes at normal operating conditions and survives at 1600 °C without large changes.	Rationale: (≤ 1600 °C) Extensive testing at 1600 °C for hundreds of hours has shown the good behavior of SiC.	Closure Criterion: None
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

The major challenge is to reproduce the SiC that performed so well in past testing. The exposure to air is expected to lead to corrosion effects rather than sintering effects. The loss of the SiC integrity is the major issue.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer: Chemical attack by air Kinetics	Rate of reaction per unit surface area as a function of temperature and partial pressure of air

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 4	Remedy: Determine chemical conditions and release time for the relevant case.
	> 1600 °C: N/A	Remedy: N/A
Rationale: The rates determine how long the SiC will last. Also, oxidation of the SiC layer will destroy its fission product retention capability. A major issue is whether SiO or SiO_2 is produced. SiO_2 will produce a layer that impedes mass transfer while SiO is volatile.	Rationale: (≤ 1600 °C) Experiments have been done with particles.	Closure Criterion: Resolution of release rates.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

This is a complex issue because of the SiO or SiO_2 issue and mass transfer. Some references:

Compilation of Fuel Performance and Fission Product Transport Models and Database for MHTGR Design, Martin, R.C., ORNL/NPR-91/6

Fuel Performance and Fission Product Behavior in Gas Cooled Reactors, IAEA-TECDOC-978 (1997)

Methods and Data for HTGR Fuel Performance and Radionuclide Release Modeling during Normal Operational and Accidents for Safety Analysis, K. Verfondern, et. al., Jul-2721

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer: Chemical attack by air	Modification of the reaction rate by fission products or impurities
	Catalysis	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	≤ 1600 °C: 1	Remedy: Estimate the potential for this to occur.
	> 1600 °C: N/A	Remedy: N/A
Rationale: A catalysis could influence the reaction rate of SiC with water or air and thus greatly increase the rate of thinning.	Rationale: (≤ 1600 °C) This is unexplored.	Closure Criterion: Resolution of the issue.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

Little is known about this, but experiments have not revealed any sort of problem. A literature review may be a way to quickly determine if this area needs to be explored more.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer: Chemical attack by air	Changes in chemical form resulting from oxidizing or reducing fission products
	Changes in chemical form of fission products	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 4	Remedy: Determine the need for this knowledge, collect as necessary.
	> 1600 °C: N/A	Remedy: N/A
Rationale: Changes in the chemical form of the fission products can greatly change their transport properties. Once the SiC fails, the potential for significant particle releases increase.	Rationale: (≤ 1600 °C) Thermochemical codes can calculate the possible chemical compounds. Little confirmation work is available.	Closure Criterion: Collect data to resolve uncertainties
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

The forms and migration of the fission products can be complex. For some information on the chemical forms see:

Fission Product Plateout and Liftoff in the MHTGR Primary System: A Review, NUREG/CR-5647

Chemical Behavior of Fission Products in Core Heatup Accidents in High-Temperature Gas-Cooled Reactors, R. Moormann, Nuclear Technology, 94 (1991), pages 56-67.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer: Chemical attack by air	Changes in diffusivity, porosity, adsorptivity, etc.
	Changes in SiC properties	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 1	Remedy: Determine if this item is relevant.
	> 1600 °C: N/A	Remedy: N/A
Rationale: The modeling is not performed at this level; generally, the layer is assumed to disappear at some rate.	Rationale: (≤ 1600 °C) Not examined in this detail.	Closure Criterion: Collect relevant detail.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

This level of detail may not be necessary if all one needs is time to significant fuel releases as the SiC fails.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer: Chemical attack by air	Release of SiC FP inventory
	Holdup reversal	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	≤ 1600 °C: 3	Remedy: Determine the conditions of interest and collect the necessary data
	> 1600 °C: N/A	Remedy: N/A
Rationale: As the SiC is removed; any inventory of fission products will be released. The inventory of this layer is low for high quality fuel.	Rationale: (≤ 1600 °C) Some air ingress work has been done.	Closure Criterion: Determine the relevance of this need and collect data.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

If the fuel performs as expected, the inventory of this layer will be very low. Thus, the actual details of its release may not be important. The greater problem is that its loss exposed the high inventory kernel. See:

Compilation of Fuel Performance and Fission Product Transport Models and Database for MHTGR Design, Martin, R.C., ORNL/NPR-91/6

Fuel Performance and Fission Product Behavior in Gas Cooled Reactors, IAEA-TECDOC-978 (1997)

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer: Chemical attack by air Temperature distribution	Impact of SiC oxidation on temperature distribution through material

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 5	Remedy: Determine if the uncertainty in the temperatures is acceptable. Refine models and collect data as necessary.
	> 1600 °C: N/A	Remedy: N/A
Rationale: The temperature determines the reaction rates and thus how fast the layer is attacked.	Rationale: (≤ 1600 °C) Enough modeling has been done to reasonably estimate the temperatures.	Closure Criterion: Adequate data for calculations.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Inner PyC Layer Gas-phase diffusion	Diffusion of gaseous fission products through layer (Knudsen and bulk diffusion through pore structure, and pressure driven permeation through structure)

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 4	Remedy: None at present
	> 1600 °C: N/A	Remedy: N/A
Rationale: Gas diffusion through the PyCs is generally quite low at the temperatures of interest. The SiC layer must be breeched for the gases to get out. If the SiC layer has been damaged, the failure likelihood of the IPyC is increased. If attack of the IPyC occurs, significant release will soon follow.	Rationale: (≤ 1600 °C) Gas diffusion through the PyCs has been shown to be quite low. The issue is the layer behavior after is has been attacked. Some integral testing has been done.	Closure Criterion: Acceptable test fuel behavior
	Rationale (> 1600 °C) N/A	Closure Criterion: Acceptable test fuel behavior

Additional Discussion

Extensive testing has been done on various fuels over a range of temperatures. The challenge is to reproduce this good material. See:

Performance Evaluation of Modern HTR TRISO Fuel, R. Gontard, H. Nabielek, HTA-1B-05/90, July 1990
Fuel Performance and Fission Product Behavior in Gas Cooled Reactors, IAEA-TECDOC-978 (1997)
Fission-Product Release During Postirradiation Annealing of Several Types of Coated Fuel Particles, R.E. Bullock, Journal of Nuclear Materials, 125 (1984), pages 304-319

The concern is how the chemical attack affects the layer. For accident models see:

Compilation of Fuel Performance and Fission Product Transport Models and Database for MHTGR Design, Martin, R.C., ORNL/NPR-91/6
Revised MHTGR High-Temperature Fuel Performance Models, R.C. Martin, ORNL/NPR-92/16
Methods and Data for HTGR Fuel Performance and Radionuclide Release Modeling during Normal Operational and Accidents for Safety Analysis, K. Verfondern, et. al., Jul-2721

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Inner PyC Layer Condensed-phase diffusion	Inter-granular diffusion and/or intra-granular solid-state diffusion

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	≤ 1600 °C: 4	Remedy: None, nothing can be done
	> 1600 °C: N/A	Remedy: N/A
Rationale: The diffusion of metallic fission products through the PyCs is known to be fairly high. Only modest credit can be taken for PyC as a barrier or release delay for metallics. Any chemical attack will only enhance the diffusion.	Rationale: (≤ 1600 °C) The PyCs are generally assumed to provide limited retention to metallic fission products at accident temperatures. Chemical attack may make the situation worse.	Closure Criterion: None
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

For a discussion of PyC and metallics see:

Nuclear Technology, 35, Number 2, Fission Product Release Section, pages 457-526

For the higher accident temperatures, the PyCs are assumed to have essentially no resistance to metallic transport. The PyC offers some impedance to metallic transport, but is not a major barrier. Chemical attack will worsen the situation, but the SiC layer is the important one.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Inner PyC Layer Pressure loading (Fission products)	Stress loading of the layer by increased pressure from fission products

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 7	Remedy: Proper design and fabrication
	> 1600 °C: N/A	Remedy: N/A
Rationale: Depending on the particular configuration, the PyC layers can help keep the SiC in compression. Loss of a PyC layer can increase the probability of SiC failure.	Rationale: (≤ 1600 °C) Pressure can be controlled by particle design, burnup, and kernel composition. Analysis and designs are available	Closure Criterion: Acceptable fuel performance
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

According to the fuel models, the PyC functions as an important load-bearing component of the fuel particle. See the PIRT Design Table for more information concerning the stresses. Loss of other layers due to chemical attack influences the structural stability of the entire particle.

A major concern is the proper material properties – see the Manufacturing Design PIRT

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Inner PyC Layer Pressure loading (Carbon monoxide)	Stress loading of the layer by carbon monoxide by increased pressure

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 7	Remedy: Control pressure by design
	> 1600 °C: N/A	Remedy: N/A
Rationale: High CO product will result in high particle pressures, especially at the higher accident temperatures. Changing the kernel composition can control CO production.	Rationale: (≤ 1600 °C) Pressure can be controlled by particle design, burnup, and kernel composition. Analysis and designs are available.	Closure Criterion: Proof testing of final fuel design
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

For a discussion on kernel design to minimize CO and immobilize key fission products see:

Stoichiometric Effects on Performance of High-Temperature Gas-Cooled Reactor Fuels from the U-C-O System, F.J. Homan, et. al., Nuclear Technology, 35, pages 428-441.

See the other PIRT Tables for fuel design issues.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Inner PyC Layer Layer oxidation	Reaction of pyrolytic graphic with oxygen released from the kernel.

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 3	Remedy: Collect relevant data
	> 1600 °C: N/A	Remedy: N/A
Rationale: Defects or cracks in the OPyC and SiC can allow air/stem to enter the particle and oxidize the IPyC. This will release fission gases and provide a direct path to the kernel.	Rationale: (≤ 1600 °C) This behavior is similar to the burn leach tests used to determine fuel quality. The rates are assumed to be the same as for OPyC	Closure Criterion: Reasonable calculational basis.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

If both the OPyC and the SiC are breeched, then the particle is releasing.

Performance Evaluation of Modern HTR TRISO Fuel, R. Gontard, H. Nabielek, HTA-1B-05/90, July 1990
Fuel Performance and Fission Product Behavior in Gas Cooled Reactors, IAEA-TECDOC-978 (1997)
Fission-Product Release During Postirradiation Annealing of Several Types of Coated Fuel Particles, R.E. Bullock, Journal of Nuclear Materials, 125 (1984), pages 304-319

For accident models see:

Compilation of Fuel Performance and Fission Product Transport Models and Database for MHTGR Design, Martin, R.C., ORNL/NPR-91/6
Revised MHTGR High-Temperature Fuel Performance Models, R.C. Martin, ORNL/NPR-92/16
Methods and Data for HTGR Fuel Performance and Radionuclide Release Modeling during Normal Operational and Accidents for Safety Analysis, K. Verfondern, et. al., Jul-2721

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Inner PyC Layer Stress state (compression/tension)	The state of the forces induced by external forces that are acting across the layer to resist movement

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: II	≤ 1600 °C: 7	Remedy: Control pressure by design
	> 1600 °C: N/A	Remedy: N/A
Rationale: Failure of the PyC can increase the likelihood of SiC failure. See the previous pressure loading entries.	Rationale: (≤ 1600 °C) Pressure can be controlled by particle design, burnup, and kernel composition. Analysis and designs are available	Closure Criterion: Proof testing of final fuel design
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

See the table entries about pressure loading and also the PIRT Design Tables.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Inner PyC Layer Cracking	Lengths, widths and numbers of cracks produced in layer during accident

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 4 (failure only, cracking is not calculated)	Remedy: Review and collect new data for the codes if necessary.
	> 1600 °C: N/A	Remedy: N/A
Rationale: Failure of the IPyC affects the likelihood of SiC failure. See the entry on stress state. The lengths, widths, and number of cracks don't really matter – the failure does. Many models assume the SiC layer will dominate the particle failure. Effects of chemical attack may not be included.	Rationale: (≤ 1600 °C) Fuel models have been developed to model normal and accident behavior. Particles are assumed to fail when they meet some weakness criteria rather based a layer stress.	Closure Criterion: Models that predict fuel behavior under normal and accident conditions. Does one need cracks or just failure? This adds a lot of complexity.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

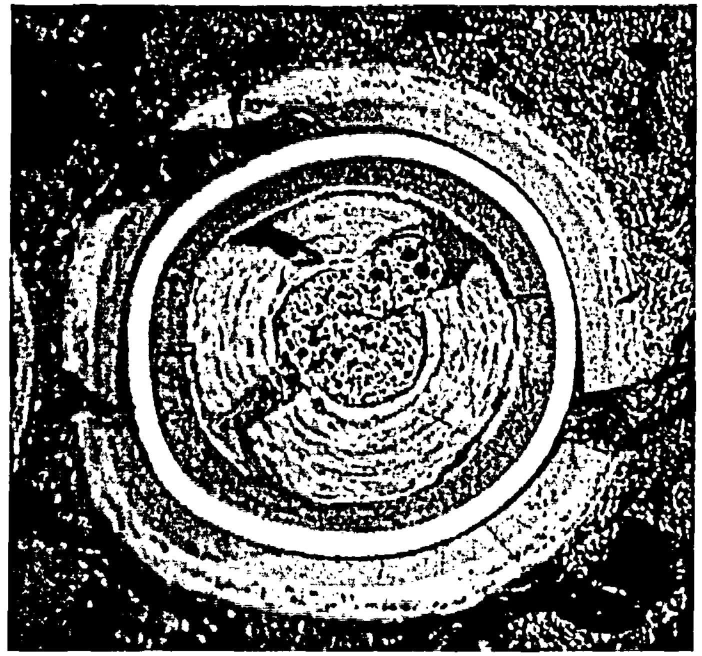
For some work on examining the effects of cracks on fuel performance and general models see:

Under accident conditions, a pressure vessel type failure model has been used with the particle failing when the pressure exceeds a critical value. The accident models may not include all the chemical attack effects.

Consideration of the Effects on Fuel Particle Behavior from Shrinkage Cracks in the Inner Pyrocarbon Layer, G.Miller, et. al., Journal of Nuclear Materials, 295 (2001), pages 205-212.
Key Differences in the Fabrication, Irradiation and Safety Testing of U.S. and German TRISO-coated Particle Fuel and Their Implications on Fuel Performance, D.A. Petti, et. al., INEEL/EXT-02-00300

MHTGR TRISO-P Fuel Failure Evaluation Report, DOE-HTGR-90390

Compilation of Fuel Performance and Fission Product Transport Models and Database for MHTGR Design, Martin, R.C., ORNL/NPR-91/6
Revised MHTGR High-Temperature Fuel Performance Models, R.C. Martin, ORNL/NPR-92/16
Methods and Data for HTGR Fuel Performance and Radionuclide Release Modeling during Normal Operational and Accidents for Safety Analysis, K. Verfondern, et. al., Jul-2721
Fuel Performance and Fission Product Behavior in Gas Cooled Reactors, IAEA-TECDOC-978 (1997)



Massive pyrocarbon failure In HRB-21 due to a design flaw (seal coats) resulted in cracks that appear to have compromised the SiC and resulted in releases. (ORNL)

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Inner PyC Layer Intercalation	Trapping of species between sheets of the graphite structure

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	≤ 1600 °C: 2	Remedy: None
	> 1600 °C: N/A	Remedy: N/A
Rationale: This layer is likely to be saturated with fission products and this effect may only make a minor difference.	Rationale: (≤ 1600 °C) This situation has not caused problems	Closure Criterion: None
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

Some modeling is looking at this situation.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Inner PyC Layer: Chemical attack by air Kinetics	Rate of reaction per unit surface area as a function of temperature and partial pressure of air

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 4	Remedy: Review data and perform tests to fill in gaps.
	> 1600 °C: N/A	Remedy: N/A
Rationale: This is the last barrier before exposing the kernel. Metals are being released, but gases are still retained.	Rationale: (≤ 1600 °C) Some testing has been done on the reaction of steam with matrix material and graphite.	Closure Criterion: Sufficient data to resolve gaps.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

Air attack of the IPyC means that the OPyC and SiC layers have all been breeched. In this case, the particle is probably just about gone. It may not be worthwhile to model this in detail as failure is near. See:

Source Term Estimation for Small-Sized HTRs: Status and Further Needs, Extracted From German Safety Analysis, R. Moormann, et. al., Nuclear Technology, 135, (2001), pages 183-193

Fuel Performance and Fission Product Behavior in Gas Cooled Reactors, IAEA-TECDOC-978 (1997)

Compilation of Fuel Performance and Fission Product Transport Models and Database for MHTGR Design, R. Martin, ORNL/NPR-91/6

Methods and Data for HTGR Fuel Performance and Radionuclide Release Modeling during Normal Operational and Accidents for Safety Analysis, K. Verfondern, et. al., Jul-2721

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Inner PyC Layer: Chemical attack by air Catalysis	Modification of the reaction rate by fission products or impurities

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	≤ 1600 °C: 1	Remedy: Determine if it is relevant or important
	> 1600 °C: N/A	Remedy: N/A
Rationale: A catalysis can increase the reaction rate in the layer and hasten its failure.	Rationale: (≤ 1600 °C) This is an unexplored area.	Closure Criterion: Collect the effects of catalysis if necessary.
	Rationale (> 1600 °C) N/A.	Closure Criterion: N/A

Additional Discussion

For the effects of trace elements on graphite H-451 see:

The Effect of Trace Elements on the Surface Oxidation of H-451 Graphite, O.C. Kopp, et. al., ORNL/NPR-92/56, December 1992
A literature search should come up with some material on catalysis for PyC. It is likely to be sensitive to the exact nature of the materials.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Instrusion	Inner PyC Layer: Chemical attack by air	Changes in chemical form resulting from oxidizing or reducing fission products
	Changes in chemical form of fission products	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 4	Remedy: Determine the need for this knowledge, collect as necessary.
	> 1600 °C: N/A	Remedy: N/A
Rationale: Changes in the chemical form of the fission products can greatly change their transport properties. Once the SiC fails, the potential for significant particle releases increase. The greatest change may come from the reaction of UC and the change in kernel structure.	Rationale: (≤ 1600 °C) Thermochemical codes can calculate the possible chemical compounds. Little confirmation work is available.	Closure Criterion: Collect data to resolve uncertainties
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

The forms and migration of the fission products can be complex. For some information on the chemical forms see:

Fission Product Plateout and Liftoff in the MHTGR Primary System: A Review, NUREG/CR-5647

Chemical Behavior of Fission Products in Core Heatup Accidents in High-Temperature Gas-Cooled Reactors, R. Moormann, Nuclear Technology, 94 (1991), pages 56-67.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Inner PyC Layer: Chemical attack by air	Changes in diffusivity, porosity, adsorptivity, etc.
	Changes in graphite properties	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	≤ 1600 °C: 2	Remedy: Determine if this level of detail is really needed for the safety case.
	> 1600 °C: N/A	Remedy: N/A
Rationale: It may not be necessary to examine the PyC to this level of detail. An integral weakening or failure rate may be sufficient.	Rationale: (≤ 1600 °C) This area has not been examined in detail. Many of the tests have been integral tests on fuel elements and particles.	Closure Criterion: Resolution of the problem and the needed data.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

The level of detail needed by the models needs to be examined. This will be expensive and difficult information to get. It is also like to be sensitive to the exact material nature.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Inner PyC Layer: Chemical attack by air	Release of graphite FP inventory
	Holdup reversal	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	≤ 1600 °C: 2	Remedy: Determine if this is really important.
	> 1600 °C: N/A	Remedy: N/A
Rationale: The destruction of this layer will expose the kernel/buffer and a large fission product inventory.	Rationale: (≤ 1600 °C) This individual parameter has not been studied in much detail.	Closure Criterion: Resolution of its importance.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

Once the particle layers have been breached, the kernel is exposed. The inventory now available for release will dwarf the minor inventories in the layers.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Inner PyC Layer: Chemical attack by air Temperature distribution	Impact of graphite oxidation on temperature distribution through material

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 4	Remedy: Determine if the uncertainty in the temperatures is acceptable. Refine models and collect data as necessary.
	> 1600 °C: N/A	Remedy: N/A
Rationale: The temperature determines the rate at which the layer is attacked.	Rationale: (≤ 1600 °C) Enough modeling has been done to reasonably estimate the temperatures	Closure Criterion: Adequate data for calculations.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Buffer Layer Gas-phase diffusion	Diffusion of gaseous fission products through layer (Knudsen and bulk diffusion through pore structure, and pressure driven permeation through structure)

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: II	≤ 1600 °C: 7	Remedy: None
	> 1600 °C: N/A	Remedy: N/A
Rationale: The buffer layer is designed to be a void to collect the gases released from the kernel. The problem would be if it weren't porous.	Rationale: (≤ 1600 °C) The buffer layer appears to work as planned. Gases are expected to diffusive through this layer.	Closure Criterion: None
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

Once this layer is exposed, the kernel is essentially exposed.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Buffer Layer Condensed-phase diffusion	Inter-granular diffusion and/or intra-granular solid-state diffusion

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 7	Remedy: None
	> 1600 °C: N/A	Remedy: N/A
Rationale: The buffer layer is essentially void volume and is not expected to offer resistance to transport. Some material may be sorbed on this layer.	Rationale: (≤ 1600 °C) The buffer layer appears to work as planned. Fission products are expected to diffusive through this layer.	Closure Criterion: None
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

Once this layer is exposed, the kernel is essentially exposed.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Buffer Layer Response to kernel swelling	Mechanical reaction of the layer to the growth of the kernel via swelling

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: II	≤ 1600 °C: 5	Remedy: None
	> 1600 °C: N/A	Remedy: N/A
Rationale: The buffer layer must be weak enough that it will deform or crush without transmitting high forces to the IPyC as the kernel distorts.	Rationale: (≤ 1600 °C) All evidence to date indicates that the buffer layer performs as expected.	Closure Criterion: None
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

In the accident fuel testing done to date, no evidence of adverse buffer reaction to kernel swelling was apparent.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Buffer Layer Maximum fuel gaseous fission product uptake	Maximum loading of fission products that can deposit from the gas phase onto surfaces of materials surrounding the fuel kernel

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 7	Remedy: None
	> 1600 °C: N/A	Remedy: N/A
Rationale: The buffer layer must have sufficient void volume to control the pressure from released fission gases and CO.	Rationale: (≤ 1600 °C) All evidence to date indicates that the buffer layer performs as expected.	Closure Criterion: None
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

This is really a design issue. See the PIRT Design Table.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Buffer Layer Layer oxidation	Reaction of buffer layer with oxide materials in the kernel.

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	≤ 1600 °C: 7	Remedy: None
	> 1600 °C: N/A	Remedy: N/A
Rationale: A small portion of the layer is oxidized by the excess oxygen released form the kernel. This is of no consequence, as the layer has no structural function. It is of no consequence if the buffer is oxidized by air/steam as the particle is already failed.	Rationale: (≤ 1600 °C) No problem ahs been observed. The basic problem is CO production that has been outlined elsewhere.	Closure Criterion: None
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

See the discussions on the use of UCO to control CO pressure.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Buffer Layer Thermal gradient	Change in temperature with distance

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	≤ 1600 °C: 7	Remedy: None
	> 1600 °C: N/A	Remedy: N/A
Rationale: During accident conditions, the particle gradient is low because the power production is low relative to operating conditions and heat transfer is no longer driven by strong convection	Rationale: (≤ 1600 °C) The codes can compute these temperatures.	Closure Criterion: None
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

It is not likely that the chemical reactions will generate thermal gradients that are comparable with normal operation.

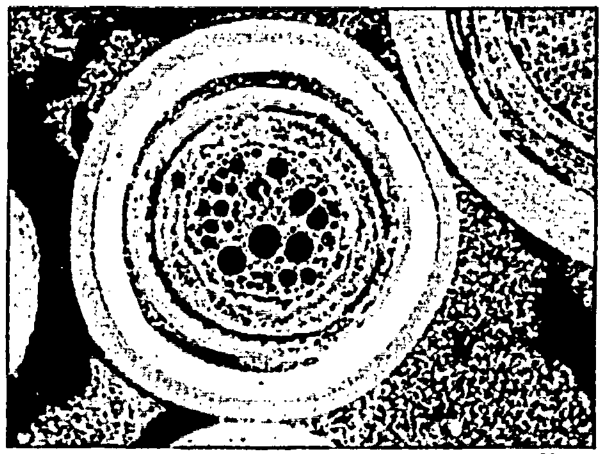
Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Buffer Layer Irradiation and thermal shrinkage	Dimension changes in the buffer layer or changes in its porosity produced by irradiation or by exposure to elevated temperatures

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	≤ 1600 °C: 6	Remedy: None
	> 1600 °C: N/A	Remedy: N/A
Rationale: Ideally, the buffer layer should isolate the kernel from the IPyC, but small cracks or limited shrinkage do not seem to cause trouble. Most of these changes would have taken place during normal operation.	Rationale: (≤ 1600 °C) Modest buffer shrinkage and small cracks don't seem to result in problems	Closure Criterion: None
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

One concern is that cracks could offer a direct path for corrosive fission products to the SiC if the IPyC also breaks. Some current modeling is looking at this.

In this high burnup Pu kernel (ORNL), considerable shrinkage took place in the buffer layer and the IPyC separated from the SiC. While one would like to see less behavior of this sort, the particle performed well under irradiation.



R71558 200x 20 μm

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Buffer Layer: Chemical attack by air Kinetics	Rate of reaction per unit surface area as a function of temperature and partial pressure of air

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	≤ 1600 °C: 3	Remedy: Determine if this affect is of any real importance.
	> 1600 °C: N/A	Remedy: N/A
Rationale: The particle has failed by the time this layer is attacked. The additional loss of the buffer may not make much difference.	Rationale: (≤ 1600 °C) Some data and modeling is available. Integral tests on particles and fuel elements have been performed.	Closure Criterion: Resolution of the importance.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

Once the other layers have been attacked, the buffer offers very little impedance to fission product migration.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Buffer Layer: Chemical attack by air	Modification of the reaction rate by fission products or impurities
	Catalysis	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	≤ 1600 °C: 1	Remedy: Determine if it is relevant or important
	> 1600 °C: N/A	Remedy: N/A
Rationale: Catalysis can increase the reaction rate in the layer and hasten its failure.	Rationale: (≤ 1600 °C) This is an unexplored area.	Closure Criterion: Collect the effects of catalysis if necessary.
	Rationale (> 1600 °C) N/A.	Closure Criterion: N/A

Additional Discussion

For the effects of trace elements on graphite H-451 see:

The Effect of Trace Elements on the Surface Oxidation of H-451 Graphite, O.C. Kopp, et. al., ORNL/NPR-92/56, December 1992
A literature search should come up with some material on catalysis for PyC. It is likely to be sensitive to the exact nature of the materials.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Buffer Layer: Chemical attack by air	Changes in chemical form resulting from oxidizing or reducing fission products
	Changes in chemical form of fission products	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 4	Remedy: Determine the need for this knowledge, collect as necessary.
	> 1600 °C: N/A	Remedy: N/A
Rationale: Changes in the chemical form of the fission products can greatly change their transport properties. The greatest change may come from the reaction of UC and the change in kernel structure	Rationale: (≤ 1600 °C) Thermochemical codes can calculate the possible chemical compounds. Little confirmation work is available.	Closure Criterion: Collect data to resolve uncertainties
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

The forms and migration of the fission products can be complex. For some information on the chemical forms see:

Fission Product Plateout and Liftoff in the MHTGR Primary System: A Review, NUREG/CR-5647

Chemical Behavior of Fission Products in Core Heatup Accidents in High-Temperature Gas-Cooled Reactors, R. Moormann, Nuclear Technology, 94 (1991), pages 56-67.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Buffer Layer: Chemical attack by air Changes in graphite properties	Changes in diffusivity, porosity, adsorptivity, etc.

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	≤ 1600 °C: 2	Remedy: Determine if this level of detail is really needed for the safety case.
	> 1600 °C: N/A	Remedy: N/A
Rationale: It may not be necessary to examine the PyC to this level of detail. An integral weakening or failure rate may be sufficient.	Rationale: (≤ 1600 °C) This area has not been examined in detail. Many of the tests have been integral tests on fuel elements and particles.	Closure Criterion: Resolution of the problem and the needed data.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

The level of detail needed by the models needs to be examined. This will be expensive and difficult information to get. It is also like to be sensitive to the exact material nature

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Buffer Layer: Chemical attack by air	Release of graphite FP inventory
	Holdup reversal	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	≤ 1600 °C: 2	Remedy: Determine if this is really important.
	> 1600 °C: N/A	Remedy: N/A
Rationale: The destruction of this layer will expose the kernel and a large fission product inventory.	Rationale: (≤ 1600 °C) This individual parameter has not been studied in much detail.	Closure Criterion: Resolution of its importance.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A.

Additional Discussion

Once the particle layers have been breached, the kernel is exposed. The inventory now available for release will dwarf the minor inventories in the layers.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Buffer Layer: Chemical attack by air Temperature distribution	Impact of graphite oxidation on temperature distribution through material

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 4	Remedy: Determine if the uncertainty in the temperatures is acceptable. Refine models and collect data as necessary.
	> 1600 °C: N/A	Remedy: N/A
Rationale: The temperature determines the rate at which the layer is attacked.	Rationale: (≤ 1600 °C) Enough modeling has been done to reasonably estimate the temperatures	Closure Criterion: Adequate data for calculations.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Kernel Maximum fuel temperature	Maximum fuel temperature attained by the fuel kernel during the accident

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 7	Remedy: Insure that core models are up to date.
	> 1600 °C: N/A	Remedy: N/A
Rationale: The SiC layer is the primary barrier, but diffusion through the kernel does delay the release somewhat. The kernel retains a considerable amount of material and release is a function of temperature.	Rationale: (≤ 1600 °C) The core codes should be good enough to calculate the temperatures.	Closure Criterion: Acceptable uncertainties.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

For a study comparing the relative contributions of core and fuel materials and fission product retention see: *An Analytical Study of Volatile Metallic Fission Product Release From Very High Temperature Gas-Cooled Reactor Fuel and Core*, S. Mitake, et. al., Nuclear Technology, 81, 7-12.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Kernel Temperature vs. time transient conditions	The time-dependent variation of fuel temperature with time

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: II	≤ 1600 °C: 7	Remedy: None, expect to watch for hot spots
	> 1600 °C: N/A	Remedy: N/A
Rationale: The temperature history of the fuel is important. Higher temperature operation even if it is followed by lower temperature operation can result in greater corrosion problems. High temperatures also increase fission product diffusion.	Rationale: (≤ 1600 °C) Modern codes can computer the time history of the fuel. The greatest problem is material property uncertainties.	Closure Criterion: Calculations within the needed uncertainties.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

This is really a core design issue.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Kernel Energy Transport: Conduction within kernel	Flow of heat within a medium from a region of high temperature to a region of low temperature

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	≤ 1600 °C: 7	Remedy: None
	> 1600 °C: N/A	Remedy: N/A
Rationale: The kernel conductivity determines the kernel peak temperature. The kernel is fairly small, so modest changes in conductivity won't matter much. Higher temperatures could result in greater diffusion of fission products out of the kernel.	Rationale: (≤ 1600 °C) These numbers have been measured for the fuels of interest. No major issues are associated with them.	Closure Criterion: None
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

Kernel conductivity depends on the kernel composition and changes as the kernel burns up. The small size of the kernel limits these effects in coated particle fuel.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Kernel Thermodynamic state of fission products	Chemical and physical state of fission products

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 4	Remedy: If fuel kernels other than UO_2 are to be used, testing is required to assure that they work as expected.
	> 1600 °C: N/A	Remedy: N/A
Rationale: The chemical state of the fission products determines how they will migrate and the temperature dependence. It is desirable to oxidize some fission products without producing CO. Air and steam could cause additional changes by reacting with the UCO.	Rationale: (≤ 1600 °C) A considerable amount of work has been done kernel composition to limit the migration of fission products and control CO pressure. However, only UO_2 has been extensively tested in a high quality fuel. Also, the kernel will oxide with air and water.	Closure Criterion: Demonstrated performance under the conditions of interest
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

For a discussion on kernel design to minimize CO and immobilize key fission products see:

Stoichiometric Effects on Performance of High-Temperature Gas-Cooled Reactor Fuels from the U-C-O System, F.J. Homan, et. al., Nuclear Technology, 35, pages 428-441.

The effect of Water Vapor on the Release of Gaseous Fission Products from High-Temperature Gas-Cooled Reactor Fuel Compacts Containing Exposed Uranium Oxycarbide Fuel, B. Myers, DOE-HTGR-88486

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Kernel Oxygen flux	Mass transport of oxygen per unit surface area per unit time

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	≤ 1600 °C: 3	Remedy: Determine if this area is of any significance
	> 1600 °C: N/A	Remedy: N/A
Rationale: The mass of oxygen from the kernel will determine the rate at which CO is formed and particle pressure. Since the particles are designed assuming maximum pressure, the rate does not seem that important, but his area is somewhat unexplored. Oxygen coming in due to air/water will oxidize the kernel. See previous entry.	Rationale: (≤ 1600 °C) Some work has been done in this area. The full implications are not clear.	Closure Criterion: Resolution of the issue.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

Tests have shown that the oxygen does not immediately leave the kernel, leading to a somewhat lower CO pressure than normally would occur. This effect is probably more important for low burnup fuel than high burnup fuel. Upcoming tests on German fuel at higher burnups should shed more light on the oxygen issue. See:

Production of Carbon Monoxide During Burn-up of UO_2 Kerneled HTR Fuel Particles, E. Proksch, et. al., Journal of Nuclear Materials, 107 (1982) pages 280-285.

Influence of Irradiation Temperature, Burnup, and Fuel Composition on Gas Pressure (Xe, Kr, CO, CO2) in Coated Particle Fuels, G.W. Horsley, et. al., Journal of the American Ceramic Society, 59, Number 1-2, pages 1-4.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Kernel Grain growth	Enlargement of grains as a result of diffusion

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	≤ 1600 °C: 3	Remedy: None at present
	> 1600 °C: N/A	Remedy: N/A
Rationale: Kernel grain growth has not been an issue. The higher burnups of coated particles fuels often results in the destruction of any structure. Gas release could be higher, but this issue hasn't come up.	Rationale: (≤ 1600 °C) The grain growth issue appears to be less important with coated particle fuel because the layers form the fission product boundary.	Closure Criterion: None at present
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

Unlike LWR fuel, the grain structure appears to be less important.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Kernel Buffer carbon-kernel interaction	Chemical reaction between carbon and the fuel (UO2 or UOC) to form UC2 and CO (gas)

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	≤ 1600 °C: 5	Remedy: None
	> 1600 °C: N/A	Remedy: N/A
Rationale: A significant problem in this area has not been observed.	Rationale: (≤ 1600 °C) Reactions of this nature can be investigated using thermochemical codes. Nothing has come up to date.	Closure Criterion: None
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

This issue is discussed to some extent in: *Stoichiometric Effects on Performance of High-Temperature Gas-Cooled Reactor Fuels from the U-C-O System*, F.J. Homan, et. al., Nuclear Technology, 35, pages 428-441.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Kernel: Chemical attack by air Kinetics	Rate of reaction per unit surface area as a function of temperature and partial pressure of air

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 3	Remedy: Determine the need for this information.
	> 1600 °C: N/A	Remedy:N/A
Rationale: As the kernel is oxidized, it can change its structure and release fission products in a small burst. The rate at which this happens may be important if a significant number of kernels are exposed or particles fail.	Rationale: (≤ 1600 °C) The details effects on kernels have not been studied. Some integral testing has been done with particles and fuel elements.	Closure Criterion: Resolve this issue for accident cases.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

For some information on fuel under oxidizing conditions see:

Compilation of Fuel Performance and Fission Product Transport Models and Database for MHTGR Design, Martin, R.C., ORNL/NPR-91/6

Fuel Performance and Fission Product Behavior in Gas Cooled Reactors, IAEA-TECDOC-978 (1997)

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Kernel: Chemical attack by air Catalysis	Modification of the reaction rate by fission products or impurities

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	≤ 1600 °C: 1	Remedy: Determine if relevant.
	> 1600 °C: N/A	Remedy: N/A
Rationale: A catalysis could increase the reaction rate and accelerate releases, but it doesn't appear that there are any good candidates.	Rationale: (≤ 1600 °C) Unknown	Closure Criterion: Collection of relevant data.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

Accelerated releases from the kernel under accident conditions due to catalysis have not been explored.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Kernel: Chemical attack by air Changes in chemical form of fission products	Changes in chemical form resulting from oxidizing or reducing fission products

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 4	Remedy: Determine the need for this knowledge, collect as necessary.
	> 1600 °C: N/A	Remedy: N/A
Rationale: Changes in the chemical form of the fission products can greatly change their transport properties. The greatest change may come from the reaction of UC and the change in kernel structure	Rationale: (≤ 1600 °C) Thermochemical codes can calculate the possible chemical compounds. Little confirmation work is available	Closure Criterion: Collect data to resolve uncertainties
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

The forms and migration of the fission products can be complex. For some information on the chemical forms see:

Fission Product Plateout and Liftoff in the MHTGR Primary System: A Review, NUREG/CR-5647

Chemical Behavior of Fission Products in Core Heatup Accidents in High-Temperature Gas-Cooled Reactors, R. Moormann, Nuclear Technology, 94 (1991), pages 56-67.

Fuel Performance and Fission Product Behavior in Gas Cooled Reactors, IAEA-TECDOC-978 (1997)

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Kernel: Chemical attack by air	Changes in diffusivity, porosity, adsorptivity, etc.
	Changes in kernel properties	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	≤ 1600 °C: 4	Remedy: Determine the relevance of this situation
	> 1600 °C: N/A	Remedy: N/A
Rationale: If the kernel restructures because of oxidation, it can release some its stored inventory of fission products, mostly gases.	Rationale: (≤ 1600 °C) Testing has been done for LWR fuel. Some of this information may be useful for HTGR fuel.	Closure Criterion: Relevance of this situation and any data.
	Rationale (> 1600 °C) N/A.	Closure Criterion: N/A

Additional Discussion

The amount of damaged fuel determines how significant this issue is. If the fuel performs as advertised, then it may not matter. See *Fuel Performance and Fission Product Behavior in Gas Cooled Reactors*, IAEA-TECDOC-978 (1997)

Appendix F.3

Detailed PIRT Submittal by the SNL Panel Member

F. A. Powers

TRISO Fuel PIRT: Accident With Subsequent Air Intrusion

This PIRT is based more on geometry than it is on phenomenology, despite the name. The PIRT seems to be attempting to identify the critical component of the coated particle fuel structure that deserves the most attention. This is done at the expense of identifying the critical phenomena that need to be understood to anticipate the behavior of the fuel in normal and off normal circumstances. As a result questions are asked repetitively about each of the major elements of the fuel perhaps to see if one or more of the elements are more vulnerable than others. The questions do not illuminate in any detail the type of information that must be derived for coated particle fuel or the types of testing that must be done to gather the information. For instance, lumped within the simple question of gas phase diffusion are bulk and Knudsen diffusion. Though the question is repeated for each layer even when the layers are very similar, such as inner and outer PyC, there is no request for details of the materials that would be essential to estimate Knudsen versus bulk diffusion such as porosity and tortuosity. There is no indication of whether tests of permeability need to be done for layers in situ or such data can be obtained from macroscopic samples of analog material. We do not know from the PIRT whether phenomena such as thermal diffusion require testing to be done in prototypic gradients or just known gradients. We do not know from the PIRT whether diffusion must be considered as approximately binary diffusion or has to be viewed as a multicomponent process. This focus on the structure at the expense of phenomena limits the utility of the PIRT for the design of fuel models and experimental studies. Perhaps, the PIRT is more useful in other respects because of its focus on structure.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Fuel Element Irradiation history	The temperature, burnup and fast fluence history of the layer

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 3	Remedy:There is a need for studies of the energetics of radiation damage to the materials making up the coated particle fuel layers. (Damage to the kernel is of lesser interest). The needed information can probably be obtained by thermal analysis of specimens irradiated under prototypic conditions for varying lengths of time. There is further need for information on the kinetics of oxidant reactions and reactions of nitrogen with the materials as functions of temperature.
Rationale: The fast fluence history of the layers will dictate how much radiation damage is built into the materials. This will affect the kinetics of reaction. Also as reaction proceeds, the radiation damage energy will be released augmenting the energy of chemical reactions with the layers	Rationale: We have some knowledge of the radiation damage that can develop in carbon materials at the operating temperatures of interest for this work. We don't have such information about the specific materials involved in the coated particle fuel. Furthermore, we don't have data or models on the effects of radiation damage on the kinetics of oxidant interactions with the materials	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Fuel Element Condensed phase diffusion	Inter grannular diffusion and/or intra-grannular solid-state diffusion

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	Level: 1	Remedy: The essential remedy is to wait until a specific and reproducible material is specified. Then the material has to be characterized in terms of grain size and orientation as well as in terms of the surface and grain boundary diffusion coefficients of irradiated material. Diffusion studies will have to take into account the fact that the material will not be isothermal. Rather there will be necessarily a temperature gradient across the material from the fuel particles (which are the source of the decay heat) and the coolant. A major issue to confront here is whether the release modeling should be so complete that it considers release limitations by the matrix material surrounding the fuel particles. It would not be an unreasonable conservatism to neglect this barrier to release since it appear unlikely that there will soon be useful experimental data to validate models of the barrier
Rationale: Grain boundary and surface diffusion of fission products will be faster mechanisms of mass transport of fission products from the perimeter of the fuel particles to the surfaces of the matrix material and into the reactor coolant system from where they can escape into the plant environment. Surface diffusion and grain boundary diffusion are notoriously sensitive to impurity concentrations of the material. They are also sensitive to the grain sizes and the preferential orientation of grains. Presumably they are also sensitive to the irradiation of the material though I am not familiar with definitive studies of this issue. Diffusion in the systems will be complicated by the presence of a thermal gradient across the material.	Rationale: The bulk matrix material has not been specified and certainly has not been characterized sufficiently to estimate diffusion coefficients for the fission products. There are of course no measured data because the specification of the material has not yet been made. Studies of generic material may provide some guidance.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Fuel Element Gas diffusion	Diffusion of gaseous fission products through layer (Knudsen and bulk diffusion through pore structure, and pressure driven permeation through structure) Other factors include holdup craking adsorption, site poisoning, permeability, sintering and annealing

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: II	Level: 4	Remedy: The gas phase mass transport across elements from multi-point sources is a sufficiently complicated process that it is probably useful to set up models now and test them against models used for catalysts and the like. Detailed analyses of the issue will have to wait until there are real data on the fuel matrix materials that will be used in the reactor. A major issue to confront here is whether the release modeling should be so complete that it considers release limitations by the matrix material surrounding the fuel particles. It would not be an unreasonable conservatism to neglect this barrier to release since it appear unlikely that there will soon be useful experimental data to validate models of the barrier
Rationale: Vapor transport through pores and voids in the matrix material will be the fastest mechanism of mass transport of fission products from the fuel particle surfaces to the boundary of the fuel elements. The transport may driven by pressure differences or it may be by diffusion (either chemical or Knudsen). The presence of a thermal gradient will affect the diffusion process. It may be necessary to develop the diffusion equations to include thermal diffusion. Certainly the mass transport will have to address multicomponent effects using something like the Stefan Maxwell equations rather than Fickian diffusion equations	Rationale: The physics of the process is relative well understood and, indeed, fairly sophisticated models of this kind of mass transport have been developed by the catalyst community. What we don't know with any detail is the speciation of the fission product vapors or the pore and void structure of the matrix material. Diffusion coefficients for the vapors can be estimated with surprisingly good reliability from simple first order Chapman Enskog theory. Second order theory must be used to estimate thermal diffusion coefficients which (continued next column)	Closure Criterion: (continued from previous column) may not be negligible if the thermal gradients are large and if there are gases that have low molecular weights relative to the fission product vapors. Application of models of this type to the issue is not possible now because we do not have data on the material such as its void and porosity structure and its permeability

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Fuel Element: Transport of metallic FPs through fuel element Chemical form	Chemical stoichiometry of the chemical species that includes the radioisotope of interest

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H A major issue to confront here is whether the release modeling should be so complete that it considers release limitations by the matrix material surrounding the fuel particles. It would not be an unreasonable conservatism to neglect this barrier to release since it appear unlikely that there will soon be useful experimental data to validate models of the barrier	Level: 4	Remedy: There needs to be an agreed upon thermodynamic data base for the important species arising in the analysis of fission product release at these gas-cooled reactors. Much of the data in this base could be borrowed from existing databases. There needs also to be a search for possible species many of which have been identified in the literature but not characterized sufficiently to include in data bases now available.
Rationale: metallic fission products are going to be transported through the matrix material primarily as vapors. The effective vapor pressures of the metallic fission products depend on their gas phase speciation. There have been fairly limited investigations of the speciation of the fission products in the strongly reducing environment of the fuel element. Certainly the elemental forms will be important. What is of interest is whether there are more exotic species such as carbonyls and carbides and even cyanides that can augment the vapor pressures significantly. A reliable database on the thermodynamics of fission product species appropriate for this kind of a reducing environment (At least prior to oxidant intrusion) has not been assembled. Existing databases treat primarily elements, oxides and in some cases hydroxides. Once the oxidant (air) intrudes, these other possible vapor species as well as vapor phase hydrides need to be considered to know the vapor pressures of the fission products	Rationale: Elemental vapor pressures are rather well established for most of the fission products. Databases exist for most oxides and some hydroxides. Hydride, carbonyl, carbide data are scattered in the literature and have not been systematized nor has there been a systematic survey to identify more exotic vapor species. Polyatomic vapor species become less important as temperatures increase and pressures decrease.	Closure Criterion:

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Fuel Element: Chemical attack by air Kinetics	Rate of reaction per unit surface area as a function of temperature and partial pressure of air

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 4	Remedy: Any model of fission product release will have to be capable of addressing the multiple effects of oxidation.
Rationale: The intrusion of oxidant, in this case air, will have several effects : Alter the ambient oxygen potential and consequently the speciation and volatility of fission products Convert carbon into carbon monoxide, etc. and in doing so open pathways for vapor transport through the fuel element to the reactor coolant system thereby facilitating release of radionuclides Impart heat to the element and alter the temperature distribution within the element The kinetics of attack on the matrix material is important since the depletion of oxidant by the reactions reduces the attack that is possible on fuel particles themselves. An interesting issue in the case of air intrusion is reactions of nitrogen. Presumably some production of cyanogens occurs. Cyanides of metals such as fission product metals are often considered analogous to the rather volatile halides of the same metals. Does the production of cyanogens alter the vapor phase speciation of fission products and enhance the volatility of fission products normally considered refractory? Unfortunately, there does not seem to have been a systematic study of the volatile cyanides of pertinent metals in the literature.	Rationale: There is a lot of information about air interactions with generic graphitic materials though obviously nothing specifically for the material that will be used in gas-cooled reactor fuel. What we know is that at lower temperatures the attack by oxidant is not uniform. Attack is along preferential locations. Catalysis can be responsible for this localized attack and catalysis is discussed further below. In the absence of catalysis oxidation of graphite seems to be at energetic sites such as those found on cracks and pore networks of the material. This means that solid material gets converted to gas to open channels for gas phase mass transport from the fuel particles through the matrix material. It also means that kinetics of oxidant attack on graphite should differ between normal material and irradiated material though it is not entirely clear how much the kinetics differ. One possibility is that irradiation will make the attack more homogeneous since the defects introduced by irradiation will be much like energetic sites on the walls of cracks and pore networks. Investigation of the kinetics of oxidation as a function of temperature is made complicated by the additional release of energy as material displace by irradiation from normal crystal sites reacts. At very high temperatures, the attack on graphite by oxidant becomes more uniform and the effects of catalysis less dominant. Still the overall issues of oxidation remain.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Fuel Element: Chemical attack by air Catalysis	Modification of the reaction rate by fission products or impurities

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 5	Remedy:Catalysis will have to recognized in modeling of the oxidation of graphite.
Rationale: the oxidation of graphite is catalyzed especially at lower temperatures. The catalysis arises because of the adsorption step O_2(gas) = 2 O (surface) That preceeds reaction with carbon and the desorption step CO(surface) = CO(gas) Catalysis is by materials deposited on the surface of the graphite. Because of this, catalytic attack is localized and leads to pits being bored into the material. The depth of attack in these pits vastly exceeds the expected uniform erosion. In the case of fuel elements, pit attack can result in oxidant boring into the regions of fuel particles. Many materials catalyze the oxidation. Common contaminants such as iron catalyze attack. Such fission products such as cesium and palladium are known to catalyze attack.	RationaleThere is information in the literature on catalytic oxidation of generic graphites. Nothing can be said to be particularly applicable to the graphite to be used in the reactors. There has not been a systematic survey of catalysts by the fission products of interest for graphite reactors. Catalysis becomes of decreasing interest at very elevated temperatures – It is difficult to investigate because the catalysts vaporize from the surface. This may not be an excuse to ignore the issue here. The transport of radionuclides will involve transient adsorption and desorption along the transport pathway. During residence on the surface the material can catalyze reaction of the surface and the opening of the flow pathway	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Fuel Element: Chemical attack by air Changes in chemical form of fission products	Changes in chemical form resulting from oxidizing or reducing fission products

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 4	Remedy Any modeling of the fission product release from gas reactor fuels will have to include a careful thermodynamic assessment of both the condensed and vapor phase speciation. It may require that this speciation assessment is spatially dependent:
Rationale: Vapor pressures of many of the fission products are strong functions of the ambient oxygen potential. In the regions of oxidant attack the oxygen potential may be much higher than the bulk average oxygen potential of the reactor core. The higher oxygen potential can enhance the vaporization of fission products like Pd, Ru, Mo. It can inhibit the vaporization of fission products like Ba, Sr, La, Ce. An intriguing concept is the possibility that nitrogen will react with carbon to form cyanogens that will subsequently react to form pseudo halides of the metals. N_2 (gas) + 2C = $(CN)_2$ $(CN)_2$ + Ru = $Ru(CN)_2$ (gas) Since pseudohalides like halides are typically quite volatile, this could enhance the vaporization of some radionuclides. At high temperatures, vapor phase nitrides (as well as carbides) could contribute to the volatility of the fission products.	Rationale: The speciation of fission products in the environment of air attack on graphite have not been explored very thoroughly though the basis for such an exploration can be done. The data base is not well established and there has not been a careful survey to identify unusual species like carbides and cyanides that might contribute to the vaporization of fission products	Closure Criterion:

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Fuel Element: Chemical attack by air Changes in graphite properties	Changes in diffusivity, porosity, adsorptivity, etc.

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 2	Remedy:This modeling of the oxidation along pathways for mass transport could be a very challenging feature of a fission product release model. Whether the development of such a model needs to be done or not depends on whether credit is taken for the barrier to fission product release provided by the matrix material.
Rationale: As noted above, especially at lower temperatures, oxidant attack on graphite is localized, not uniform and the localized attack is on the regions that will facilitate gas phase mass transport of fission product vapors through the fuel matrix like cracks and pore networks, the attack opens these pathways and makes transport easier	Rationale: The prediction of the effects of oxidant attack on the pathways is challenging. There has been some work in the chemical engineering field on analogous issues that could serve as a basis for modeling this phenomenon.	Closure Criterion:
	The effects of oxidant attack on cracks and pore networks become less important as temperature become very high and the attack becomes more uniform.	

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Fuel Element: Chemical attack by air Holdup reversal	Release of graphite FP inventory

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 5	Remedy: It is not clear that this phenomenon needs to be included in a model. Certainly it does not need to be included if the barrier to release presented by the matrix is neglected as a conservative measure that considerably relieves the challenges in estimating releases for risk assessments.
Rationale: It is known that energetic sites will adsorb fission product vapors and create some holdup of the release of radionuclides. It is not evident that there are enough of these sites to cause the holdup of a significant fraction of the radionuclide inventory. It is known that chemical reactions that destroy energetic sites or even the intrusion of polarizable gases that will compete for site occupancy can result in the release of the adsorbed fission products. But, if the desorption does not involve a large fraction of the inventory of particular class of fission products the phenomenon is not significant	Rationale We probably do not have sufficient data on the holdup to make quantitatively defensible estimates of the holdup. We do know enough to make simple qualitative arguments about its significance Holdup on the matrix surfaces is less important at high temperatures because of the high vapor pressures of the fission product species of interest. Though we certainly know less about holdup on the surfaces at high temperature than we know at low temperatures, we probably know enough to say that if the importance of the phenomenon is questionable at low temperatures, it certainly is unimportant at very high temperatures.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Fuel Element: Chemical attack by air Temperature distribution	Impact of graphite oxidation on temperature distribution through material

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 6	Remedy: If the barrier to fission product release posed by the matrix material is to be considered a fairly sophisticated model of gas phase mass transport will be needed. (A completely similar model will be needed also for mass transport in the fuel particles themselves. Once developed the same model can be used in both places) Modeling of fission product transport by gas phase processes will be important both because these are the fastest transport processes and because it is unlikely that we will ever have good, reproducible data on the release of fission products from fuel elements for the range of accidents that will be of interest for risk assessments.
Rationale: Temperature distributions along the transport paths for fission products will affect the vapor pressures of these fission products. The temperature gradients will also affect the gas phase mass transport of fission products (It will also affect condensed phase mass transport though here this process is taken to be much less important than gas phase mass transport) the effect is both to the chemical diffusion of vapors and to the thermal diffusion	Rationale: Given the details of the gas phase mass transport paths (which are not currently available) it should be possible to estimate the effects of temperature distribution on the transport of fission product vapors from the fuel particles to the surfaces of the fuel element exposed to the atmosphere of the reactor coolant system. Many things will have to be estimated. Fickian diffusion may not be the appropriate basis for the calculation of transport of multicomponent gas which may include light molecular weight species such as CO along with heavy molecular weight species like the fission product (continued next column)	Closure Criterion: (Continued from previous column) vapors. Though we can estimate chemical diffusion coefficients using perturbations of Chapman Enskog theory, it is more challenging to estimate the thermal diffusion coefficients of polyatomic species (Third order expansion of determinants versus first order expansion). A further complication will be the need to allow for Knudsen diffusion and pressure driven flow in the case of very limited flow pathways for release. Though the problem is doable, it is not trivially doable.
	The reliability of predictions of gas phase mass transport decreases with increasing temperature because of the increasing influence of inelastic collisions Otherwise things are the same as above though Knudsen diffusion becomes more important at higher temperatures	

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Outer PyC Layer Gas Phase Diffusion	Diffusion of gaseous fission products through layer (Knudsen and bulk diffusion through pore structure, and pressure driven permeation through structure)

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 6	Remedy: Any model of fission product transport within the fuel particle will have to include a gas phase mass transport model recognizing bulk diffusion, pressure driven flow and Knudsen diffusion
Rationale: These gas phase mass transport processes are the fastest ways for fission products released from the kernel to cross the Outer PyC layer.	Rationale: Given the geometry and nature of the pore and crack network in the layer it is possible to calculate the gas phase mass transport across the layer. We can estimate most of the gas phase diffusion coefficients. The mass transport is probably not modeled well by Fickian diffusion and one will have to develop a multicomponent diffusion model much like the membrane models that have been developed in the chemical engineering literature. It may be necessary to include in these models the effects of thermal diffusion especially if the gas includes both low molecular weight species such as CO (MW=28) and fission product vapor species (MW>100) and temperature gradients are significant as they surely must be to get decay heat out of the particle. The most complicated part of the modeling will be to treat the geometries of the layer as a (continued next column)	Closure Criterion: (continued from previous column) whole and the pore, crack and void network in the layer. We know the layers will not by spherically symmetric. Does the deviation from symmetry have a significant effect on the rate of transport? Similarly the layers will not be uniformly thick and this may create short circuits or preferred pathways for mass transport. We do not have good data on the pore and void network. We are not likely to get adequate data from microscopic analysis. The cracks pores and voids that are of interest are too small to readily identify and detect and microscopic examinations will never yield anything but a biased estimate of the concentration and sizes of the networks. Transport data are needed, but it is not readily apparent how such data are obtained for the microscopic layers of the particles.
	The situation is much the same at elevated temperatures though gas phase mass transport becomes an even more dominant mechanism simply because the gas phase concentrations are higher. The ability to estimate diffusion coefficients and thermal diffusion coefficients for polyatomic vapor species begins to degrade because inelastic collision become more important	

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Outer PyC Layer Condensed phase diffusion	Intergrannular diffusion and'or intra-grannular solid-state diffusion

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	Level: 2	Remedy: Any model of fission product transport across the Outer PyC layer will have to include these process though it is likely that even with only modest vapor pressures the gas phase mass transport processes will be more important mechanisms. The diffusion process has the same problems discussed above. Spherical symmetry may be an overly crude approximation as may be the assumption that the layer is uniformly thick.
Rationale: Fission products that are not volatile will be transported across the barrier posed by the outer PyC layer by the condensed phase diffusion processes. Bulk diffusion is the slowest of these a low temperatures, but it has the highest activation energy so it does eventually become the dominant process. Even if the metals have only small vapor pressures, gas phase mass transport of fission products may still be the dominant mechanism for most fission products. There do appear to be some exceptions such as the transport of Ag.	Rationale: We donot have surface and grain boundary diffusion coefficients for the fission products and materials of interest here and surface and grain boundary diffusion are likely to be the dominant condensed phase transport processes. These coefficients cannot be estimated. They have to be measured and they are notoriously sensitive to impurities accumulated on the grain surfaces and at the grain boundaries At sufficiently high temperatures (and it by no means established that 1600 is sufficiently high) bulk diffusion of fission products will be dominant transport processes for nonvolatile species. We do not have useful bulk diffusion coefficients for irradiated material. The need for irradiated material is to be emphasized since it is known that radiation defects can act as traps for diffusing species	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Outer PyC Layer Layer oxidation	Reaction of pyrolytic graphite with oxygen released from the kernel

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 2	Remedy: Analysis of fission product release during air intrusion or water intrusion accidents will have to account for the effects of oxidant on the integrity of the outer PyC layer. It will have to be a kinetic analysis so that the analyst will know how much oxidant survives the interaction with the layer to attack other regions of the fuel particle.
Rationale: Oxidant can reach the Outer PyC layer either coming from oxygen evolved from the fuel kernel or oxidant intruding into the core (air or water). It is likely that the source of oxidant coming form the fuel will be sufficiently weak that most of this oxidant will be consumed by reactions with graphite etc. before it can reach the Outer PyC layer in any form other than CO. Oxidant from intrusive sources will have to survive reactions with graphitic materials along its transport path to the fuel particle. When it does survive this transport the results can be catastrophic with respect to fission product transport across the PyC layer. The oxidant will thin the layer, but more importantly localized attack on energetically preferred sites will result in widening and smoothing the cracks and pores through the layer thereby facilitating gas phase mass transport across the layer. The oxidation reactions can also heat the layer	Rationale: The oxidation reactions kinetics are enormously sensitive to impurities that can catalyze reactions. Fission products themselves may act as catalysts. Though we have some data on the oxidation reactions, we do not have data on the specific material. Without these data accurate quantitative analysis of the oxidation process at the Outer PyC layer is really not possible The situation becomes a little simpler at very high temperatures where the kinetics are less affected by the catalytic processes and proceed in a more uniform process. Still we donot have validated kinetic models.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Outer PyC Layer Stress state (compression/tension)	The state of the forces induced by external forces that are acting across the layer to resist movement

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 2	Remedy: it isn't clear that any remedy is needed
Rationale:This is a more important issue during normal operations since it can result in rupture of the layer prior to the accident . Thermal expansion may cause some stresses on the layer and it would be of interest to know if rupture can occur	RationaleWe really don' t know much about these forces	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Outer PyC Layer Intercalation	Trapping of species between sheets of the graphite structure

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 2	Remedy: no remedy needed
Rationale: It is known that energetic sites in the PyC layer will provide sites for fission product deposition and holdup. There can be a preference for fission products to migrate toward the basal planes of the graphite structure and be intercalated. It is not apparent that sufficient concentrations of sites will be formed to holdup a significant fraction of the radionuclide inventory of the fuel particle. Eventually oxidation or thermal annealing will eliminate these energetic sites and lead to the desorption of fission products that have been attracted to the sites. The elevated temperatures will eventually move fission products from the intercalation sites as well.	Rationale: We don't really know how much holdup can occur At sufficiently high temperatures there really will not be any holdup since the vapor pressures of the fission products will be so high	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Outer PyC Layer Trapping	Adsorption of fission products on defects

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 2	Remedy: no remedy needed
Rationale: It is known that energetic sites in the PyC layer will provide sites for fission product deposition and holdup. There can be a preference for fission products to migrate toward the basal planes of the graphite structure and be intercalated. It is not apparent that sufficient concentrations of sites will be formed to holdup a significant fraction of the radionuclide inventory of the fuel particle. Eventually oxidation or thermal annealing will eliminate these energetic sites and lead to the desorption of fission products that have been attracted to the sites. The elevated temperatures will eventually move fission products from the intercalation sites as well.	Rationale: We don't really know how much holdup can occur At sufficiently high temperatures there really will not be any holdup since the vapor pressures of the fission products will be so high	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Outer PyC Layer Cracking	Lengths, widths and numbers of cracks produced in layer during accident

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 1	Remedy:It is clear that any model of fission product transport through the fuel particles has to recognize the possibility of cracks in the material providing a short pathway for transport. Whether the cracking has to be modeled or cracking is input to the transport model is a decision that must be made. This decision may well rest on whether cracking occurs during the accident transient or is primarily a process that occurs during normal operations.
Rationale: Cracks through the layer facilitate gas phase mass transport of fission products across the layer	Rationale: It is not apparent that we are in any position to predict the cracking of the layers under any circumstances let alone under accident circumstances. It may not be practical to predict cracking and we will have to rely on empirical evidence for cracks. This is a challenge since cracks that can affect fission product release rates may be very difficult to detect microscopically	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Outer PyC Layer:Chemical attack by air Kinetics	Rate of reaction per unit surface area as a function of temperature and partial pressure of air

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 2	Remedy: Analysis of fission product release during air intrusion or water intrusion accidents will have to account for the effects of oxidant on the integrity of the outer PyC layer. It will have to be a kinetic analysis so that the analyst will know how much oxidant survives the interaction with the layer to attack other regions of the fuel particle.:
Rationale: Oxidant can reach the Outer PyC layer either coming from oxygen evolved from the fuel kernel or oxidant intruding into the core (air or water). It is likely that the source of oxidant coming form the fuel will be sufficiently weak that most of this oxidant will be consumed by reactions with graphite etc. before it can reach the Outer PyC layer in any form other than CO. Oxidant from intrusive sources will have to survive reactions with graphitic materials along its transport path to the fuel particle. When it does survive this transport the results can be catastrophic with respect to fission product transport across the PyC layer. The oxidant will thin the layer, but more importantly localized attack on energetically preferred sites will result in widening and smoothing the cracks and pores through the layer thereby facilitating gas phase mass transport across the layer. The oxidation reactions can also heat the layer	Rationale: The oxidation reactions kinetics are enormously sensitive to impurities that can catalyze reactions. Fission products themselves may act as catalysts. Though we have some data on the oxidation reactions, we do not have data on the specific material. Without these data accurate quantitative analysis of the oxidation process at the Outer PyC layer is really not possible The situation becomes a little simpler at very high temperatures where the kinetics are less affected by the catalytic processes and proceed in a more uniform process. Still we do not have validated kinetic models.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Outer PyC Layer: Chemical attack by air Catalysis	Modification of the reaction rate by fission products or impurities

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 4	Remedy: Models of fission product transport that include the effects of oxidation will have to take into account catalysis. That is oxidation of pure material cannot be the kinetic data base the model uses.
Rationale: catalysis by impurities will affect the oxidation rates of the PyC layer. Catalysis can be caused by fission products. Defects introduced by the irradiation of the layer may also accelerate the reaction kinetics in such a way that the catalytic effects are not detectable. However, the biggest effect of catalysis is to open up pore networks and facilitate the transport of radionuclides across the layer. Defects and reactive sites are very likely to be most concentrated in these networks.	Rationale: We don't have good models of the catalysis of oxidation of the materials of specific interest by the fission products or the radiation defects. Catalysis is much less important at high temperatures where the reaction rates are inherently high and the fission products are quite volatile. Though we don't know more about high temperature catalysis, we don't need to know as much so our relative knowledge level is higher	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Outer PyC Layer: Chemical attack by air Changes in chemical form of fission products	Changes in chemical form resulting from oxidizing or reducing fission products

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 5	Remedy: Fission product transport models will have to have the capability to evolve the chemical forms of the fission products as the ambient conditions change with respect to both chemical potentials and temperatures.
Rationale: The high local oxygen potential will change the fission product chemical form making some more volatile and some less volatile	Rationale: We have databases that will allow us to do some exploration of the change in chemical form of the fission products in the vicinity of regions of higher oxidation potential. We do not have information on more exotic species like pseudo halides such as cyanides that may affect the volatility of some of the more refractor fission products.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Outer PyC Layer: Chemical attack by air Changes in graphite properties	Changes in diffusivity, porosity, adsorptivity, etc.

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 3	Remedy: Oxidation effects on fission product transport will have to be considered. Data on the change in the permeability of material as reactions progress would be useful.
Rationale: The important effect of oxidation aside from changing the volatilities of the fission products is to open pathways for the transport of the fission products from the fuel kernels to the outside of the fuel particles.	Rationale It is difficult to predict quantitatively how the oxidation will change the transport pathways	Closure Criterion:
	same as above, however at higher temperature when oxidation kinetics are rapid, the reactions take place more uniformly and act more to ablate material (shorten the transport distance) than to open the flow pathways	

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Outer PyC Layer: Chemical attack by air	Release of graphite FP inventory
	Holdup reversal	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 4	Remedy: It is not evident a remedy is needed until there is some demonstration that the holdup is significant from a risk perspective
Rationale: oxidation reaction will destroy energetic sites that have absorbed fission products and thus release the fission products. It is not apparent that absorption of fission products on energetic sites holdups enough of the releasable inventory of fission products for this reactive desorption process to be risk important	Rationale: We don't have data on the adsorption. We do know that reactions will reverse it	Closure Criterion:
	At such high temperatures the adsorption of fission product vapors has probably been thermally reversed prior to reaction	

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Outer PyC Layer: Chemical attack by air Temperature distribution	Impact of graphite oxidation on temperature distribution through material

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 3	Remedy:Any fission product transport model will require good, local temperature descriptions including the effects of chemical reactions on these temperatures
Rationale: Chemical reactions can heat the layer and change the thermal gradients across the layer – both of which will affect fission product transport	Rationale: We generally know enough about the heat of reaction. Combining this with the less well known kinetics of reaction and the heat that comes from destroying irradiation produced defects should allow a calculation of the effects of reaction on temperatures. The thermal conduction calculation is a challenge as delineated above	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer Gas phase diffusion	Diffusion of gaseous fission products through layer (Knudsen and bulk diffusion through pore structure, and pressure driven permeation through structure)

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 6	Remedy: Any model of fission product transport within the fuel particles will have to include an gas phase mass transport model recognizing bul diffusion, pressure driven flow and Knudsen diffusion The mechanistic detail with which a model could be constructed is probably not supported by adequate characterization of the irradiated layer. It may be necessary to adopt a more empirical modeling retaining perhaps the functional forms suggested by the theory of mass transport through porous materials.
Rationale: Gas phase mass transport across the SiC layer through cracks or through the pore and void network in the material will be by far the fastest mechanism for mass transport of fission products across this layer	Rationale: Given the geometry and nature of the pore and crack network in the layer it is possible to calculate the gas phase mass transport across the layer. We can estimate most of the gas phase diffusion coefficients about as accurately as they can be measured. The mass transport probably cannot be calculated using Fickian diffusion and neglecting temperature gradients in the material. A multicomponent model similar in nature to the models of mass transport across membranes used widely in the chemical engineering field will have to be used. It may be necessary to recognize the effects of thermal diffusion if the temperature gradients are large and there are significant differences in the molecular weights of gases. This may well be the case especially inside the SiC layer which will be	Closure Criterion: (continued from previous column)
	The situation is largely the same at high temperatures as at low temperatures though the speciation of the gas phase fission products becomes more complicated.	

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer Condensed phase diffusion	Inter-grannular diffusion and/or intra-grannular solid-state diffusion

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	Level: 2	Remedy: Modeling of fission product transport will have to include the modeling of condensed phase mass transport.
Rationale: Fission products that are not volatile will transport across the layer by diffusion. At low temperatures, grain boundary diffusion and surface diffusion will be the more rapid processes. Because the activation energy for bulk diffusion is highest, it will become, eventually the dominant mechanism of mass transport as the temperature is increased. Still, even if the fission product has only a very small vapor pressure, gas phase mass transport may outstrip condensed phase diffusion processes. There are some exceptions to this. Ag seems to be capable of fast transport across the layer and this fast transport has been ascribed to condensed phase diffusion although there are not the data necessary to conclusively demonstrate this.	Rationale: We really don't have good condensed phase diffusion coefficients for fission products during bulk, surface or grain boundary diffusion for the specific material that is of interest. Bulk diffusion coefficients from analogous materials may be adequate IF the defects in the crystal lattices produced by irradiation don't act as traps for diffusing species. Grain boundary and surface diffusion coefficients depend so much on the impurity levels at surfaces and grain boundaries where these impurities accumulate, that it would be difficult to ascribe significance to data sets for anything except the actual material of the layer including the correct crystallite orientation etc. pressurized with CO from the reaction of carbon (continued next column)	Closure Criterion: (continued from previous column) materials with the urania fuel kernel. Complication in the analysis come about if the deviations from spherical symmetry of the layer are significant and if the variations in the layer thickness is significant. Characterization of the pore, void or crack network in the layer is most important and quite challenging since the voids or cracks that can be effective for mass transport are not easily detected by microscopic examination. It is furthermore quite difficult to average sets of visual observations of cracks and voids to come up with a suitable 'average' description for the analysis of mass transport. What would really be desirable would be permeability measurements of the layer. It is of course not practical to make such measurements.

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer Thermal deterioration/decomposition	Decline in the quality of the layer due to thermal loading

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	Level: 3	Remedy: no remedy may be needed.
Rationale: SiC is a most peculiar material. There have been reports of phase changes in the material from cubic to hexagonal at elevated temperatures. Modern phase diagrams do not reflect this phase change. It may be more important that the material is subject to polytypism based on the hexagonal structure. If the formation of the layer does not yield the thermodynamically stable product, thermal annealing during the temperature transient of an accident could cause some restructuring that will create pathways for gas phase mass transport. It might also be possible during a thermal transient for the heavily radiation damaged material to restructure to relieve the accumulation of strain energy of the irradiation defects (A sort of analogy to the formation of the rim in heavily irradiated fuel!). This restructuring could well lead to gas phase mass transport paths that will facilitate the transport of fission products released from the fuel kernel across the layer.	Rationale: To quantitatively examine this issue we would have to have considerable data on the product of the particle formation process to see if polytypism occurs and also to see if radiation restructuring can occur during an accident temperature transient. Then we would need data to see how annealing affected the permeability of the layer The situation is the same as above for lower temperatures	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer Fission product corrosion	Attack of layer by fission products, e.g., Pd

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 3	Remedy: At this juncture it appears to me that holdup by chemical reaction with the SiC layer can be neglected until there is evidence that this important for more important radionuclides than Pd.
Rationale: Chemcial attack on the layer by fission products will affect transport across the layer and certainly may affect the transport of the fission product doing the transporting since it will be converted to a more stable form which may be less volatile. It is however to become excessively concerned over this since the fission product inventory of the kernel is not large enough to produce massive damage to the layer that will affect the transport of all fission products. There is only one example of significant attack and that is with Pd which is not an especially important fission product from an accident consequences view point. The attack by Pd may suggest other noble metals such as Ru and Mo will produce similar attack. There would have to be substantial evidence of this to rate the process of higher signficance.	RationaleWe don't have a comprehensive survey of the attack on SiC by fission products in part because SiC under reducing conditions is not an especially reactive material.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer Heavy metal diffusion	Diffusion of heavy metals through layer

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	Level: 2	Remedy: Modeling of fission product transport will have to include the modeling of condensed phase mass transport
Rationale: Fission products that are not volatile will transport across the layer by diffusion. At low temperatures, grain boundary diffusion and surface diffusion will be the more rapid processes. Because the activation energy for bulk diffusion is highest, it will become, eventually the dominant mechanism of mass transport as the temperature is increased. Still, even if the fission product has only a very small vapor pressure, gas phase mass transport may outstrip condensed phase diffusion processes. There are some exceptions to this. Ag seems to be capable of fast transport across the layer and this fast transport has been ascribed to condensed phase diffusion although there are not the data necessary to conclusively demonstrate this.	Rationale: We really don't have good condensed phase diffusion coefficients for fission products during bulk, surface or grain boundary diffusion for the specific material that is of interest. Bulk diffusion coefficients from analogous materials may be adequate IF the defects in the crystal lattices produced by irradiation don't act as traps for diffusing species. Grain boundary and surface diffusion coefficients depend so much on the impurity levels at surfaces and grain boundaries where these impurities accumulate, that it would be difficult to ascribe significance to data sets for anything except the actual material of the layer including the correct crystallite orientation etc.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer Layer oxidation	Uptake of oxygen by the layer through a chemical reaction

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 5	Remedy: No remedy needed.
Rationale: I distinguish here between the reaction of SiC with oxidant to form CO and SiO and the uptake to form nominally SiOC. This later uptake can only progress to the point of saturation. It will only be important if it causes swelling or decrepitation of the SiC layer and I can find no evidence that it does. All my experience is with higher oxygen potentials where SiO is not stable and SiO2 is the condensed product of reaction and this SiO2 does act to occlude surfaces which would interfere in gas phase mass transport at the highest temperatures. SiO, a vapor in the temperature ranges of interest could condense elsewhere in the particle and have some ramifications on the transport of fission products.	Rationale: There is a lot of information about the response of SiC to oxidizing conditions of various oxygen potentials. I don't' find information that indicates processes during uptake that would affect fission product transport (but see below when reaction is discussed)	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer Fission product release through defects	Passage of fission gas from the buffer region through defects in the SiC layer

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 1	Remedy: This mechanism probably cannot be modeled mechanistically. It will have to be treated by providing empirical evidence of the change in layer permeability as irradiation progresses.
Rationale: Defects introduced into the SiC lattice by manufacture or by irradiation will become mobile at elevated temperatures and accumulate to form dislocations that themselves will lead to the formation of porosity networks. These networks will provide a pathway for gas phase mass transport that will be the dominant mechanism for fission product transport across the layer.	Rationale: We don't have the information to assess this process now	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer Fission product release through failures, e.g. craking	Passage of fission gas from the buffer region through regions in the SiC layer that fail during operations or an accident

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 4	Remedy: Mechanistic modeling of gas phase mass transport across a failed layer of SiC may not be undertaken though it can be done. A true failure of the layer may be taken somewhat but not greatly conservatively as meaning the layer no longer poses a barrier to fission product transport.
Rationale: SiC layer failure will permit the venting of accumulated fission product vapors and the ongoing releases of fission product vapors as they escape the fuel kernel and reach the SiC layer	Rationale: We don't have information that allows us to know when SiC layers fail or how massive the failures are. If we had this information it should not be difficult to model the gas phase mass transport across the layer through the failure locations.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer Thermodynamics of the SiC-fission product system	Include solubility, intermetallics, and chemical activity

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	Level: 2	Remedy: The remedy is some compatibility studies of fission products with SiC
Rationale: Fission products that dissolve in the SiC lattice will be stabilized and will be held from release at least temporarily. It does not appear, however, that this is major factor in the release of the more important, volatile fission products like I, Cs, Xe, Kr, Te etc. It may be more important for some of the transition metal fission products. Certainly Pd actually can react with SiC. Similarly Zr might react. It would also be of interest to know if other materials interacted badly with SiC, but even if we knew of some bad interactions involving materials other than fission products, we would have to have some idea of how these materials came into contact with the SiC within a fuel particle.	Rationale: There is amazingly little information about the phase relationships in the Si-C-FP systems of interest.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer Sintering	Change of graphite microstructure as a function of temperature

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 6	Remedy no remedy necessary:
Rationale: I do not find anything to suggest that changes in the microstricture of graphite will affect the SiC layer there may be some information suggesting that bonding of the graphite to the SiC affects the integrity of this layer, but it has nothing to do with microstructure issues	Rationale : there is really quite a lot of information about the sintering of SiC in the literature. It does not necessarily cover the entire region of interest nor does it address the effects of the fission product species on the sintering process. It should, however, be sufficient to estimate the magnitudes of any effects attributable to sintering on fission product transport. Far more important than simple, classic sintering will the thermal annealing of the radiation-induced defects in the SiC structure	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer: Chemical attack by air Kinetics	Rate of reaction per unit surface area as a function of temperature and partial pressure of air

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 4	Remedy: The key issues are whether sufficient oxidant survives transport through the core and the matrix material to reach the SiC and whether oxidant in the viscinity of the SiC layer will react to open pathways for gas phase mass transport across the layer or only leads to homogeneous ablation of layer material as the gases SiO and CO. Clearly actual data are needed and these should be collected for irradiated material since the dislocations produced by the irradiation should be more reactive than normal materials
Rationale: The rate of oxidation will be important to know. The rate will be complicated in regions of oxygen potential where there is a change from both products of oxidation being gases (SiO and CO) and higher oxygen potentials where the silicon-bearing product is condensed SiO2. More important than the homogeneous reaction kinetics will be how the reaction rates are affected by radiation-produced defects and the presence of pores and voids in the SiC. We will want to know if there is preferential attack in the voids that leads to the opening of pathways for gas phase mass transport of fission products through the layer or simple material ablation thinning the transport path across the layer. It will also be of interest to know if the SiC will react with the nitrogen component of air once the oxygen has been depleted to form silicon nitride and cyanogens, etc.	Rationale: there is some data in the literature on the air oxidation of SiC. Most of these data are for higher oxygen potentials than are likely to exist at the layer within the fuel particle. The database does not include information on highly irradiated material. A further complication is that SiC produced in a dynamic fashion such as is done in the manufacture of the coated particle fuels may still exhibit polytyism and not be in the stable crystallographic state for which measurements of reaction kinetics done in other technical disciplines have been directed. Especially at temperatures in excess of about 1800 K, and at higher oxygen potentials, product SiO2 will be liquid and will occlude the surface so that oxidation rates are controlled by transport across the viscous layer.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer: Chemical attack by air Catalysis	Modification of the reaction rate by fission products or impurities

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 2	Remedy No remedy needed:
Rationale: I am not aware of data indicating that the oxidation of SiC is catalyzed. There are some indications that impurities, notably iron, can accentuate the rates of attack and lead to attack along the grain boundaries, but this is really not catalysis.	Rationale: I am not aware of a data base that would suggest catalysis	Closure Criterion:
	The situation at higher temperatures is much the same as above and catalysis becomes less important at higher temperatures where reaction rates can be sufficiently fast that mass transport of oxidant will control the rate of reaction	

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer: Chemical attack by air	Changes in chemical form resulting from oxidizing or reducing fission products
	Changes in chemical form of fission products	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 6	Remedy:It will be essential in the analysis of fission product transport to track the speciation of the fission products as changes in ambient temperature, pressure and chemical potentials occur including the ambient potentials of oxygen
Rationale:An elevated oxygen potential can lead to changes in the chemical forms of the fission products making some more volatile and some less volatile. There is a reasonable understanding of this. Less certain is whether nitrogen from air can react with the fission products or carbon to produce species such as cyanides that have higher vapor pressures than would otherwise be expected. Vapor phase nitrides are now getting substantial attention in the molecular vapor literature. Solid thermochemical databases have not been developed for these species though it is known that some fission products can form stable vapor phase nitrides.	Rationale: There is a reasonable data base to calculate the speciation of fission products as a function of the oxygen potential. The issue may focus on the local oxygen potential and not the core wide average oxygen potential which will be dictated by the equilibrium: $2\,CO = CO_2 + C$ There has not been a systematic survey of the effects of species like cyanogens and the formation of pseudohalides of the fission product elements to produce elevated vapor pressures	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer: Chemical attack by air Changes in SiC properties	Changes in diffusivity, porosity, adsorptivity, etc.

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	Level: 2	Remedy A more far ranging data base on the oxidation of SiC and its effects on bulk material permeability would help resolve whether this is an issue of concern or not.:
Rationale:The clear concern is that oxidation of SiC opens pathways for gas phase mass transport because the attack is preferentially at pores, and void networks. I am not aware of data that shows this to be the case, but it is certainly possible for this to happen since the material at the boundaries of porosity in the SiC will be more energetic and reactive than material in the bulk. Also, because reactions with SiC are essentially slow there may be some preferential attack. Its significance depends both on the nature of SiC oxidation and the availability of oxidant to reach the SiC	Rationale: No data base for oxidation of the particular material in the coated particle fuels which will certainly be badly defected by irradiation and may exhibit some polytypism that makes it different than bulk annealed materials	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer: Chemical attack by air	Release of SiC FP inventory
	Holdup reversal	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 1	Remedy no remedy needed:
Rationale: Chemical reaction of oxidant with energetic sites that have adsorbed fission products will destroy the site and release any retained, volatile fission product. It is not clear that adsorption will retain a sufficient fraction of the radionuclide inventory to make this oxidative release of risk significance.	Rationale There appear to be only anecdotal accounts of fission product retention on the dislocations introduced by irradiation and no quantitative data on the adsorption isotherms	Closure Criterion:
	The issue becomes of less interest at elevated temperatures both because energetic sites anneal thermally and because the vapor pressures of important fission products become so high that there is no significant retention even on energetic sites	

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer: Chemical attack by air	Impact of SiC oxidation on temperature distribution through material
	Temperature distribution	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 6	Remedy: Fission product transport analyses will require a detailed prediction of the temperature distributions throughout the coated particle fuel.
Rationale: The oxidation of SiC is not iso-enthalpic so we know that the temperature distribution will be changed by chemical reaction. As noted elsewhere temperature distributions can affect both the volatility and the transport of fission products across a layer	Rationale: It should be possible to calculate the effect of oxidation on the temperature distributions across the layer since the heats of reaction are known for the bulk material and may be estimated when the involve the destruction of a radiation induced defect in the SiC lattice. It is necessary to have detailed knowledge of the reaction kinetics to do this calculation	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Inner PyC Layer Gas Phase Diffusion	Diffusion of gaseous fission products through layer (Knudsen and bulk diffusion through pore structure, and pressure driven permeation through structure)

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 6	Remedy: Any model of fission product transport within the fuel particle will have to include a gas phase mass transport model recognizing bulk gaseous diffusion, pressure driven flow and Knudsen diffusion
Rationale: Gas phase mass transport is the fastest mechanism to move fission products release from the fuel kernel across the barrier posed by the inner PyC layer	Rationale: Given the geometry and nature of the pore and crack network through the layer it should be possible to calculate the gas phase mass transport across the layer. We can estimate the gas phase diffusion coefficients for most of the dominant gaseous species. The diffusion process itself probably cannot be modeled as strictly Fickian diffusion. One will have develop a multicomponent diffusionmodel much like the membrane modesl that have been developed in the chemical engineering literature. It may be necessary to include in these models the effects of thermal diffusion especially since we will have low molecular weight species (CO MW=28) migrating along the same paths as the high molecular weight (>100) fission product vapor species. The importance of this will depend on the magnitude of the thermal gradients across the layer which surely must be significant given the relatively high conductivity and the need to move the decay heat away from the fuel kernel.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Inner PyC Layer Condensed phase diffusion)	Inter-grannular and/or intra-grannular solid-state diffusion

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	Level: 2	Remedy: Any model of fission product transport across the inner PyC layer will have to include the condensed phase mass transport process to account for mass transport of fission products when the layer does not have pore and crack networks to facilitate gas phase mass transport across the layer
Rationale: Fission products that are not volatile will be transported across the inner PyC layer by the condensed phase diffusion processes. Bulk diffusion is the slowest of these at low temperatures but it has the highest activation energy so it does eventually become the dominant process. Even if the metals have only small vapor pressures, gas phase mass transport of fission products may still be the dominant mechanism for mass transport	Rationale We do not have surface and grain boundary diffusion coefficients to model the mass transport of fission products across the layer at lower temperatures. These cannot be estimated or transferred from studies of analogous materials since they are notoriously sensitive to the precise grain structure and the nature of impurities at the grain boundaries. We don't even have a data set of bulk diffusion coefficients for the PyC layer of demonstrated reliability. The most complicated part of the modeling will be a realistic portrayal of the layer geometry and the pore and crack networks. It is tempting to model the layer as a spherical shell, but this Continued next column	Closure Criterion: (continued from previous column) is only justified if the deviations from spherical are not sufficient to provide a short circuit pathway in some regions. Similarly, it will be tempting to treat the layer as uniform in thickness though it never will really be. We do not have meaningful data on the pore and crack network. These networks may change if there is reaction with the intruding gases. We may not be able to derive useful descriptions of the pore and crack networks through the layer from microscopic examinations of these networks. Cracks and channels to small to be readily identified in microscopic analyses can be effective in the transport of material across the layer.
	At sufficiently high temperatures bulk diffusion will be the dominant condensed phase mass transport process This process is very sensitive to the presence of defects produced by irradiation acting as traps for diffusing species and we don't seem to have data on this.	

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Inner PyC Layer Pressure loading (Fission products)	Stress loading of the layer by fission products by increased pressure

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 2	Remedy to evaluate the pressure drop one would have to have some estimate of the permeability of the layer:
Rationale: Pressure loading will more likely be by CO pressure produced by the reaction of carbon with the fuel kernel. The loading will probably be on the SiC layer rather than the inner PyC layer though it is possible that there will be some pressure drop across the layer	Rationale: We need permeability data that seem not to exist to estimate the pressure drop across the layer. If this is significant then the layer can act at least temporarily as a barrier to fission product transport. But, if the pressure drop is significant then the layer is likely to rupture and completely lose its effectiveness as a barrier as the accident progresses and additional pressurization from both CO build up and fission product release occurs	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Inner PyC Layer Pressure loading (Carbon monoxide)	Stress loading of the layer by carbon monoxide by increased pressure

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 2	Remedy:no remedy needed
Rationale:The loading by CO should dominate that by fission products. Still it is not evident that the layer will have a substantial pressure retaining capability and the SiC layer is a more important layer for this.	Rationale: We need permeability data that seem not to exist to estimate the pressure drop across the layer. If this is significant then the layer can act at least temporarily as a barrier to fission product transport. But, if the pressure drop is significant then the layer is likely to rupture and completely lose its effectiveness as a barrier as the accident progresses and additional pressurization from both CO build up and fission product release occurs)	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Inner PyC Layer Layer oxidation	Reaction of pyrolytic graphite with oxygen released from the kernel

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 2	Remedy: Analysis of fission product transport will have to treat the effects of oxidants and ascertain if oxidants can reach the inner PyC layer. If so, the possibility of preferential and even catalyzed oxidation of the layer will have to be considered. Decent data sets on the reactions of the specific materials with oxidants are really needed.
Rationale: This high importance is assigned under the presumption that oxidant can reach the layer. The oxidant that comes is more likely to be from the fuel kernel than from the gases intruding in the accident scenario. Intruding gases will have to pass over an awful lot of reactive material before they can reach the inner PyC layer. On the other hand oxidant from the fuel will have to pass through a buffer layer of carbon to reach the inner PyC layer. If the oxidant reaches the material it can cause thinning of the layer (probably not especially important) or opening of the pathways for gas phase mass transport of fission products making the transport by gas phase processes even more rapid.	Rationale: The layer really does not take up oxidant. It reacts to form CO (and other equivalent species such as C2O and C2O3) that vaporize. The reactions are enormously sensitive to catalysis and fission products can act as catalysts. We don't have a lot of data on which fission products will produce catalysis, We do know that Cs can catalyze the oxidation of C. We also know that irradiation makes the material more reactive. More than just rate of reaction data for the specific material, we need to know if the reaction takes place uniformly over the surface or if there is preferential reaction especially to open pathways for the gas phase transport of fission products across the layer	Closure Criterion:
	same as above though catalysis is not an issue at very high temperatures where the oxidation reaction are rapid	

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Inner PyC Layer Stress state (compression/tension)	The state of the forces induced by external forces that are acting across the layer to resist movement

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 2	Remedy: Models or data to predict rupture of the layer are needed. These models may be nothing more than criteria identifying conditions for which layer integrity can no longer be assured.
Rationale: It is known that stress state can affect both condensed phase and gas phase diffusion across a layer, but this is a pretty subtle effect. More important is whether the layer stays in tact or is ruptured and allows essentially unimpeded gas phase mass transport across the layer, but this is treated in other questions	Rationale:We don't really know much about the forces and especially forces induced by the radiation caused growth of materials	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Inner PyC Layer Cracking	Lengths, widths and numbers of cracks produced in layer during accident

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 1	Remedy: Any model of the fission product transport across the inner PyC layer will have to admit to the possibility of cracks – perhaps quite narrow cracks – developing in the layer from radiation-induced growth or thermal expansion or mechanical forces on the layer including pressurization examined above.
Rationale:Any cracking of the layer will create effective pathways for gas phase mass transport across the layer	Rationale: We are not really in the position to predict cracking of the layer. Though there are data in abundance for PyC they are not for the specific material in the fuel particle and not for the material subjected to thermal transients and irradiation of the type that will be seen by the PyC layer	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Inner PyC Layer Intercalation	Trapping of species between sheets of the graphite structure

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	Level: 2	Remedy: WE need some sort of data or analyses to show whether intercalation will be an effective holdup mechanism for fission product release.
Rationale: Intercalation could act as a holdup mechanism for fission products. Intercalation usually occurs during the simultaneous condensation of vapors and graphitic material. Intercalation could occur because of the radiation displacements of materials. Intercalation is known to be an effective way to trap potassium in graphite and so it might be effective in trapping Cs in the graphite. Still, it is not evident that so much of the radionulcide inventory can be trapped in the layer that this is risk-significant issue	Rationale: I have no data on intercalation as a dynamic process either during an accident or during fuel operations Intercalation will reverse at very high temperatures and not be an issue	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Inner PyC Layer: Chemical attack by air Kinetics	Rate of reaction per unit surface area as a function of temperature and partial pressure of air

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 5	Remedy: kinetic data on both the reactions of oxygen and the reactions of nitrogen with the specific material of the inner PyC layer will be needed. As important as the spedific reaction kinetics – which may be just mass transport limitations for this particular case – will be information on the nature of the attack and in particular whether the attack is uniform or is localized so that it enhances the pathways available for gas phase mass transport through the layer.
Rationale: A rating of « high » is given to this issue under the assumption that it is conditional upon oxidant actually getting to the Inner PyC layer after having passed over and through a lot of reactive material. Though it is possible for the oxidant to do this, it may not be especially likely. IF, indeed. oxidant reaches the PyC surface it can react exothermically – thereby increasing the driving force for fission product vaporization – reactions will remove layer material and facilitate transport of fission products across the layer – and it will affect the volatility of the fission products – accentuating the vapor pressures of some fission products and reducing the vapor pressures of others.	Rationale: There is quite a lot of information about the interactions of air with carbon analogous to the carbon that makes up the inner PyC layer though none, apparently, for the specific material. At low temperatures the attack on carbon can be localized rather than uniform. The reactions can be catalyzed. There is much less information of the reactions of nitrogen from air that has been depleted of its oxygen by reactions prior to reaching the inner PyC layer. Certainly, one can hypothesize the reactions of nitrogen to form cyanogens and this would certainly affect temperatures in the particle, remove material from the layer and affect the volatility of radionuclides through the formation of vapor phase cyanides which could be viewed as pseudo halides Continued next column	Closure Criterion: (continued from previous column) The situation at higher temperatures is much the same as above though the potential for reaction of the layer with nitrogen increases. Also, at higher temperatures the reactions should become more homogeneous so that they work primarily to thinning the layer rather than to enhancing the facility of gas phase mass transport across the layer.

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Inner PyC Layer: Chemical attack by air Catalysis	Modification of the reaction rate by fission products or impurities

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 3	Remedy: Models of graphit oxidation will have to account for catalysis and a more comprehensive base of data on catalytic agents will have to become available
Rationale: there is information suggesting that the rates of reaction of oxidant with graphite can be catalyzed and this catalysis can lead to preferential attack on the layer – perhaps enhancing gas phase mass transport across the layer	Rationale: It is known that some materials such as Cs and Fe will catalyze the oxidation of carbon. The effects of these catalytic materials or the catalytic effectiveness of other fission products on the reactions of the specific material are not reported in literature that I have seen.	Closure Criterion:
	Catalysis is less of an issue at higher temperatures where the reactions rates are inherently more rapid – eventually becoming limited only by the availability of oxidant. It is not that we know more about catalytic reactions at high temperature, it is that we need to know less that leads to relative scoring of the two temperature regimes.	

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Inner PyC Layer: Chemical attack by air Changes in chemical form of fission products	Changes in chemical form resulting from oxidizing or reducing fission products

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 5	Remedy:The data bases used to calculate fission product speciation need to be reliable or at least known. Codification of the data base to be used for NRC would be beneficial. There also needs to be an examination of the literature and even molecular calculations concerning the likely importance of vapor phase nitrides and cyanides.
Rationale: It is well established that the ambient oxygen potential can strongly affect the volatility of many fission products – enhancing the vapor pressures of some such as Ru, Mo and Te, and depressing the vapor pressure of others such as Ba, Sr, Ce, and La. Of additional interest for this particular location is the enhancement of the vapor pressures of fission products caused by an ambient partial pressure of nitrogen or the products of nitrogen reactions with carbon.	Rationale: We have the technical capability to assess the effects of oxygen potential on the vapor pressures of fission products as long as we confine or interest to oxides and elemental forms of the fission products. We don t have much of a data base to assess the effect of nitride formation and the formation of pseudo halides like cyanides on the vapor pressures of fission products. Modern methods of molecular orbital calculations have advanced to the point that it ought to be possible to explore computationally for stable species of these types that have not been systematically investigated experimentally	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Inner PyC Layer: Chemical attack by air	Changes in diffusivity, porosity, adsorptivity, etc.
	Changes in graphite properties	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 1	Remedy:Models of PyC layer oxidation will have to recognize the possibility of localized attack that increases the porosity or permeability of the material. Mechanistic models or even bounding models of mass transport across the inner PyC layer will have to recognize that the porosity and permeability of the material is time dependent when there is oxidation taking place.
Rationale: Again given that oxidant can reach the inner PyC layer this is a high importance issue especially at low temperatures. Oxidant does not attack carbon homogenously. There is preferential attack at energetic sites and the concentrations of energetic sites are points where catalysts reside and in cracks and pores. Attack on surfaces in cracks and pores will enhance vapor phase mass transport of fission products across the layer.	Rationale: There appears to be little information on the localized attack on PyC by oxidants and its effects on the effective permeability of the material to gases	Closure Criterion:
	Localized attack becomes less important at elevated temperatures where reactions become faster.	

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Inner PyC Layer: Chemical attack by air	Release of graphite FP inventory
	Holdup reversal	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 2	Remedy: no remedy needed
Rationale: It is known that fission products can adsorb on energetic sites in graphite. It is also known that chemical reactions with these sites can release the adsorbed material. What is not evident is whether the adsorption of fission products on energetic sites in the inner PyC layer can involve sufficient amounts of fission products to be risk significant.	Rationale: We don't have information for quantifying the holdup of fission products on the energetic sites created by irradiation or by cracking in the inner PyC layer. What holdup does occur will be reversed at the rate of oxidation reaction.	Closure Criterion:
	Holdup by adsorption is much less important at high temperatures because the vapor pressures of the interesting fission products are so high.	

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Inner PyC Layer: Chemical attack by air Temperature distribution	Impact of graphite oxidation on temperature distribution through material

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 3	RemedyAny fission product ttransport model will require goo, local temperature descriptions including the effects of chemical reactions on these temperatures
Rationale: If oxidant can get to the inner PyC layer, its reactions will be exothermic and will affect temperature distributions. As noted above these temperature distributions affect both the volatilities of the fission products and their transport across the layer	Rationale: We know enough in principle to calculate the effects of chemical reactions on the temperature distributions if we know the kinetics of reaction. Certainly we know the heats of reaction with pristine material and these heats need to modified to account for the additional energy coming from the reaction of defects introduced by irradiation. A key to the calculation of temperature distributions is the thermal conductivity of the porous, defected and possibly cracked material.	Closure Criterion:
	The situation at higher temperatures is much the same as above except radiation heat transfer becomes more of an issue and the ambient atmosphere of CO will participate in the radiation heat transfer.	

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Buffer Layer Gas phase diffusion	Diffusion of gaseous fission products through layer (Knudsen and bulk diffusion through pore structure, and pressure driven permeation through structure)

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 4	Remedy a fairly sophisticated model of the layer porosity will be needed as will a very sophisticated model of mass transport across the layer:
Rationale: Gas phase mass transport across this layer will be the dominant transport mechanism for volatile fission products because the temperatures are high and because the material is quite porous.	Rationale Given the nature of the porosity in the layer it should be possible to calculate the gas phase mass transport quite well. We can estimate the diffusion coefficients for most vapor species. The analysis probably cannot treat the diffusion as Fickian. A multicomponent model will have to be considered because there will be a flow of CO across the layer that may be, in fact, pressure driven rather than diffusion. Diffusion may have to be augmented by consideration of thermal diffusion because of the large temperature gradient and the mixture of molecular weights of the gaseous species. Other complexities in the analysis include lack of spherical symmetry of the layer and the variations in the layer thickness	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Buffer Layer Condensed phase diffusion	Inter-grannular diffusion and/or intra-grannular solid-state diffusion

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 1	Remedy:no remedy needed
Rationale: Fission products that reach the interface between the buffer carbon and the fuel kernel will have all escaped the kernel as some sort of a vapor species through the interconnected pore network in the urania. (The flux of fission products from the fuel via intragrannular diffusion is really quite small at temperatures that are well below the urania melting point) It does not seem likely that significant transport of even species with very modest vapor pressures would switch to a condensed phase process upon encountering the highly porous buffer region.	Rationale: Don't have definitive condensed phase diffusion coefficients for the material Condensed phase mass transport rather than vapor phase mass transport is even less likely to be dominant at higher temperatures and the condensed phase diffusion coefficients are even less known at elevated temperatures	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Buffer Layer Response to kernel swelling	Mechanical reaction of the layer to the growth of the kernel via swelling

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	Level: 4	Remedy:Because integrity of the layer is not critical, it may not be necessary to develop a very detailed understanding of the mechanical properties of the buffer layer. It may not even be present in future incarnations of coated particle fuel pellets
Rationale: cracking and otherwise opening pathways for gas phase mass transport as a result of mechanical interactions could facilitate fission product transport across the buffer region, but the region is already quite porous so the incremental effects of cracking on gas phase mass transport are not likely to be as dramatic as cracking of the more compact structural barriers in the coated particle fuel.	RationaleWe have been shown some evidence that in the current inadequate fuels mechanical interactions can rupture the buffer layer. We have not been shown any indication that this process can be predicted in a quantitative way. There are data on the mechanical properties of materials analogous to materials in the buffer region, but these data may not be applicable to the thin layer that can bond to either the kernel or to the bounding PyC layer	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Buffer Layer Maximum fuel gaseous fission product uptake	Maximum loading of fission products that can deposit from the gas phase onto surfaces of materials surrounding the fuel kernel

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 3	Remedy no remedy needed:
Rationale: It is likely that some fission products will deposit in the buffer region at least temporarily and this effect has to be considered in developing the modeling of the fission product transport. But it does not appear likely that the fraction of the released fission product inventory that can deposit in this region will be sufficiently large to be of risk significance	Rationale We know deposition can take place. We don't have quantitative information on the density of active sites for deposition or adsorption desorption isotherms for the fission products	Closure Criterion:
	Adsorption on active sites become even less important at elevated temperatures first because the vapor pressures at such elevated temperatures are so high and second because at elevated temperatures active adsorption sites are being thermally annealed. So it is not that we know more about the situation at high temperatures, it is that relatively we need to know less.	

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Buffer Layer Layer oxidation	Reaction of pyrolytic graphite with oxygen released from the kernel

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 2	Remedy Easily one of the most important characteristics to understand for coated particle fuels is the reaction of carbon with the urania fuel. This may well be a heterogeneous reaction of gas phase oxidant with carbon. It may also involve a homogeneous direct reaction of two solid materials especially under conditions of irradiation. The reaction will be dependent on the ambient CO pressure. In fact leakage of the CO from the coated particle fuel may well dictate the extent of reaction
Rationale: The 'uptake' is really the reaction of oxygen from the fuel reacting with carbon in the buffer layer to form CO that pressurizes and possibly ruptures the compact barriers with the fuel particle such as the PyC layer and the SiC layer. Rupture of these layers will allow the venting of the vapor phase fission products within the particle and provide a facile pathway for the gas phase mass transport of fission products out of the fuel particle as the accident progresses. The reaction could also damage the crystal structure of urania at the surface of the kernel – converting it into UCO and eventually UCx. The crystallographic changes are sufficiently large that fission products within grains of the surface fuel will be expelled and ready to vaporize without mass transport limitations that affect release of fission products from grain surfaces within the fuel kernel.	Rationale Reactions of carbon with urania are thermodynamically possible at sufficiently low CO partial pressures even at low temperatures. They do appear to be slow. Irradiation of the carbon may create energetic sites that are more reactive than might be expected based on tests with unirradiated materials. Still the empirical evidence is that the reactions are slow in absence of some sort of catalyst. Always a concern is that the fission product species may act as catalysts under circumstances not so far encountered in the studies of coated particle fuels Reactions of carbon with urania definitely occur at more elevated temperatures. I am not aware of definitive rate data for the reactions	Closure Criterion:

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Buffer Layer Thermal gradient	Change in temperature with distance

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 4	Remedy: Modeling of fission product transport in the coated particle fuels will require that there be a detailed model of the local temperatures and temperature gradients. To do this for the buffer layer will first require that the porosity of the layer be characterized and then some heat transfer modeling be done to develop expressions for the thermal conductivity of the material.
Rationale: Thermal gradients across the buffer layer – which could be substantial in magnitude – will affect the fission product release both by chemical diffusion of vapors and by thermal diffusion of vapors	Rationale: In principle we can calculate the mass transport across the layers given the temperature distributions. Calculations of the thermal distributions are made complicated by the poor knowledge of the material thermal conductivity and the effects of radiation defects and pores or cracks on the thermal conductivity. It is unlikely that simple corrections of material thermal conductivity using things like the Loeb correction will be adequate since the layer is so thin the bulk averaging inherent in the Loeb correction and similar corrections simply will underestimate the effects of porosity. Something much more sophisticated will have to be done. The situation is largely the same at elevated temperatures except that radiation heat transfer within the layer becomes more of an issue. It is not simple to calculate because the ambient CO cannot be taken as transparent to the radiation.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Buffer Layer Irradiation and thermal shrinkage of buffer	Dimension changes in the buffer layer or changes in its porosity produced by irradiation or by exposure to elevated temperatures

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 5	Remedy: The only real issue that must be borne in mind is whether the dimensional changes are sufficient to cause rupture and then this is of concern only if holdup of fission products in the buffer layer is actually credited in the transport process.
Rationale: The effects are small enough that they will probably be safely neglected in the modeling of fission product transport. Of course, if the changes open pathways for gas phase mass transport of fission products they facilitate this transport as discussed above.	Rationale: We know that the buffer layer material will grow as a result of radiation-induced defects in the material. Thermal expansion during accident transients will affect the material. While w e don't have data for the specific material, we do have data for analogous materials	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Buffer Layer: Chemical attack by air Kinetics	Rate of reaction per unit surface area as a function of temperature and partial pressure of air

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 2	Remedy: no remedy really needed.
Rationale: It really begins to stretch the imagination of how oxidant intruding from outside the core could penetrate to the buffer layer rather than react with other carbon materials along the pathway. Besides, if oxidant is this far it has reached the fuel kernel and the game is up. Oxidation of fuel will initiate massive release of fission products. It does not seem useful to give great attention to the oxidation of the buffer layer from external gases. The more important issue is reaction of the buffer with oxygen from the fuel kernel and this has been discussed above.	Rationale Detailed reaction kinetic data for the specific material are not available and probably are not really needed. If models are really needed it may be adequate to assume reaction proceeds at the rate of mass transport of oxidant to the buffer region which cannot be very fast even if the other parts of the fuel particle have been completely ruptured.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Buffer Layer: Chemical attack by air Catalysis	Modification of the reaction rate by fission products or impurities

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 4	Remedy no remedy needed:
Rationale: See discussion above. The reactions just are not likely to be important for this layer	Rationale: reactions of carbon with oxidants are catalyzed and fission products can be catalysts. This may more important for oxidants coming from the fuel kernel rather than intruding oxidants like air and water vapor.	Closure Criterion:
	Catalysis is just less important at very high temperatures where the rates of reactions especially of gases are intrinsically high.	

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Buffer Layer: Chemical attack by air	Changes in chemical form resulting from oxidizing or reducing fission products
	Changes in chemical form of fission products	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue ***Closure Criteria***
Rank: L	Level: 6	Remedy: no remedy needed
Rationale: oxidant intrusion to this depth in the coated particle fuel structure is hard to believe. If it does occur the higher oxidant partial pressures will affect the speciation and consequently the vapor pressures of the fission products – enhancing some and depressing others.	Rationale: As discussed above for other layers there is some technical basis for at least estimating the effects of oxidants on the speciation and consequently the vapor pressures of fission products	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Buffer Layer: Chemical attack by air	Changes in diffusivity, porosity, adsorptivity, etc.
	Changes in graphite properties	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 3	Remedy: no remedy needed
Rationale: again, it just is not apparent that oxidant is likely to intrude to the buffer layers	Rationale: see discussions above for the effects of oxidants on pathways for gas phase mass transport. Even if oxidant gets to this point and does react preferentially in local areas, the incremental effect on the facility of gas phase mass transport across the layer is likely to be very much less than it is for localized reactions in other layers that are more compact and less porous.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Buffer Layer: Chemical attack by air	Release of graphite FP inventory
	Holdup reversal	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 2	Remedy: no remedy needed
Rationale: Again, we just don't believe for most accident sequences that oxidant will penetrate to the buffer layer and if it does little details like the release of holdup inventory in the layer will hardly matter.	Rationale: Don't know the concentrations of the active sites for adsorption nor do we know the adsorption/desorption isotherms for the material with the radiation induced sites. It is not apparent however that in any case the fractional holdup could be risk significant.	Closure Criterion:
	There is likely to be little to release since active sites will thermally anneal at elevated temperatures and vapor pressures are so high that adsorption on defects that remain may be small.	

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Buffer Layer: Chemical attack by air	Impact of graphite oxidation on temperature distribution through material
	Temperature distribution	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	Level: 4	Remedy: Any modeling of fission product transport in the coated particle fuel will require a detailed model of the temperature distributions in the layers including the buffer layer.
Rationale: As noted above, it is unlikely that oxidant will penetrate to the buffer layer itself and so chemical reactions of oxidant with this layer will not distort temperature distributions. But to some small extent the temperature distributions in the buffer layer will be affected by the chemical reactions of intruding oxidant with other layers. The effect is not likely to be large since the buffer layer thermal conductivity will not be huge.	Rationale: The pertinent knowledge bases are those discussed in connection with reactions of other layers and the modeling of thermal conductivity in the buffer layer.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Kernel Maximum fuel temperature	Maximum fuel temperature attained by the fuel kernel during the accident

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 6	Remedy:
Rationale: Temperature is well known to be one of the dominant variables controlling the release of fission products form urania kernels	Rationale: In principle, it should be possible to calculate the maximum kernel temperature fairly accurately. Even so, errors on the order of 50 degrees are possible. Definitive, defensible calculations for credible accidents have not yet appeared.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Kernel Temperature vs. time transient conditions	The time-dependent variation of fuel temperature with time

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 4	Remedy:
Rationale: Fission product release is a strong function of both time and temperature	Rationale: Though fairly reliable temperature histories are in principle possible to predict defensible calculations have not yet been produced. Most existing calculations are hopelessly optimistic about heat loss pathways.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Kernel Energy Transport: Conduction within kernel	Flow of heat within a medium from a region of high temperature to a region of low temperature

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	Level: 3	Remedy:
Rationale: Conduction as well as decay heat generation determine the temperature history of the kernel during the event	Rationale: Conduction in moderately porous urania is known with some accuracy. But, the porosity of the urania kernels can become heroic during extended operations and the events of the accident could easily produce porosities and configurations of the kernels that are quite intractable for conduction calculations.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Kernel Thermodynamic state of fission products	Chemical and physical state of fission products

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 5	Remedy:
Rationale: Fission product release depends on the chemical activity of the fission products. Completely diluted in the urania matrix, the fission product activities could be quite low. But, when the segregate into separate phases such as uranate phases or metallic nodules, chemical activities can be driven up substantially – orders of magnitude.	Rationale: We have a useful understanding of chemical activities of fission products in urania fuel at moderate burnups. At the higher burnups expected for some gas reactor fuels, our knowledge and predictive capabilities begin to fail us	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Kernel Oxygen flux	Mass transport of oxygen per unit surface area per unit time

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	Level: 3	Remedy:
Rationale: Diffusion of fission products will occur simultaneously with the diffusion of oxygen from the kernels to the reactive graphite at the buffer-kernel interface. The release is far more a multicomponent process than we have encountered in the case of fission product release from conventional fuels. The gettering of oxygen by reaction with the carbon is not passivating as is the case with gettering of oxygen by reaction with zirconium in the case of conventional fuels. It is not evident, then, that the usual Fickian diffusion approximation can be made incaustiously to predict release from the kernels	Rationale: Release analysis recognizing the multicomponent nature of the transport within fuel grains have not been published. In multicomponent systems remarkable things can be predicted that appear counter-intuitive when viewed within the context of binary diffusion.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Kernel Grain growth	Enlargement of grains as a result of diffusion

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 8	Remedy:
Rationale: Grain growth is largely unimportant because of the grain boundary pinning effects of fission products and especially separated phases of fission products	Rationale: It has not been essential to consider grain growth in models of fission product release from conventional reactor fuels, though some codes include such models.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Kernel Buffer carbon-kernel interaction	Chemical reaction between carbon and the fuel (UO2 or UOC) to form UC2 and CO (gas)

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: II	Level: 3	Remedy:
Rationale: The reaction of the buffer with the kernel can be responsible for the pressurization perhaps to failure of the SiC layer. The reaction can also lead to fission product release as the reactive refinement of the urania progresses	Rationale: Details of the reaction process and even the phase relations in these systems are not known well.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Kernel: Chemical attack by air Kinetics	Rate of reaction per unit surface area as a function of temperature and partial pressure of air

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 9	Remedy:
Rationale: Air attack on the kernel would produce catastrophic release of fission products. But, if the fuel particle was so damaged that air could reach the kernel, there would have already have been catastrophic release of fission products	Rationale: We have a growing knowledge of fission product release from fuel exposed to air. We also know that carbon will react with air well before it is possible for the air to reach the kernel.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Kernel: Chemical attack by air Catalysis	Modification of the reaction rate by fission products or impurities

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 1	Remedy:
Rationale: Air attack is unimportant and there is not a lot of evidence that air attack on urania is catalyzed	Rationale: Not aware of information on catalysis of air attack on urania at temperatures that would lead to extensive fission product release	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Kernel: Chemical attack by air Changes in chemical form of fission products	Changes in chemical form resulting from oxidizing or reducing fission products

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 5	Remedy:
Rationale: Should air reach the fuel, it can cause changes to the volatility of fission products by changes in the chemical forms of these fission products. It is just not obvious that air will reach the kernels and if air does reach the kernels, core damage may be so extensive there will be few fission products left that can react with the air.	Rationale We certainly know of possible changes to the chemical forms of fission products exposed to air.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Kernel: Chemical attack by air Changes in kernel properties	Changes in diffusivity, porosity, adsorptivity, etc.

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 8	Remedy:
Rationale: The changes in the thermophysical properties of urania when it is exposed to air are quite significant. But, as noted above, such changes are not likely to be of importance either because air cannot get to the urania or because the fission products have already been released once the air arrives.	Rationale: Huge amounts of information about the changes to urania exposed to air exist.	Closure Criterion:

Additional Discussion

APPENDIX G
AIR INGRESS STUDY

G.1 Background

As part of the PIRT process, the NRC panel members felt that calculations of the postulated air ingress event were needed to better inform the panel members about the potential conditions that fuel pebbles experience in a postulated air ingress event. A MELCOR model has been under development for the past few years at the INEEL to scope out the important phenomena related to air ingress events in a pebble bed reactor. These results were presented recently at a gas reactor conference [G-1]. The results showed that a significant amount of the pebble bed core would not be exposed to air. The factors, which contributed to this calculated result, include the large flow resistance between the postulated breach location and the core, the extended time for natural convection to begin, the limited oxygen available in the reactor containment, and the large amount of lower reflector graphite available for oxidation, which acts as a sink for any oxygen in the air.

The MELCOR model has been improved and now includes the effect of neutron fast fluence on the thermal conductivity of the pebble bed core and detailed modeling of the region between the reactor pressure vessel (RPV) and reactor cavity cooling system (RCCS). As a result, the analyses conducted for the PIRT panel are different than earlier scoping results. Calculations were performed for alternate scenarios that could result in varying amounts of air entering the active region of the core to determine what conditions the fuel could hypothetically experience in this event. The calculations are not intended to be a best estimate calculation of such an events in a PBR. The calculation are intended to provide realistically conservative basis for understanding the accident condition and identifying the important phenomena that could affect fuel performance and fission product transport. The calculations also aid in the understanding of the potential interactions between the system thermal hydraulics, core thermal response and oxidation behavior under a wide range of scenarios. The following eight cases were analyzed:

- Case 1: Base case.
- Case 2: Reduced effective thermal conductivity of the pebble bed core
- Case 3: Significant leak in the upper head of the reactor vessel (to investigate its effects on early initiation of natural convection in the vessel).
- Case 4: Reduction in the flow resistance in the core by a factor of 10 (to investigate increased air flow into the core).
- Case 5: No structural graphite oxidation in the lower reflector region (to maximized unreacted air in the active core region).
- Case 6: Thermal conductivity of the side reflector reduced by 50% (to investigate the effects of higher core temperature on core oxidation).
- Case 7: Infinite containment volume (to investigate ultimate unmitigated long term behavior).
- Case 8: A combination of all seven previous cases as the most conservative case.

G.2 Introduction

A MELCOR model of a reference pebble-bed reactor (PBR) was developed to explore the environmental conditions for oxidation in the PBR core in the event that fuel elements and graphite core structural components are exposed to air due to a catastrophic break in the cross flow duct connecting the reactor pressure vessel (RPV) with the power conversion systems vessel. The break is assumed to occur outside of the reactor vessel between the RPV and the high-pressure turbine. The MELCOR model presented in this appendix is sufficiently representative of PBR designs to scope out environmental conditions in the core during an air ingress accident.

The MELCOR [G-2] code used for this analyses is a severe accident code being developed at Sandia National Laboratory for the U. S. Nuclear Regulatory Commission to model the progression of severe accidents in light-water nuclear power plants. The modeling approach used by MELCOR, like other thermo-hydraulic codes, is based on the use of control volumes, heat structures, control functions and material property tables to build system models. Because of the general and flexible nature of the code, other concepts such as the pebble-bed reactor can be modeled with some simple modifications to the code. The latest released version of MELCOR is 1.8.5; however, for the analysis presented in this report a modification of the earlier 1.8.2 version of the code was used. The modifications to MELCOR 1.8.2 were the implementation of multi-fluid capabilities, a graphite oxidation model, and a simple molecular diffusion model. The multi-fluid capabilities allow MELCOR to use fluids other than water, such as helium, as the primary coolant for low Mach number flows (gases that can be treated as an incompressible fluid). This capability is documented in Reference [G-3]. The capability to analyze the oxidation of graphite structures was also added to MELCOR and will be discussed later in this appendix as will the molecular diffusion model.

G.3 PBR MELCOR Model

The PBR reactor considered for this study was assumed to have a core diameter of 3.5 m and a height of 8.0 m, yielding a total core volume of 76.97 m^2. The active core of the reactor was divided into three radial zones and eight axial zones for a total of 24 core control volumes, as shown in Figure G-1. The inner radial zone consists of 8 control volumes representing the inner reflector region (non heat generating). The remaining 16 core control volumes represent the active core. The core control volumes are cylindrical and are centered about the core centerline. The inner radial zone (inner reflector) contains 72,247 non-heated pebbles[1]. The two outer radial zones contain a total of 342,944 heat-generating pebbles producing a total of 270 MW of thermal energy. The pertinent dimensions for this model are given in Table G-1.

For nominal operating conditions the coolant enters the bottom of the reactor (CV111) at ≈ 450°C (723 K) and flows up an annular flow channel located between the reactor side reflector and the core barrel. Control volumes 101 through 110, and 211, 212, 213 as shown in Figure G-1 represent this flow channel. The coolant then flows radially along the top of the

[1] The most recent core design for the PBMR involves a fixed cylindrical graphite central column rather than moving solid graphite (unfueled) pebbles

reactor (CV 100), exiting into a small plenum located just above the core, represented by control volumes 25, 26, and 27.

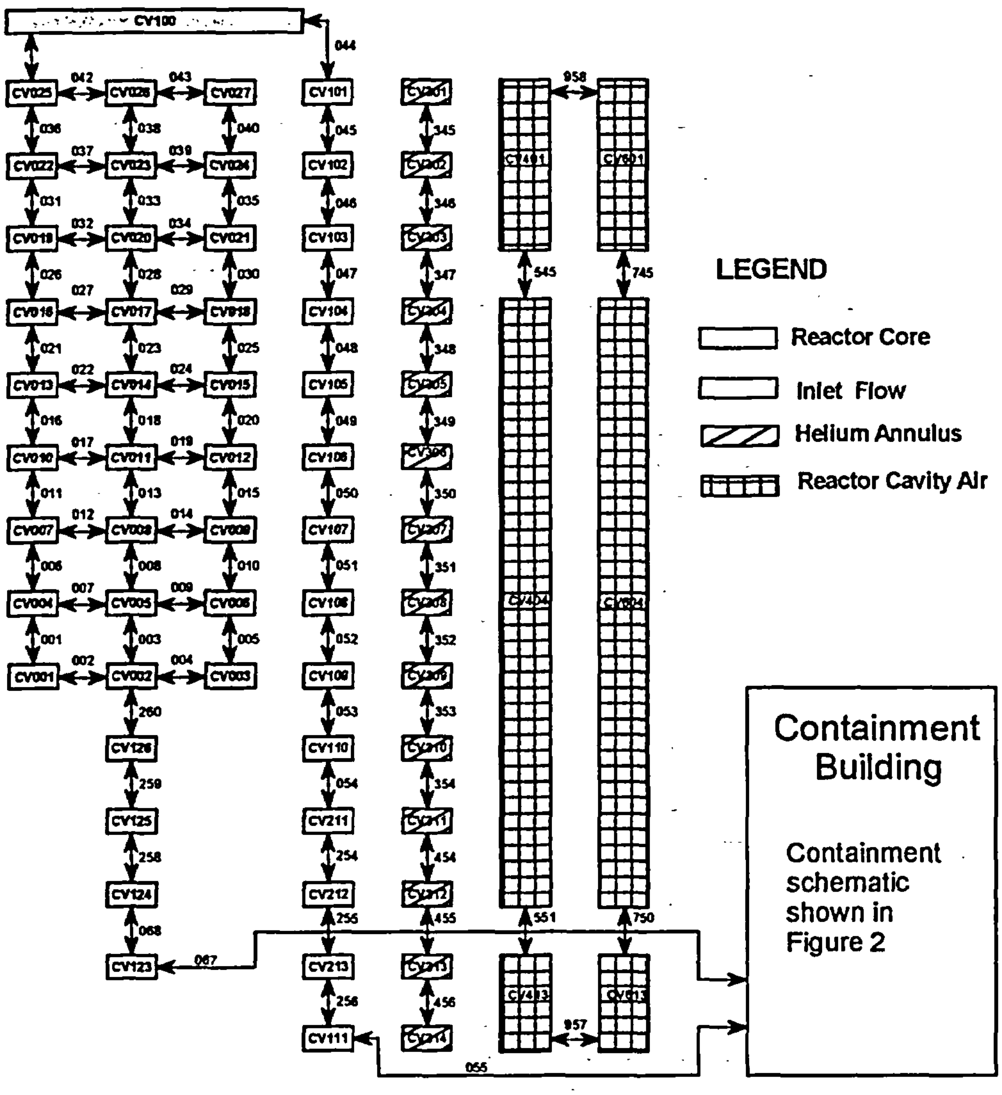


Figure G-1 PBR control volume diagram

From the plenum the coolant flows down through the core and exits the bottom of the core (CV126) at 850°C (1123 K). The coolant then flows down through the lower support structure (CVs 126, 125, 124, and 123) to the power conversion unit, which is represented simplistically by control volumes 112 through 122 (refer to Figure G-2). The double-ended rupture of both the inlet and outlet pipes as shown in Figure G-2 occurs in control volumes 112 and 122. The pipe break is represented in the model as two valves, which are connected to containment volumes 500 and 501 (not shown in figure) and are opened at the beginning of the loss of coolant accident (LOCA). This accident is sometimes referred to as a depressurized conduction cool down event.

For the base case model and all models used in the sensitivity study unless noted, the containment volume is assumed to be 27,000 m^3. This value was estimated from preliminary drawings of the containment region, thus the actual containment volume might be smaller. The large containment volume allows more oxygen to be available for oxidation of the core graphite.

Table G-1 Summary of Basic Modeling Parameters for Air Ingress Sensitivity Study

Parameters	PBR Base Case	Units
Thermal Power	270.0	MW
Core coolant inlet temperature	450.0	°C
Core coolant outlet temperature	850.0	°C
Outer radius of inner flow zone [inner reflector]	0.73	m
Outer radius of middle flow zone	1.21	m
Outer radius of outer flow zone	1.75	m
Outer radius of radial reflector	2.50	m
Outer radius of inlet coolant channel	2.80	m
Outer radius of core barrel	2.83	m
Outer radius of gas annulus	2.90	m
Outer radius of pressure vessel	3.00	m
Inner radius of reactor cavity cooling system	4.27	m
Height of HS 124, 111, 714, 314, 414	1.20	m
Height of HS 223, 210, 713, 313, 413	0.80	m
Height of HS 224, 211, 712, 312, 412	0.50	m
Height of HS 225, 212, 711, 311, 411	0.50	m
Height of HS 226, 213, 710, 310, 410	0.50	m
Height of CV 01, 02, 03	0.06	m
Height of CV 04, 05, 06	0.06	m
Height of CV 07, 08, 09	0.18	m
Height of CV 10, 11, 12	0.18	m
Height of CV 13, 14, 15	0.36	m
Height of CV 16, 17, 18	2.39	m
Height of CV 19, 20, 21	2.39	m
Height of CV 22, 23, 24	2.39	m
Height of CV 25, 26, 27	0.50	m
Number of non-fuel pebbles in reactor (inner reflector)	72247	-
Number of fuel pebbles in reactor	342944	-
Active height of core	8.00	m
Total volume of core	76.97	m^3
Active core volume	63.57	m^3
Core mean power density	5.51	MW/m^3
Core mass flow rate (steady state)	131.00	kg/sec

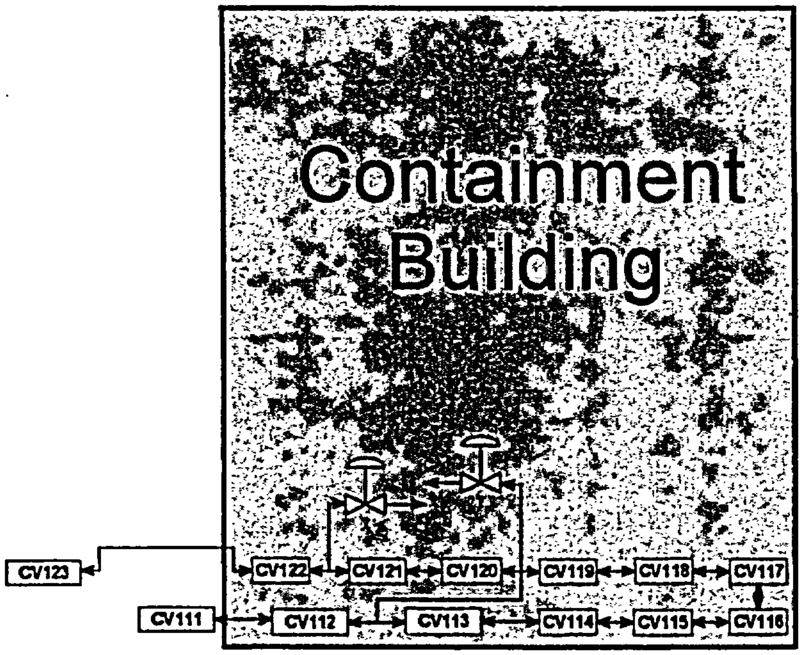


Figure G-2 PBR control volume diagram continued

The heat transfer from the pebbles is dominated by convection during normal operation. However, for the LOCA when the forced circulation flow in the core decreases to zero, the decay heat generated by the pebbles is removed primary by radial conduction and radiation to the graphite reflector, which surrounds the core. The heat is then conducted through the reflector, radiated and conducted to the primary reactor vessel (RPV) wall, conducted through the vessel wall, and is finally convected and radiated to the reactor cavity cooling system (RCCS), which for the purposes of this study was modeled as a 27°C (300 K) heat sink.

The reactor pebbles, and core structures such as the top, bottom, and side graphite reflectors, core barrel, reactor pressure vessel, and lower graphite support structures are modeled using the MELCOR heat structure package. The heat structure package calculates one-dimensional heat conduction through a solid structure and the energy transferred across its boundary surfaces into surrounding control volumes. Each heat structure has two boundary surfaces and a boundary condition must be specified for each surface. One of six different boundary condition can be specified depending on the modeling assumptions used at the boundary. For most of the surfaces in the model the heat transfer package calculates a convective heat transfer coefficient based on the flow conditions in the adjacent control volume and the geometry of the heat structure. Most of the heat structures used in the model are shown in Figure G-3 and are represented in the figure as rectangular boxes. An identifier beginning with the prefix HS denotes each heat structure. Each heat structure is coupled to at least one or two control volumes, which are identified on the figure as numbers in parentheses with the top number identifying the control volume located on the inside of the heat structure and the number on the bottom identifying the control volume on the outside of the heat structure. The wire like coupling between the heat structures represent radiation and conduction paths and are defined by control functions which will be discussed below.

The pebbles in the core are modeled as spherical heat structures, one heat structure per control volume. The convective heat transfer from one pebble is then multiplied by the number of pebbles in the control volume to get the overall convective heat transfer from all the pebbles in the volume to the fluid.

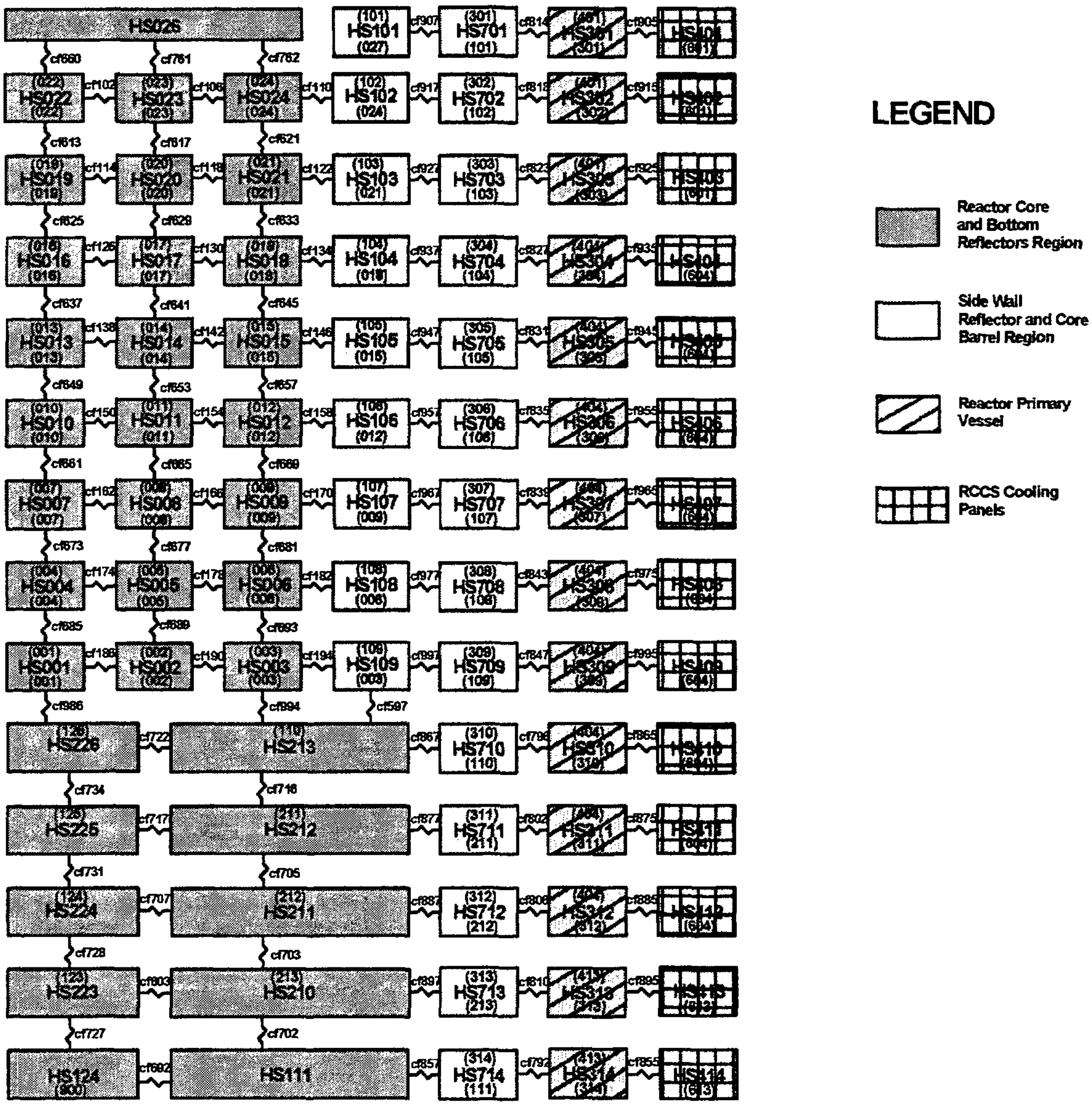


Figure G-3 PBR heat structure diagram

A control function in conjunction with a user-defined subroutine is used to model the axial and radial conduction and radiation heat transfer between the heat structures representing the pebbles in the core. The radial heat transfer rate between the heat structures in the core is governed by

$$\dot{Q}_{radial} = \frac{2\pi \cdot l \cdot k_{eff} \cdot \left(T_{r,z} - T_{r+1,z}\right)}{\ln\left(\frac{r_{r+1,z}}{r_{r,z}}\right)} \quad (1)$$

and the axial heat transfer rate between heat structures is governed by

$$\dot{Q}_{axial} = \frac{k_{eff} \cdot A_{cross}}{L}\left(T_{r,z} - T_{r,z+1}\right) \quad (2)$$

where $\dot{Q}_{radial}$ is the total radial heat transfer between CV(r,z) and CV(r+1,z), l is the height of the control volume, $r_{r+1,z}$ is the center radius of CV(r+1,z), $r_{r,z}$ is the center radius of CV(r,z), k_{eff} is the effective thermal conductivity of the pebble bed, $\dot{Q}_{axial}$ is the the total axial heat transfer rate between CV(r,z) and CV(r,z+1), A_{cross} is the cross sectional area between CV(r,z) and CV(r,z+1), and L is the length between the center of CV(r,z) and CV(r,z+1). The total radial heat transfer rate to CV(r+1,z) from CV(r,z) is divided by the number of pebbles in CV(r+1,z) to obtain the heat transfer rate per pebble entering CV(r+1,z). The total radial heat transfer rate from CV(r,z) to CV(r+1,z) is divided by the number of pebbles in CV(r,z) to obtain the heat transfer rate per pebble leaving CV(r,z). The same process is applied to the axial heat transfer rate. The heat source term is then added or subtracted to obtain the net heat conduction per pebble in appropriate control volumes per unit time. The effective thermal conductivity used in this study accounts for the radiation and conduction through the bed in both the axial and radial direction.

G.4 Effective Thermal Conductivity

The active core of a pebble bed reactor is an annular packed bed of spherical fuel pebbles with each fuel pebble element containing many fuel particles. The heat from the pebbles is transported simultaneously by a combination of mechanisms. These mechanisms are radiation through the gas regions between the pebbles, conduction through the gas surrounding the pebbles, and the conduction through the pebbles. As described in Reference [G-4] the overall effective conductivity is calculated from three different individual effective conductivities. The individual effective conductivities are summed to obtain the overall effective conductivity of the core region. These three individual effective conductivities are defined as (1) void radiation plus solid conduction, (2) gas conduction plus solid conduction, and (3) contact conduction plus solid conduction.

Equation (3) describes the effective conductivity due to void radiation plus solid conduction and is based on the cell model defined by Zehner and Schlüender [G-5] and modified by G. Breitbach and Barthels [G-6].

$$\lambda_{er} = \left[\left(1-\left(1-\varepsilon_p\right)^{\frac{1}{2}}\right)\cdot\varepsilon_p + \left(\frac{\left(1-\varepsilon_p\right)^{\frac{1}{2}}}{\frac{2}{\varepsilon_r}-1}\right)\cdot\frac{B+1}{B}\cdot\frac{1}{1+\frac{1}{\left(\frac{2}{\varepsilon_r}-1\right)\cdot\Lambda}} \right]\cdot 4\sigma T^3 d \qquad (3)$$

where

$$B = 1.25\left(\frac{1-\varepsilon_p}{\varepsilon_p}\right)^{\frac{10}{9}} \qquad (4)$$

$$\Lambda = \frac{\lambda_s}{4\sigma T^3 d} \qquad (5)$$

The variables in Eq.'s (3), (4) and (5) are σ the Stefan-Bolzmann constant, λ_s the thermal conductivity of the pebble matrix material, ε_p the porosity of the pebble bed (0.39), ε_r the emissivity of the pebble matrix material (0.8), d the diameter of the pebbles (6 cm), and T is the average temperature of the pebbles in the control volume.

The second term describes the effective conductivity due to gas conduction plus solid conduction. This equation was formulated by Zehner and Schlüender and tested by V. Prasad et, al [G-7].

$$\lambda_{eg} = \left[1-\sqrt{1-\varepsilon_p}+\frac{2\cdot\sqrt{1-\varepsilon_p}}{1-\lambda\cdot B}\cdot\left(\left(\frac{(1-\lambda)\cdot B}{(1-\lambda\cdot B)^2}\right)\cdot\ln\left(\frac{1}{\lambda\cdot B}\right)-\left(\frac{B+1}{2}\right)-\left(\frac{B-1}{1-\lambda\cdot B}\right)\right)\right]\cdot\lambda_g \qquad (6)$$

where

$$\lambda = \frac{\lambda_g}{\lambda_s} \qquad (7)$$

In equations (6) and (7) λ_g is the thermal conductivity of gas in the space between the pebbles in the pebble bed.

The third term describes the effective conductivity due to contact conduction between pebbles plus solid conduction within the pebbles. The effective conductivity component is the result of compressive loads on the spheres due to the weight of the particles in the bed.

$$\lambda_{ec} = \left[\frac{3\cdot(1-\mu_p^2)}{4\cdot E_s}\cdot f\cdot\frac{d}{2}\right]^{\frac{1}{3}}\cdot\frac{1}{0.531\cdot S_s}\cdot\left(\frac{N_A}{N_L}\right)\cdot\lambda_s \qquad (8)$$

where

$$f = p\frac{S_F}{N_A} \qquad (9)$$

For a bed assumed to have a simple cubic arrangement of the spheres, S_S, S_F, N_A and N_L are given as $S_S = 1$, $S_F=1$, $N_A = 1/(4R^2)$, $N_L=1/(2R)$ where R is the radius of a pebble. In Eq. (8) $\mu_p = 0.136$ and $E_S = 9.0E09$ (N/m^2). These two values are Poisson's ratio and Young modulus respectively. The variable p is the external pressure and is estimated by the weight of the pebbles in the pebble bed.

The effective thermal conductivity of the bed is the sum of the three terms given above:

$$k_{eff} = \lambda_{er} + \lambda_{eg} + \lambda_{ec} \qquad (10)$$

The above equations were programmed into Mathcad [G-8] using temperature dependent helium[2] and graphite thermal conductivity to generate the effective thermal conductivity used in the pebble bed for this study. The effective thermal conductivity is shown in Figure G-4 and is labeled new effective conductivity in the figure. The effective conductivity model presented here has been validated by the SANA benchmark experiments (pebble bed experiments) performed in Germany and reported in Reference [G-4].

Also shown in the figure is a second curve (Old Effective Conductivity) corresponding to values calculated from a second correlation. The values corresponding to the second curve were used in one of the MELCOR calculations to obtain the sensitivity of the pebble bed oxidation to bed effective conductivity. The second effective thermal conductivity curve was calculated using the following equation, which is an old correlation, developed in the 1950s by General Electric as reported in Reference [G-9]. It was used in our original calculation presented in Reference [G-1].

$$k_{eff} = 1.1536\times10^{-4}(T-T_o)^{1.6632} \qquad (11)$$

where k_{eff} has units of W/m-K and the temperature T has units of K. T_o is a reference temperature equal to 273.16 K.

[2] The effect of air on the effective thermal conductivity of the core was not included in this study, however its effect would be to lower the effective thermal conductivity. The influence of air results should be bracketed by the two different effective thermal conductivity curves used in this study.

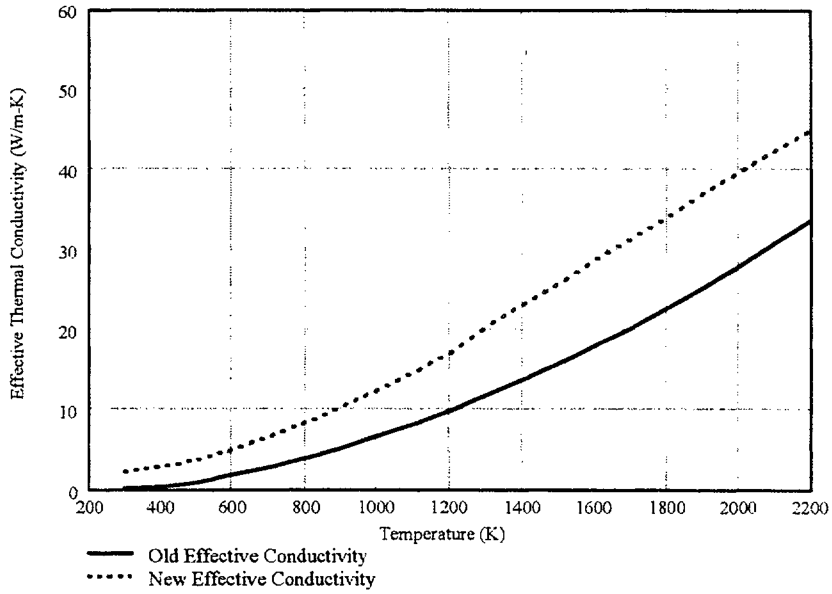


Figure G-4 Pebble bed effective thermal conductivity

The thermal conductivity of the fuel matrix used in equations (5), (7), and (8) was obtained from Reference [G-10] and is a function of both fast fluence, and the temperature at which the irradiation occurred. The fuel matrix thermal conductivity correlation presented in [G-10] was developed from experimental data from Germany and the United States. The equations presented in [G-10] were programmed into Mathcad and thermal conductivity curves (shown in Figure G-5) were generated. When compared to Figure 2.2 in Reference [G-10] the plots are identical.

Using a fast fluence of 1.5E21 neutrons/cm^2 for the core at an average core temperature of 923 K, the fuel matrix thermal conductivity curve shown in Figure G-6 was generated. The core fast fluence level was obtained from PEBBED, a neutronics code developed at the INEEL specifically for PBRs [G-11], [G-12]. The graphite conductivity for the side reflector was calculated (also shown in Figure G-6) using the same correlation for a 10-year fast fluence of 4.6E20 neutrons/cm^2 at an average temperature of 823 K. The side reflector fluence is lower than the fast fluence in the core region because of the very low fast flux in the reflector and was also obtained from the PEBBED code. The peak fast flux in the side reflector drops off rapidly with radius, thus a weighted average fluence value was calculated for use in calculating the outer reflector thermal conductivity. Shown in Table G-2 are fast flux values for five radial locations at the core midplane. The five fast flux values are area weighted and multiplied by 3.154E08 seconds to obtain a 10-year fluence value of 4.6E20 neutrons/cm^2

Table G-2 Side Reflector Fast Flux Values

Radius (cm)	Fast flux (neutrons/cm^2*sec)	Cross sectional area (cm^2)	Columns 2*3 neutrons/sec
182.5	6.09E12	1.720E04	1.047E17
197.5	1.63E12	1.861E04	3.034E16
212.5	4.39E11	2.003E04	8.792E15
227.5	1/17E11	2.144E04	2.509E15
242.5	2.65E10	2.286E04	6.057E14
Total		1.001E05	1.470E17

$$\text{Fast Fluence} = \left(\frac{1.470\text{E}17}{1.001\text{E}05}\right) \cdot 3.154\text{E}08 = 4.6\text{E}20 \frac{\text{neutrons}}{\text{cm}^2}$$

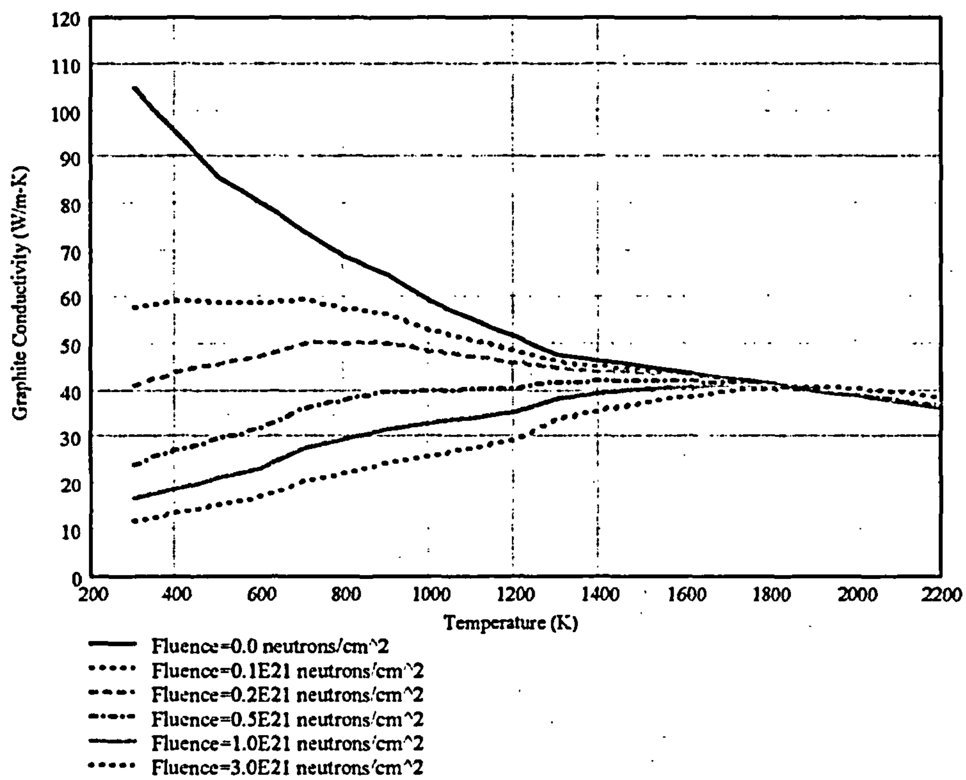


Figure G-5 Graphite thermal conductivity as a function of temperature and fast fluence

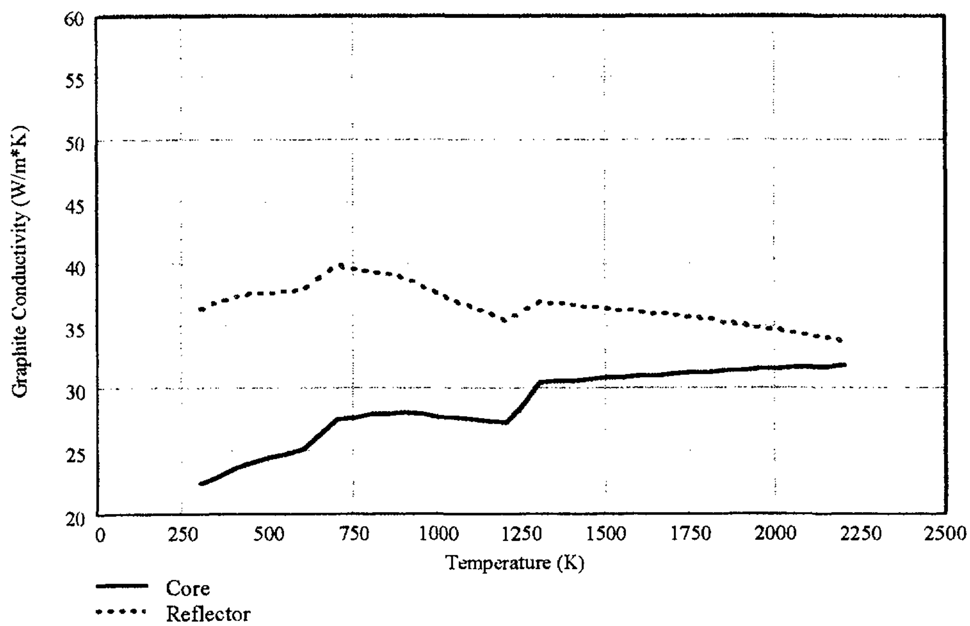


Figure G-6 Core and reflector graphite weighted average thermal conductivity verses temperature used in model

G.5 Oxidation

Early experiments performed by Wicke [G-13] and Rossberg and Wicke [G-14] showed that the reactions between porous carbon and air could be divided into three reaction zones (regimes). The three zone are (1) the low temperature zone where the reaction is controlled by the reactivity of the carbon, (2) the intermediate temperature zone where the reaction is controlled by the diffusion of oxygen through the solid and (3) the high temperature zone where the reaction is controlled by the mass transport of the oxygen through the boundary layer surrounding the carbon specimen.

A subsidiary objective of this study was to understand the importance and sensitivity of graphite oxidation in the lower reflector and in attenuating the degree of oxidation in the other core regions caused by air ingress resulting from a LOCA. The oxidation model used for this study is based on the graphite oxidation rates data obtained experimentally at the INEEL [G-15, G-16]. The two-oxidation curves from References [G-15] and [G-16] are shown in Figure G-7, one corresponding to INEEL data generated in 1988 using a more porous graphite and the other to data generated in 2002 at the INEEL using a highly engineered carbon fiber composite (CFC). The reaction rates generated by the experiments in 2002 only covered the chemical kinetic control regime (Regime I) and the in-pore oxygen diffusion-controlled regime (Regime II). In order to cover all three regimes, the data from the 2002 experiment were combined with the data from the 1988 experiments. This resulted in a correlation that could be used over the entire temperature range and allowed a smooth transition between each regime. The resulting reaction rate curve for all three regimes, henceforth referred to as the INEEL-2002I curve, is presented in Figure G-7 and is the oxidation model used in this study. For the convenience of reading the data the same data is plotted in Figure G-8 using a linear temperature scale for the x-axis as opposed to the inverse temperature scale used in Figure G-7.

For comparison purposes, some reaction rate data for German fuel pebble matrix material [G-17] are plotted in Figure G-8. The data are a function of the free stream velocity flowing past a pebble. Three curves are shown in Figure G-8 for free stream velocities of 0.043, 0.023 and 0.012 m/s. The German reaction rate data are higher in Regime I than the INEEL 2002 data. The reaction rates in Regime III are an order of magnitude lower than the INEL 1988 data. The German data are also limited to temperatures between 600 and 1200°C. Furthermore, the actual oxidation rate of graphite in the lower reflector is expected to be less than the German fueled pebbles shown here because the higher graphitization temperature of the reflector graphite should make the reflector graphite less reactive. Our earlier work using both the 1998 and 2002 INEEL reaction rate data showed that these differences in reaction rates were of less importance in the oxidation transient because the amount of the core involved in the oxidation is quite limited and the reaction at these temperatures becomes starved of air fairly quickly. The ability to get air into the core was critical. As seen from the data presented in Figure G-8 there is a large variation in the experimental data. The reaction rate for the specified fuel pebble matrix material and selected reflector graphite for a specific application would be needed to more accurately assess the behavior in an air ingress event. The INEEL 2002I oxidation curve was chosen for this study because the lower reaction rates in Regime I will allow more unreacted oxygen from the natural convecting airflow to reach the core. Most of the graphite temperatures in the lower reflector region are low enough that they fall within Regime I. Thus, the INEEL 2002I correlation was judged to be acceptable for these scoping studies.

The reaction rate equations programmed into MELCOR for the three regimes are:

Regime I: ($525 \le T < 710$ °C)

$$R_{ox} = 1.4754E07 \cdot \exp\left(-\frac{2.6128E04}{T}\right) \quad (12)$$

Regime II: ($710 \le T < 1175$ °C)

$$R_{ox} = 36.308 \cdot \exp\left(-\frac{1.3475E04}{T}\right) \quad (13)$$

Regime III: ($1175 \le T \le 1720$ °C)

$$R_{ox} = 1.57E-02 \cdot \exp\left(-\frac{2260.0}{T}\right) \quad (14)$$

The rate equations (12, 13, and 14) are based on the oxygen content in air at standard atmospheric conditions; thus, in the MELCOR model as a first-order approximation, the oxidation rates are assumed to vary linearly with the oxygen partial pressure as shown below:

$$R_{rate} = \frac{P_{ox}}{0.181E05\,Pa} R_{ox} \tag{15}$$

where P_{ox} is the partial pressure of the oxygen in the flow and the constant 0.181E05 Pa is the atmospheric partial pressure of oxygen at the INEEL where the experiments were conducted.

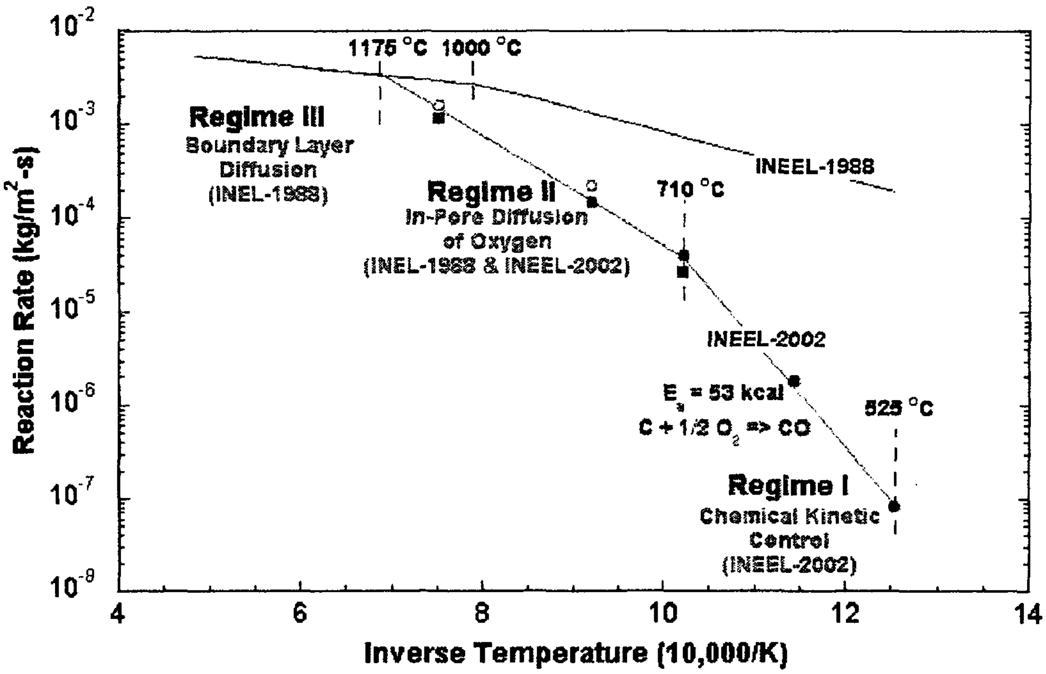


Figure G-7 CFC-air reaction rate curve for air ingress sensitivity studies.

The heat generated per pebble from the oxidation reaction is

$$q_{ox} = R_{rate} \cdot \Delta H_f \cdot A_{surface} \tag{16}$$

where ΔH_f is the heat of formation of carbon dioxide and $A_{surface}$ is the surface area of the pebble. The heat of formation of carbon dioxide is given as

$$\Delta H_f = 0.09516 \cdot \left(-93690. - 0.7077 \cdot T + 7.0E-07 \cdot T^2 - \frac{4.6E05}{T^2} \right) \text{(kJ/kg)} \tag{17}$$

The temperature has the units of K.

During the oxidation of graphite, some CO will likely be generated but is not included in the graphite oxidation model that is presently in MELCOR. At these temperatures the CO may oxidize in the boundary layer. This assumption is conservative from the standpoint of maximum pebble temperatures since the heat of formation of CO_2 is greater than the heat of formation of CO.

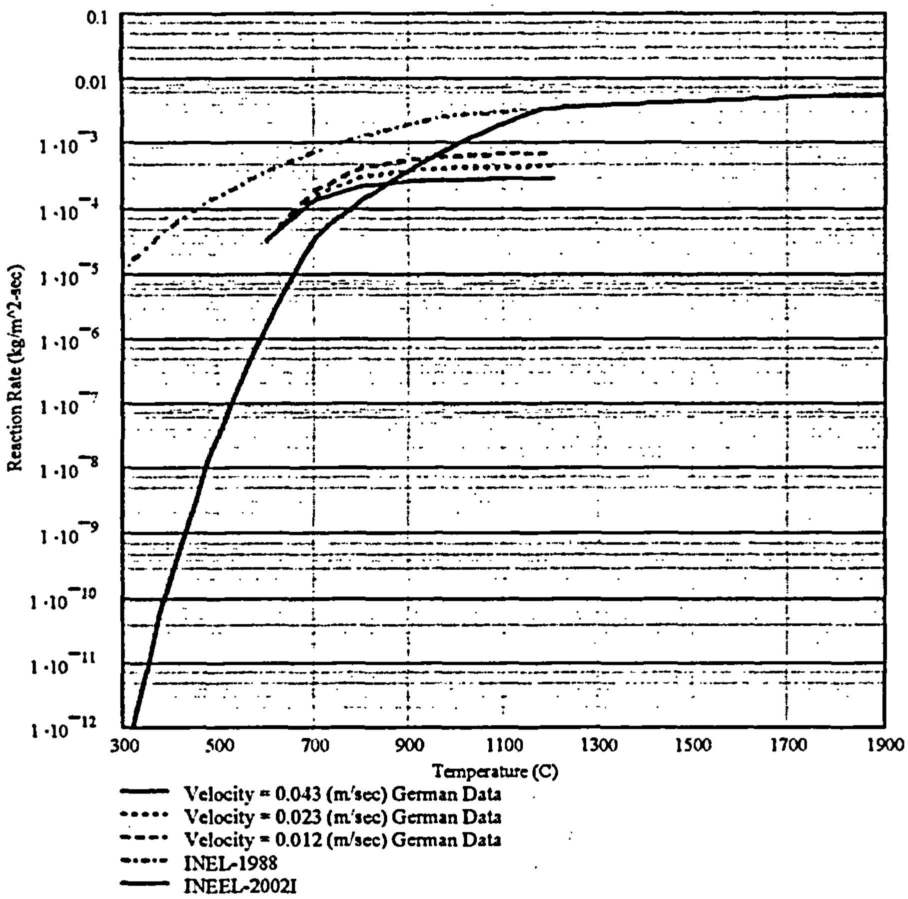


Figure G-8 Comparison of oxidation rate curves for INEEL-2002I, INEL-1988 and German pebble fuel element matrix data

G.6 Diffusion Model

A diffusion model was added to the MELCOR code in order to simulate the molecular diffusion process, which occurs as air slowly diffuses into the helium present in the core prior to the onset of natural convection.

The differential equation expressing conservation of mass for the "ith" material solved by MELCOR [G-18] for the atmospheric phase of the fluid flow is:

$$\frac{\partial \rho_A^i}{\partial t} + \nabla \bullet (\rho_A^i v_A) = \Gamma_A^i \qquad (18)$$

where
ρ^i_A = atmosphere material density (kg/m^3)

v_A = atmosphere flow velocity (m/s)
Γ^i_A = atmosphere material source term[3] (kg/m^3-s)

Equation (18) was modified by adding a gaseous diffusion term that obeys Fick's Law of diffusion as follows:

$$\frac{\partial \rho^i_A}{\partial t} + \nabla \bullet (\rho^i_A \mathbf{v}_A) = \nabla \bullet \rho_A D^i_A \nabla \omega^i_A + \Gamma^i_A \quad (19)$$

where

D^i_A = mass diffusivity (m^2/s) for the "ith" material diffusing through the atmosphere phase (A) of the fluid flow
ω^i_A = mass fraction of the "ith" material = ρ_i/ρ_A

In MELCOR these equations are solved for control volumes (volumes defined by average material properties such as rooms) that are interconnected by flow paths (connections between volumes such as piping). After integrating Equation (19) over the "jth" control volume, the result is as follows:

$$\frac{\partial M^i_{j,A}}{\partial t} = \sum_k \sigma_{j,k}\, \alpha_{k,A}\, \rho^{i,d}_{k,A} v_{k,A}\, F_k\, A_k + \sum_k \rho_{k,A}\, D^i_{k,A} \left(\frac{\omega^i_{m,A} - \omega^i_{j,A}}{L_k} \right) \alpha_{k,A} F_k\, A_k + \dot{M}^i_{j,A} \quad (20)$$

Here, as described in Reference [G-18], M is the total mass; subscript k refers to a given flow path, with $\sigma_{j,k}$ accounting for the direction of flow in flow path k with respect to volume j; $\alpha_{k,A}$ is the volume fraction of the atmospheric phase in flow path k; superscript d denotes "donor", corresponding to the control volume from which the material is flowing; A is the flow path area; F is the fraction that the flow area is open; L_k is the length of flow path k; subscript m refers to the volume connected to volume j by flow path k, and $\dot{M}$ includes all sources of mass. The diffusion coefficients for Equation 20 are calculated by MELCOR as described in Reference [G-19].

The diffusive term of Equation (20) is evaluated explicitly in time prior to each time advancement by MELCOR, and added to the mass source term as follows:

$$\dot{M}^{i\ \ t_o+\Delta t}_{j,A} = \sum_k \rho_{k,A}\, D^i_{k,A} \left(\frac{\omega^i_{m,A} - \omega^i_{j,A}}{L_k} \right) \alpha_{k,A} F_k\, A_k + \dot{M}^{i\ \ t_o}_{j,A} \quad (21)$$

where t_o is the time (s) at the start of a given computational time interval, and Δt is the size of the next computational time interval (s) MELCOR has decided to take. Because an explicit update of the diffusive term has an upper stability limit regarding time interval size, defined per flow path as $L_k^2/D^i_{k,A}$, the maximum allowed time interval is determined for all flow paths and if the MELCOR adopted time interval exceeds this diffusive limit then the calculation is terminated

[3] Includes changes resulting from chemical reactions

with an error message stating that the maximum diffusive time step size has been exceeded. The remaining terms of Equation (20) are advanced in time as described in Reference [G-18].

G.7 Core Pressure Drop

A significant determinant of the mass flow rate of air (oxygen) through the core following the onset of natural convection flow is the pressure drop through the core. The friction pressure drop ΔP_f through a pebble bed of height H can be expressed as

$$\Delta P_f = \psi \cdot \frac{H}{d_h} \cdot \frac{\rho_{ave}}{2} \cdot U_p^2 \tag{22}$$

where ψ is the pressure drop coefficient, H is the height of the core, d_h is the hydraulic diameter, ρ_{ave} is the average density of the fluid in the core, and U_p is the mean velocity in the gaps between the particles. The pressure drop coefficient is a function of the Reynolds number, which is defined as

$$Re_h = \frac{d_h \cdot U_p \cdot \rho_{ave}}{\mu} \tag{23}$$

where μ is the dynamic viscosity of the fluid.

The dependency of ψ on the Reynolds number is

$$\psi = \frac{320}{\frac{Re}{1-\varepsilon}} + \frac{6}{\left(\frac{Re}{1-\varepsilon}\right)^{0.1}} \tag{24}$$

where

$$Re = \frac{d \cdot U \cdot \rho_{ave}}{\mu} = (1-\varepsilon) \cdot Re_h \tag{25}$$

In version 1.8.2, MELCOR calculates the frictional pressure drop through the core as

$$\Delta P_f = \frac{1}{2} \cdot \rho_{ave} \cdot U^2 \cdot \left(\frac{4 \cdot f \cdot H}{D}\right) \tag{26}$$

where f is the Fanning friction factor. In the MELCOR model, the pebble bed friction pressure drop (Equation 22) was approximated by a defined laminar flow coefficient for the specific flow path. For laminar flow in a pipe, the value of the laminar flow coefficient is 16 and the Fanning friction factor equals this flow coefficient divided by the Reynolds number (e.g., f = 16/Re). For this study the Fanning laminar flow coefficient for the pebble bed region of the model was set at 175, which results in a pressure drop through the core of ≈ 46 Pa (shown in Figure G-9) for a mass flow of 0.125 kg/sec. This value of the laminar flow coefficient was found by programming Equations (22), (23), (24), and (25) into Mathcad and employing an iterative procedure to converge the flow coefficient to give the correct pressure drop at a specified mass flow rate. For a mass flow of 0.125 kg/sec the Mathcad model calculated the pressure drop as 43.2 Pa, which is in good agreement with the pressure drop calculated by MELCOR. This mass flow rate is approximately three times larger than calculations presented in Reference [G-17], which shows mass flow rates of 0.04 kg/sec for similar diameter breaks. However, for this scoping study, the larger mass flow rates are considered adequate for the oxidation and the maximum temperatures in the core for what are considered reasonably conservative assumptions.

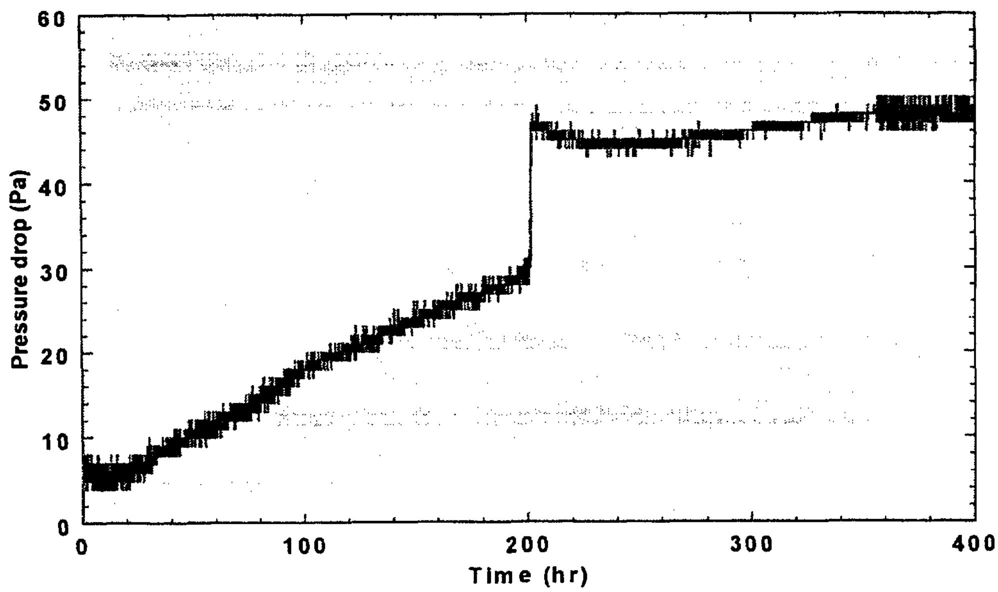


Figure G-9 Calculated core pressure drop following a large break LOCA

Equations (22), (23), (24), and (25) were programmed into Mathcad and for a mass flow of 0.125 kg/s, the pressure drop calculated was 43.2 Pa which is in good agreement with the pressure drop calculated by MELCOR.

G.8 Results

The results for a base case analysis and seven sensitivity analyses where some factors were varied about their nominal values will be presented in this section. The base case model was constructed using nominal values for the reactor input variables such as the effective thermal conductivity in the core, the thermal conductivity of the graphite reflector sounding the core, the size of the containment containing the power conditioning equipment, and the flow resistance in the core. A listing of the parameters that were varied is contained in Table G-3 as well as some of the results from the study. For the convenience of presenting the results the sensitivity calculations will be referred to as Case 1, Case 2 through Case 8. The cases are identified in Table G-3.

Table G-3 Time and maximum temperatures by sensitivity analyses factor

Case	Sensitivity analyses factors	Lower region of lower reflector	Upper region of lower reflector	First (bottom) layer of pebbles			Upper active core region		
		Max Temp °C	Max Temp °C	Max Temp °C	Time Max Temp Occurred (hr)	Time above 1600 °C (hr)	Max Temp °C	Time Max Temp Occurred (hr)	Time above 1600 °C (hr)
1	Nominal value	840	862	1611	209	0.3	1402	46	0
2	Thermal conductivity in core varied	840	852	1742	183	4.4	1499	52	0
3	Small leak in upper head	840	1087	1464	26	0.0	1388	42	0
4	Core flow resistance reduced	840	862	1745	228	3.1	1404	41	0
5	No oxidation in lower reflector	840	862	1611	209	0.3	1404	46	0
6	Thermal conductivity in side reflector reduced by 50%	848	867	1630	196	0.8	1529	61	0
7	Infinite containment volume	840	1317	1754	153	4.2	1407	46	0
8	Factors all combined	840	1091	1986	33	19.5	1618	64	46

The results from the base case analysis are presented in detail. The results from the other cases are presented in relation to their variation from the base case results.

G.8.1 Case 1 – Base Case

The accident, which results in air ingress into the core and thus oxidation of the hot fuel pebbles, is a hypothetical loss of coolant accident (LOCA). The LOCA simulation was initiated at 1000 seconds by opening two valves in the MELCOR model (used to simulate the break in the pipes) that connect the hot and cold legs to the containment. The circulator tripped at 1000 seconds and the reactor was scrammed at the same time. The simultaneous double-ended rupture of the hot and cold legs causes a rapid depressurization of the primary coolant system. The pressure in the reactor equalizes with the containment pressure (0.15 MPa) in less than 3 seconds.

The mass flow rate of air through the core is shown in Figure G-10. After the depressurization stage, hot helium occupies the core, the upper and lower plenums, and the inlet coolant annulus of the reactor with cool heavy air at the entrance of the pipe breaks. In this configuration there is insufficient buoyancy force to support natural convective flow. Thus, little or no mass flow of air from the power conversion system building to the core and from the core to the power conversion system building occurs for a number of hours. During this phase of the accident, air from the power conversion system building is mainly transported to the reactor by molecular diffusion. Japanese and German experimental results support this delay or "incubation time" prior to the onset of natural convection [G-20, G-21].

The mass flow rate of air through the core is essentially zero until approximately 200 hrs. At this time, the mass fraction of air (nitrogen) has equalized between the core and the containment building causing the flow to suddenly increase from zero to 0.125 kg/s indicating the onset of natural circulation through the core. The flow rate through the core remains between 0.125 kg/s and 0.075 kg/s from 200 to 400 hours, the time when the transient was terminated.

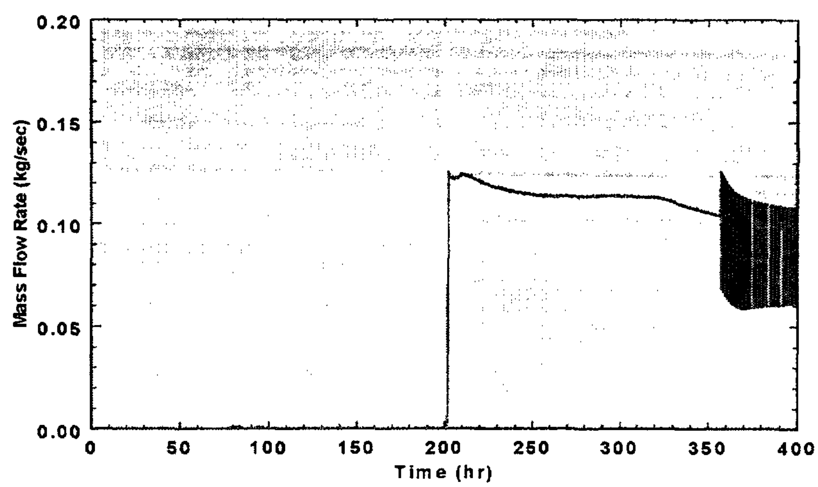


Figure G-10 Mass flow in the core after initiation of LOCA base case

The mole fraction of air (nitrogen) in the core and upper plenum of the reactor calculated by MELCOR gradually increases (shown in Figure G-11) until the buoyancy force is large enough to initiate natural circulation. The flow of air is from the hot leg to the cold leg upward through the core. As depicted in the figure, the mole fraction of nitrogen in the core gradually increases from zero at the beginning of the accident to ≈ 0.45 by means of molecular diffusion. At this point natural convection starts and the mole fraction of nitrogen increases rapidly to 0.62, which is the value of the mole fraction of nitrogen in the containment after blow down. When natural convection starts, the mole fraction of oxygen in the containment immediately starts to decrease with a corresponding increase of carbon dioxide in the containment. This increase in carbon dioxide indicates that oxidation of the graphite in the reactor is occurring. The decrease in oxygen in the containment results from the assumption that there is no significant in leakage or out leakage of air in the containment building (i.e. the containment is assumed to reclose or be reclosed within a few days after the LOCA).

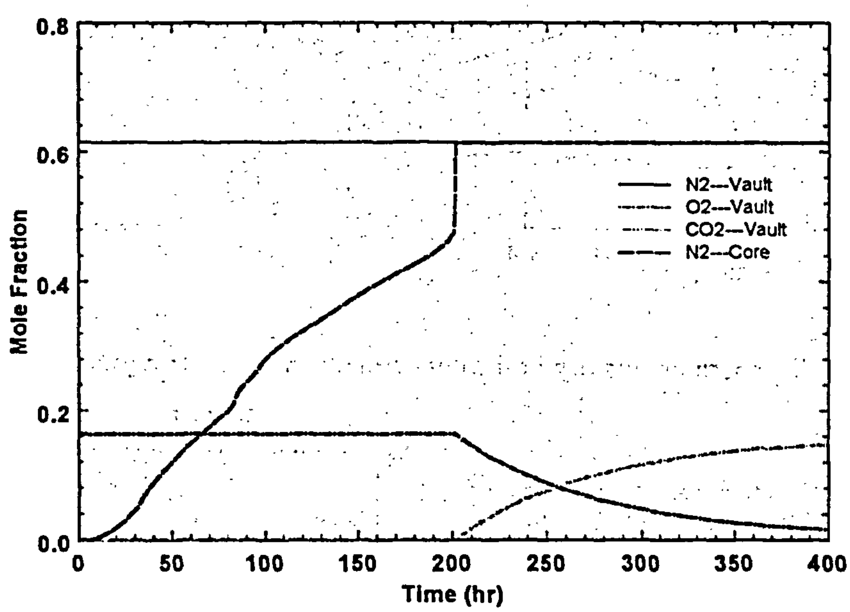


Figure G-11 Mole fraction of gas components in the reactor and containment

Figure G-12 is a schematic of the core and lower reflector region with arrows providing a correspondence between the temperature calculated by MELCOR and the physical location in the reactor. The temperature curves in all the figures to be discussed pertain to this schematic. When natural circulation of the air through the core begins, the temperature of the upper region of the lower reflector graphite (located below the active fueled core) immediately experiences a sharp rise in surface temperature as shown in Figure G-12. This rise in temperature is due mainly to conduction and radiation from the pebbles located at the entrance to the core as is discussed later when the results from the case of no oxidation in the lower reflector region is presented. As shown in Figure G-12, the temperature of the graphite reflector surface increases, from 490 °C to a maximum of

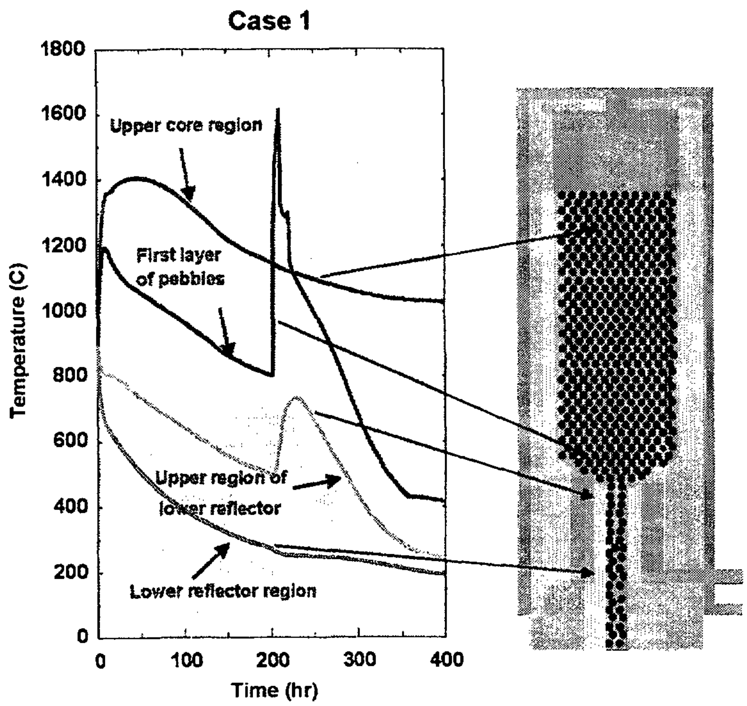


Figure G-12 Temperature history of the core and lower reflector region (base case)

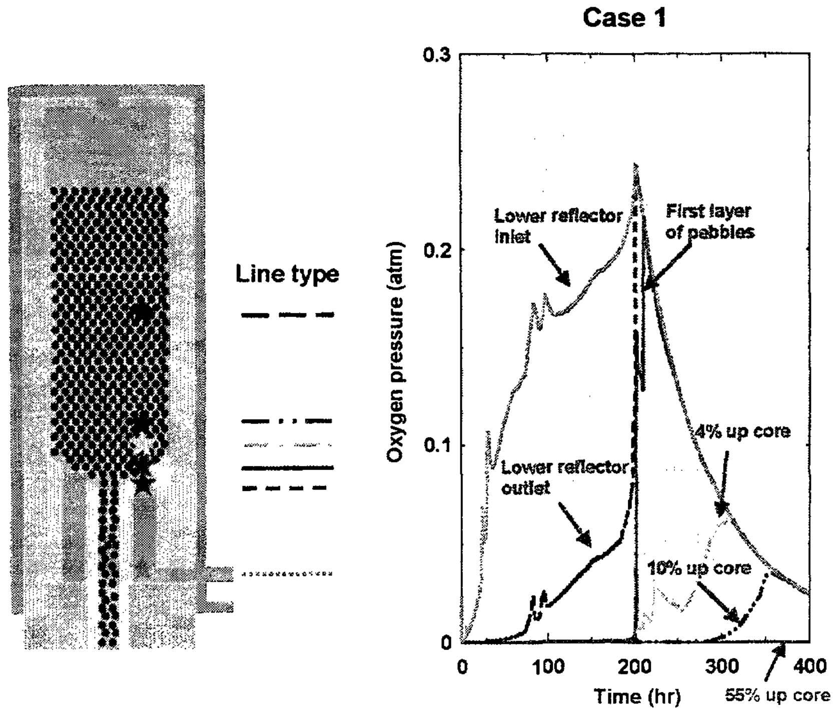


Figure G-13 Oxygen partial pressure history of the core and lower reflector region (base case)

733°C in 26 hours. At 226 hours the upper region of lower reflector graphite starts to cool down because the temperature of the pebbles in lower region of the core start to cool down. The graphite in the lower region of the lower reflector experiences initial no oxidation because the surface temperature of the graphite at the time of air ingress is 267 °C. This is substantially below the temperature at which significant oxidation takes place. This is consistent with the low oxidation rates (below 10^{-12} kg/m^2-sec) presented in Figure G-8 for temperature below 300 °C.

During the first 200 hrs of the event, the bottom layer of pebbles in the reactor core initially increases significantly and reaches a temperature of 1200°C at 9 hours and then begins to cool down reaching a temperature of 500°C at 200 hours. At 200 hours, natural convection starts and the surface temperature of the pebbles in the bottom layer rapidly increases as a result of oxidation of the graphite. The temperature increases from 500°C at 200 hrs to 1611°C by 209 hours. The temperature then begins to decrease again because the oxygen in the containment is depleted, i.e., the partial pressure of the oxygen in the first layer region has started to decrease as seen in Figure G-13. The pebble temperatures in CV(002) of the first layer are only above 1611°C for approximately 0.3 hours. The heated pebbles in the radially adjacent control volume (CV(003)) remain below 1600°C. As seen in Figure G-12 the pebbles in the upper core region experience no oxidation as indicated by no perturbation in the surface temperature plot. The maximum temperature that the pebbles in the upper region of the core experience during the transient is 1400°C. This temperature occurs at 45 hours and is due entirely to decay heating. In the base case only the control volume associated with the bottom layer of pebbles experience temperatures (slightly) in excess of 1600°C[4]. This control volume corresponds to 0.3% of the total fuel pebbles in the core.

Figure G-13 is a schematic of the lower reflector and core region. The stars (*) indicate the locations in the reactor where the partial pressure curves apply. The partial pressure curves in all the figures for all the cases to be discussed can be referenced to the star location in this schematic. Also shown in Figure G-13 is a plot of oxygen partial pressures at various locations in the lower reflector region and the core for the base case. The oxygen partial pressure curves are for the lower reflector inlet, the lower reflector outlet, the first layer of pebbles, 4% of the way up the core (Top of CV(008)), 10% of the way up the core (Top of CV(014)), 55% of the way up the core (Middle of CV(020)). The partial pressure at the lower reflector inlet slowly increases from 0.0 to 0.24 atm due mainly to molecular diffusion over the 200-hour period when there is no airflow to the core. An oxygen partial pressure of 0.24 atm is the value of the partial pressure in the containment before natural convection begins. As indicated in Figure G-13 there is little oxidation occurring in the lower region of the lower reflector. Thus, the decrease of oxygen partial pressure in this region is due to the corresponding decrease of oxygen partial pressure in the containment.

The oxygen partial pressure in the upper region of the lower reflector increases slowly due to molecular diffusion at a rate controlled by the concentration of oxygen in the lower region of the lower reflector. Although oxygen is available, the concentration (partial pressure) and the temperature of the graphite are low enough that no noticeable oxidation occurs prior to the onset of natural convection. When natural convection occurs the partial pressure of the oxygen

[4] In all cases time above 1600°C is presented as an indicator of the potential degradation of fuel

increase immediately to 0.24 atm, then follows the same partial pressure curve as the containment. Viewing Figure G-13 we see that very little oxygen is transported above 4% of the core (CV(008)). Thus, for the base case most of the oxygen is consumed in the bottom 4% of the core.

G.8.2 Case 2 - Reduced Core Effective Thermal Conductivity

The sensitivity analysis corresponding to Case 2 consisted of using a different correlation for the effective core thermal conductivity resulting in a drop in the thermal conductivity of the pebble bed (see Figure G-4) that is approximately 30 to 35% lower in the temperature range of 1200 K to 1800 K than that used in the base case analysis. The temperature and oxygen partial pressure results for Case 2 are shown in Figures 14 and 15. Each figure has Case 1 results included for ease of comparison. The reduced core effective thermal conductivity results in approximately a 100 K increase in the core maximum temperatures. The flow of air from the containment to the core starts at 175 hours as opposed to 200 hours for the base case. As a result of the earlier occurrence of air flow to the core and the higher core temperatures, the temperature of the bottom layer of pebbles peaks at 1742°C and remains above 1600°C for 4.4 hours. The maximum temperature in the upper core peaks at 1500°C due to decay heating with no indication of any oxidation occurring in the upper regions of the core.

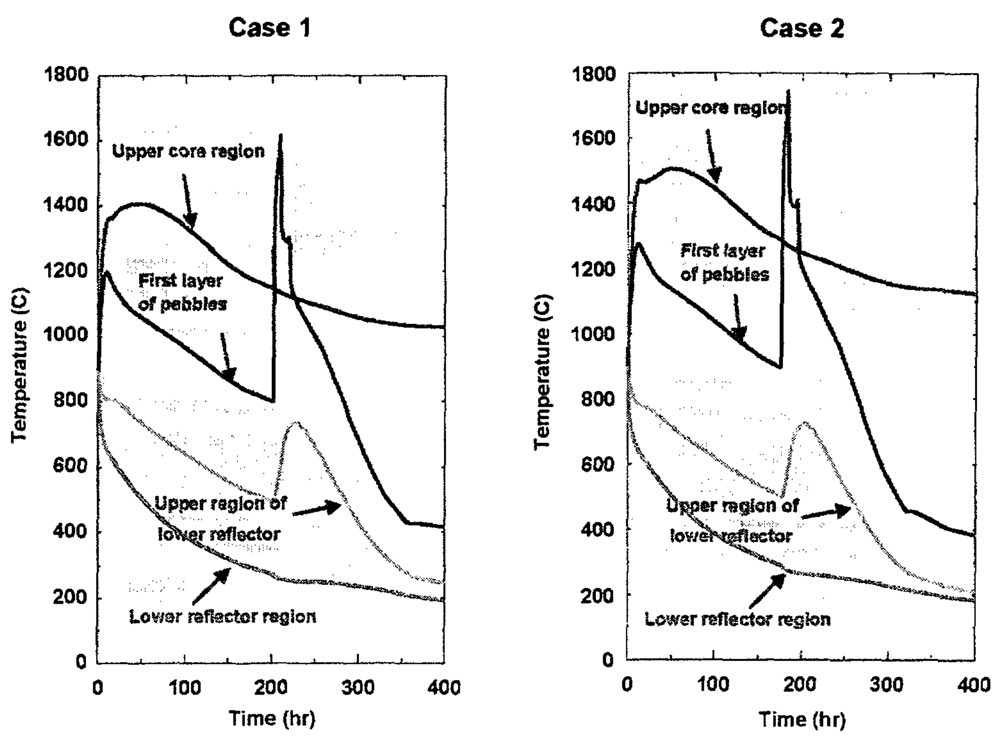


Figure G-14 Temperature history of the core and lower reflector region (Case 2)

Viewing Figure G-15, there is very little difference in the general shape of the oxygen partial pressure curves between Case 2 and the base case. The partial pressure of oxygen 4% of the way up the core is 0.057 atm for Case 2 and is 0.060 atm for Case 1. Due to the higher temperature in the first several layers of pebbles more oxygen is consumed in the lower regions of the core for Case 2 than in the base case. Only approximately 0.3% of the core experiences temperatures in excess of 1600°C.

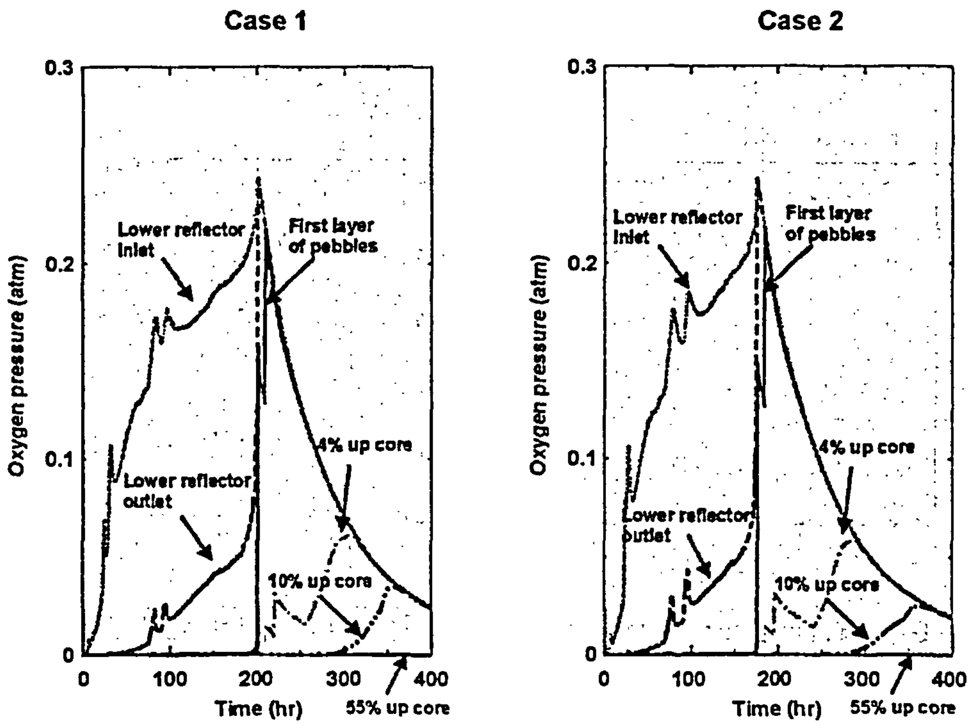


Figure G-15 Oxygen partial pressure history of the core and lower reflector region (Case 2)

G.8.3 Case 3 - Significant Leak in the Reactor Vessel Upper Head

Case 3 assumes a significant leakage in the upper head of the reactor at the time of the LOCA. The leak results in a 15% per day loss of helium mass from the reactor to the air between the RPV and containment building for a maximum pressure differential of 6.9 MPa. This leak causes the onset of natural convection to occur much earlier (22 hours) in the event when compared to the base case (200 hours). The temperature and oxygen partial pressure results corresponding to Case 3 are presented in Figures 16 and 17 respectively. The temperatures in the lower region of the lower reflector are approximately the same as in the base case because the temperatures are too low for any oxidation to occur. The time-temperature history of the bottom layer of pebbles is substantially different between Case 3 and Case 1. The temperature of the bottom layer of pebbles immediately starts to increase as the flow of oxygen from the containment reaches the bottom of the core. However the temperature of the pebbles in the bottom

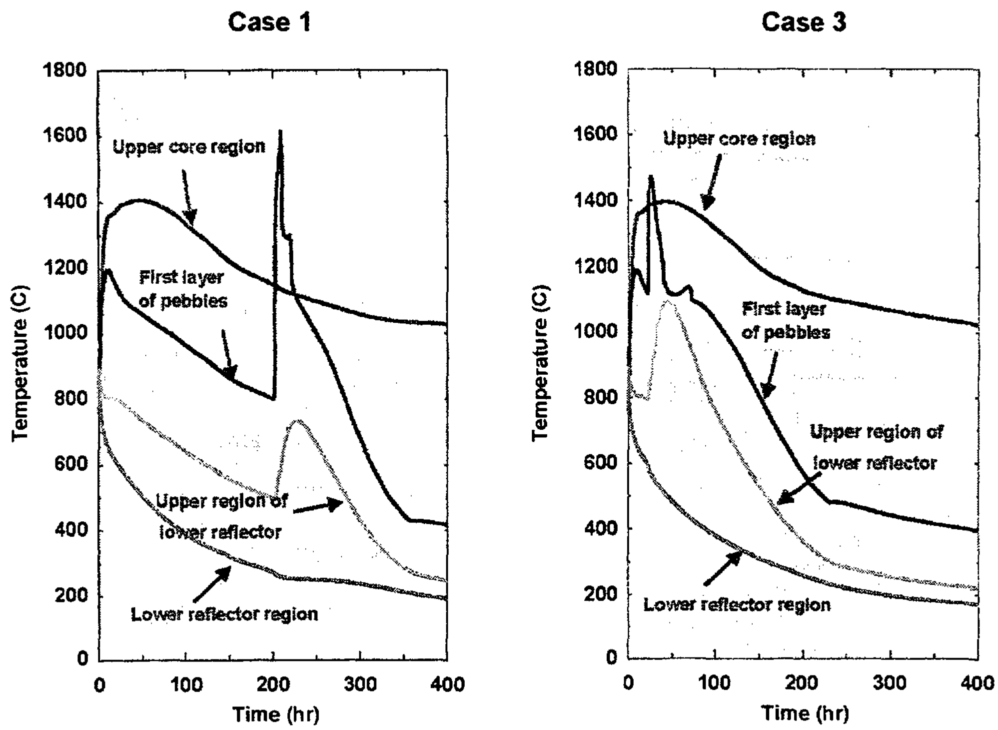


Figure G-16 Temperature history of the core and lower reflector region (Case 3)

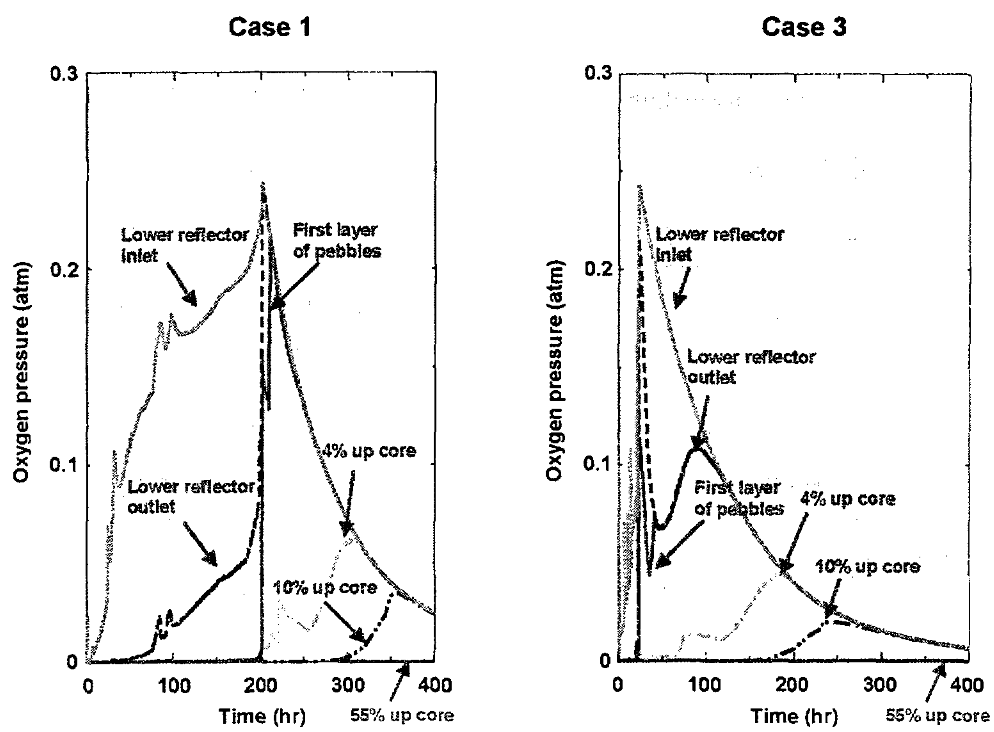


Figure G-17 Oxygen partial pressure history of the core and lower reflector region (Case 3)

layer peaks at 1464°C, which is 145 degrees lower than the peak temperature in the base case. The reason for this is that most of the oxygen is consumed in the upper regions of the lower reflector as is indicated by the oxygen partial pressure curves shown in Figure G-17. The temperatures in the upper core region are essentially the same for Case 3 and the base case because no oxidation occurs in this region of the core. Since more of the oxygen is consumed in the lower reflector region, the maximum partial pressure of oxygen above the first few layer of pebbles is lower than that presented for the base case. From Figure G-17, the partial pressure of oxygen 4% of the way up the core is 0.043 atm compared to 0.060 atm for the base case. No fuel experience temperatures in excess of 1600°C in this case.

G.8.4 Case 4 - Reduced Core Flow Resistance

Case 4 corresponds to a reduction in the flow resistance in the core by a factor of 10. Temperature and oxygen partial pressure results for this case are presented in Figures 18 and 19. As shown in Figure G-18, the mass flow rate through the core increased from 0.125 kg/s (base case) to 0.214 kg/s as a result of the reduction of the resistance through the core. The onset of natural convection for this case occurs at 220 hours, which is 20 hours later than the base case. This delay in the onset of natural convection is probably due to the localized redistribution of nitrogen in the core. In general the temperature histories are similar to Cases 1 and 2. The pebble temperatures in the first layer peak at 1745°C, which is 134 degrees higher than in the base case but is almost the same as Case 2.

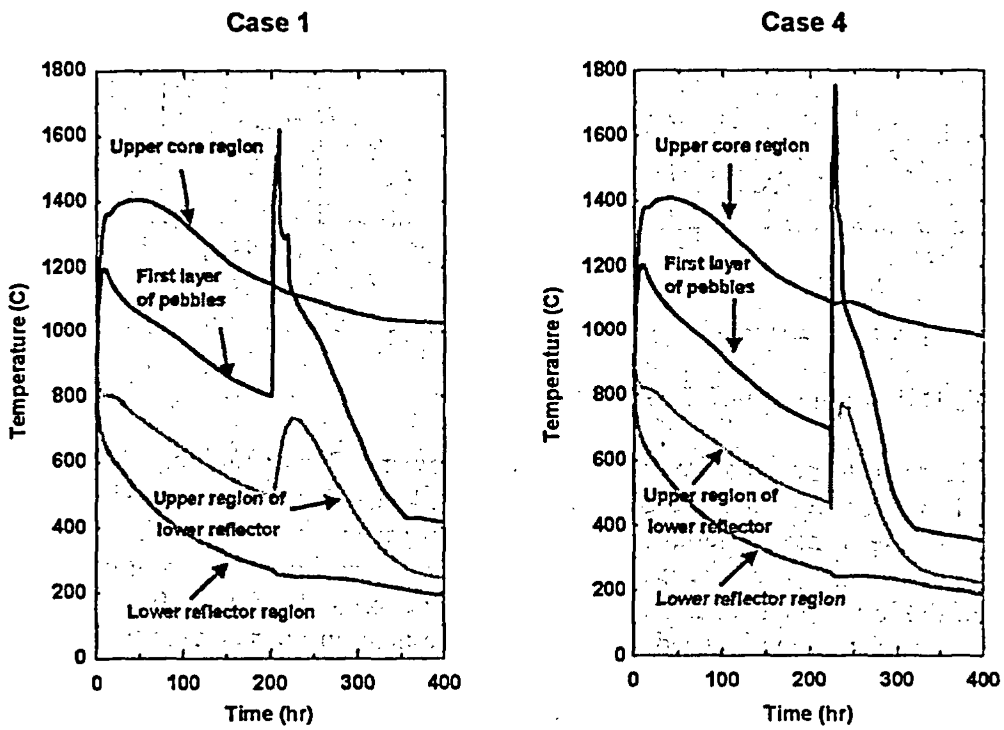


Figure G-18 Temperature history of the core and lower reflector region (Case 4)

This is the result of transporting more oxygen from the containment to the core in roughly the same time period. The pebbles in the bottom layer are above 1600°C for 3.1 hours.

The peak partial pressure of oxygen 4% up the core is 0.064 atm due to the higher transport rate of oxygen to the core. However the maximum temperature in the upper region of the core is the same as for base case thus no oxidation is occurring in this region. As shown in Figure G-19 the oxygen partial pressure 55% of the way up the core is zero. Again only 0.3% of the fueled pebbles experience temperatures in excess of 1600°C.

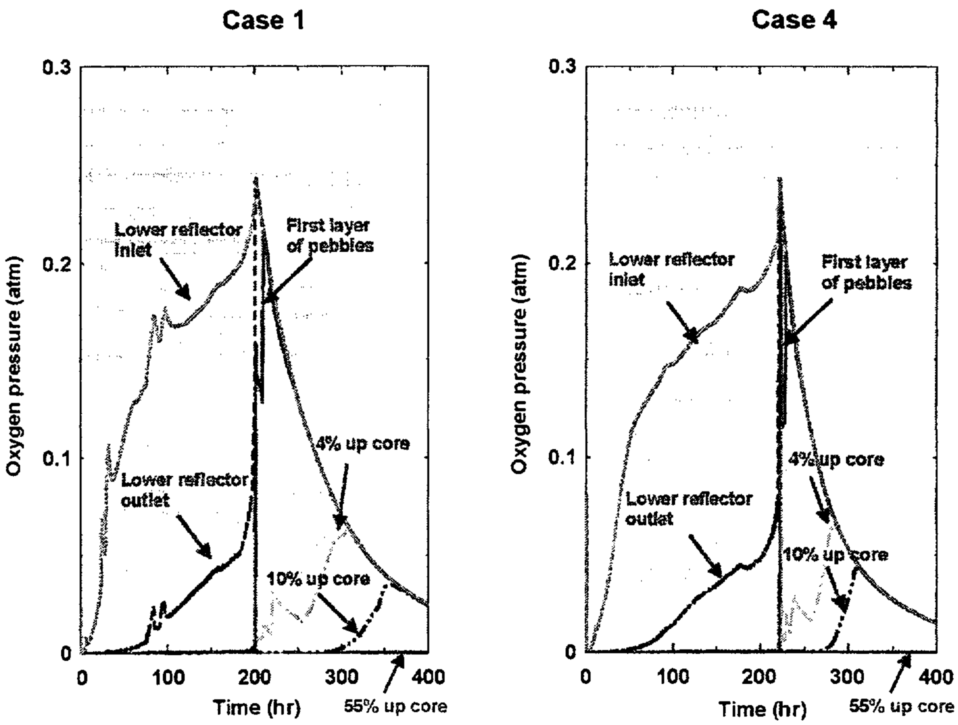


Figure G-19 Oxygen partial pressure history of the core and lower reflector region (Case 4)

G.8.5 Case 5 - No Oxidation in the Low Reflector Region

Case 5 results correspond to no graphite oxidation in the lower reflector region. Temperature and oxygen partial pressure results for Case 5 are presented in Figures 20 and 21. Viewing Figures 20 and 21 it is seen that the temperature and oxygen partial pressure results for Case 5 are identical to the base case. The results from this case show that the temperature increase of the upper region of the lower reflector is due mainly to conduction and radiation from the lower core region. For the oxidation model used in this study the oxidation rates corresponding to the predicted temperatures in the lower reflector region are too small to support any noticeable oxidation of the graphite in the lower reflector. Oxidation models having higher oxidations rates at lower temperature such as the German data and the INEL 1988 correlation would consumed most of the

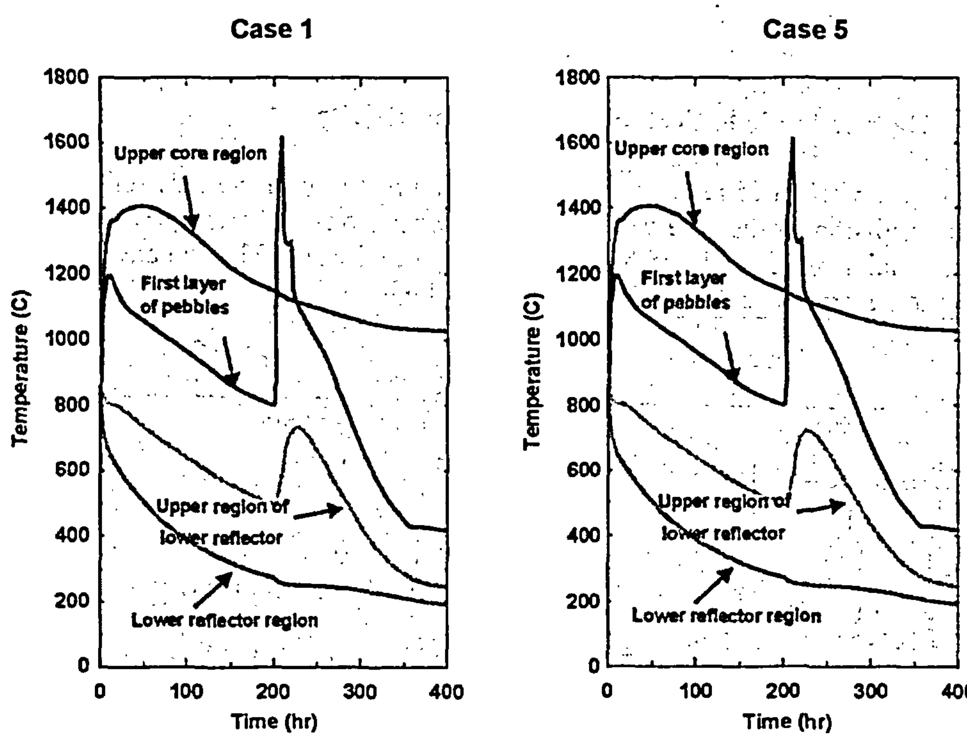


Figure G-20 Temperature history of the core and lower reflector region (Case 5)

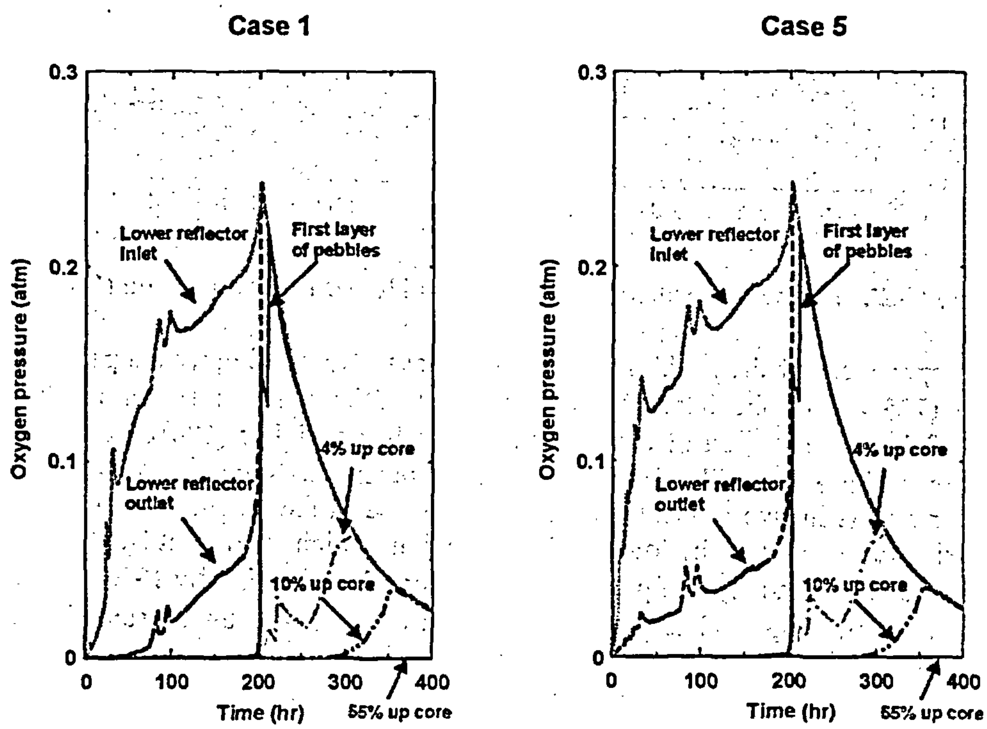


Figure G-21 Oxygen partial pressure history of the core and lower reflector region (Case 5)

oxygen in the air before it reached the pebbles in the core as shown in previous results [G-1]. Again only 0.3% of the fueled pebbles experience temperatures in excess of 1600°C.

G.8.6 Case 6 - Reduced Side Reflector Thermal Conductivity

Case 6 considered the effect of reducing the thermal conductivity in the side reflectors by 50% on the graphite oxidation in the core and lower reflector regions. The temperature and oxygen partial pressure results for Case 6 are presented in Figures 22 and 23 respectively. Again the results for Case 6 are similar to the result presented for the base

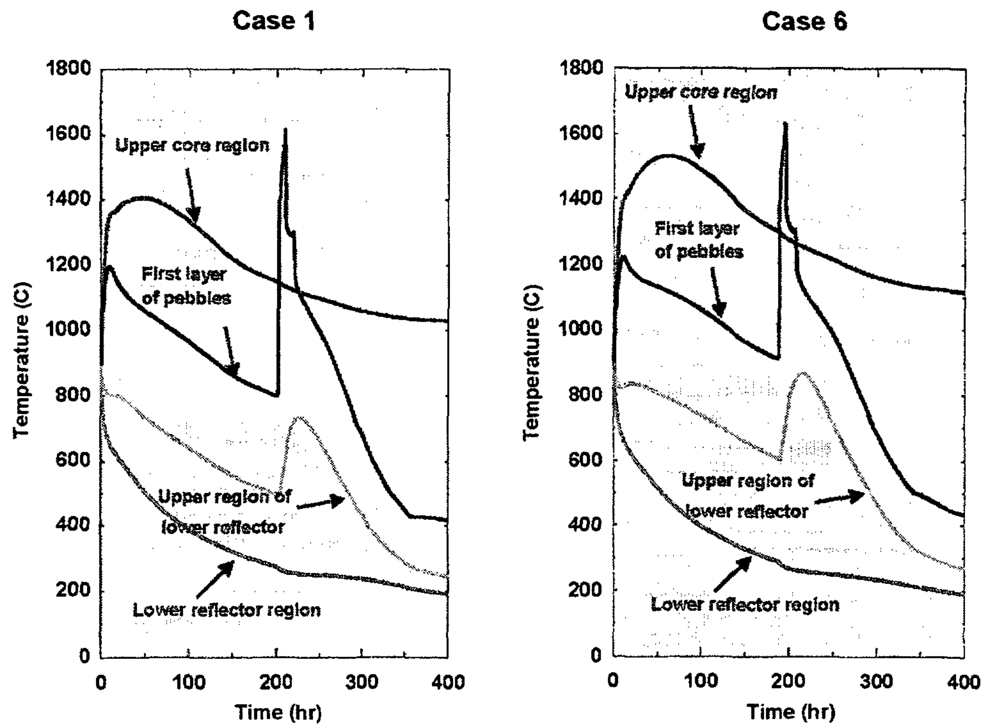


Figure G-22 Temperature history of the core and lower reflector region (Case 6)

case. The temperatures of the pebbles in the bottom layer are at a higher temperature (904°C) compared to (795°C) for the base case at the onset of natural convection resulting in the temperature of the upper region of the lower reflector being higher (600°C) compared to the 500°C value in the base case. This 100°C increase in the temperature of the upper region of the lower reflector results in two orders of magnitude increase in the oxidation rate. Thus, in this case some oxidation occurs in the lower reflector region, which is evident by the fact that the peak temperature in the first layer of pebbles only exceeds the base case by 19°C although it was initially 100°C hotter. Figure G-23 also indicates that oxygen is being consumed in the upper region of the lower reflector. The oxygen partial pressure histories are vary similar to the base case. Here as well only 0.3% of the fuel pebbles experience temperatures in excess of 1600°C.

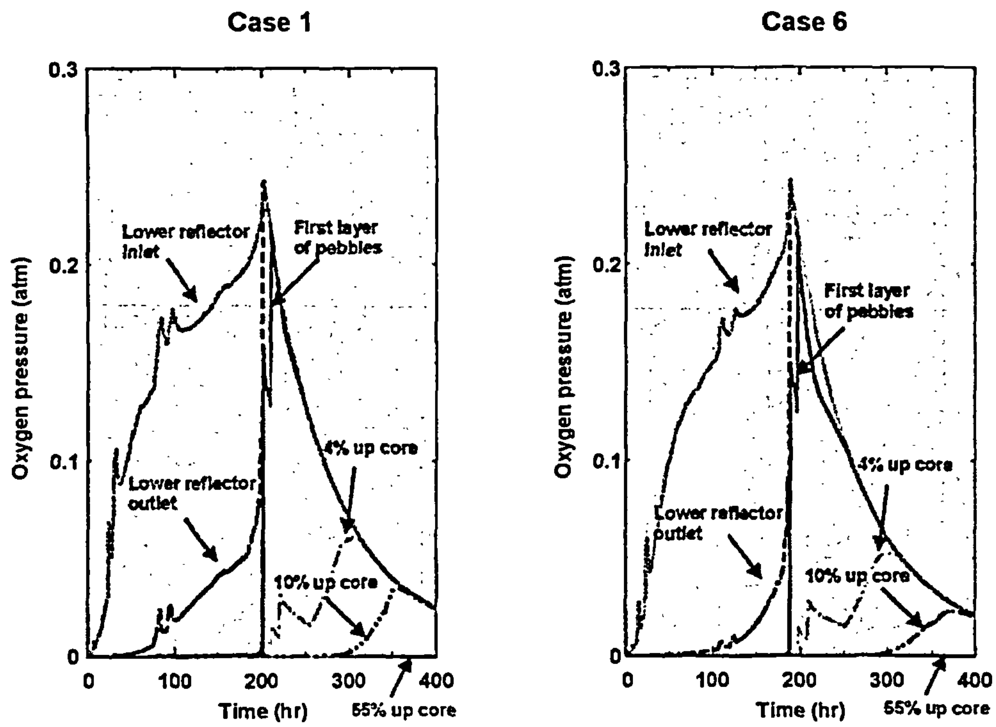


Figure G-23 Oxygen partial pressure history of the core and lower reflector region (Case 6)

G.8.7 Case 7 - Infinite Containment Volume

Case 7 considers the effect of having an infinite supply of air available for graphite oxidation in the lower reflector and core regions. The temperature and oxygen partial pressure results for Case 7 are presented in Figures 24 and 25 respectively. The major difference between this case and previous cases is that the upper region of the lower reflector experiences substantial oxidation due to the unlimited supply of air. The temperature of the upper region reaches a temperature of 1275°C at 200 hours. The temperature remains at approximately 1275°C for the remainder of transient indicating that the heat generated by oxidation is balanced by the heat removal through the sidewalls of the reactor. The temperature of the bottom layer of pebbles reaches a maximum temperature of 1754°C shortly after the beginning of natural convection (≈ 146 hours). The reflector graphite then cools down to 1060°C where it remains for the remainder of the transients. The temperature of the first layer of pebbles remained above 1600°C for 4.2 hours. The temperature of the upper core region is the same as shown in Case 1 indicating that no oxidation is occurring in the upper regions of the core at least out to 400 hours.

From Figure G-25 it is seen that the partial pressure in the bottom layer of pebbles is the same as in the upper region of the lower reflector. This indicates that all the graphite in the bottom layer of pebbles is consumed by 180 hours. The partial pressure of oxygen 4% of the way up the core (CV(008)) increases to the same level as in the upper region of

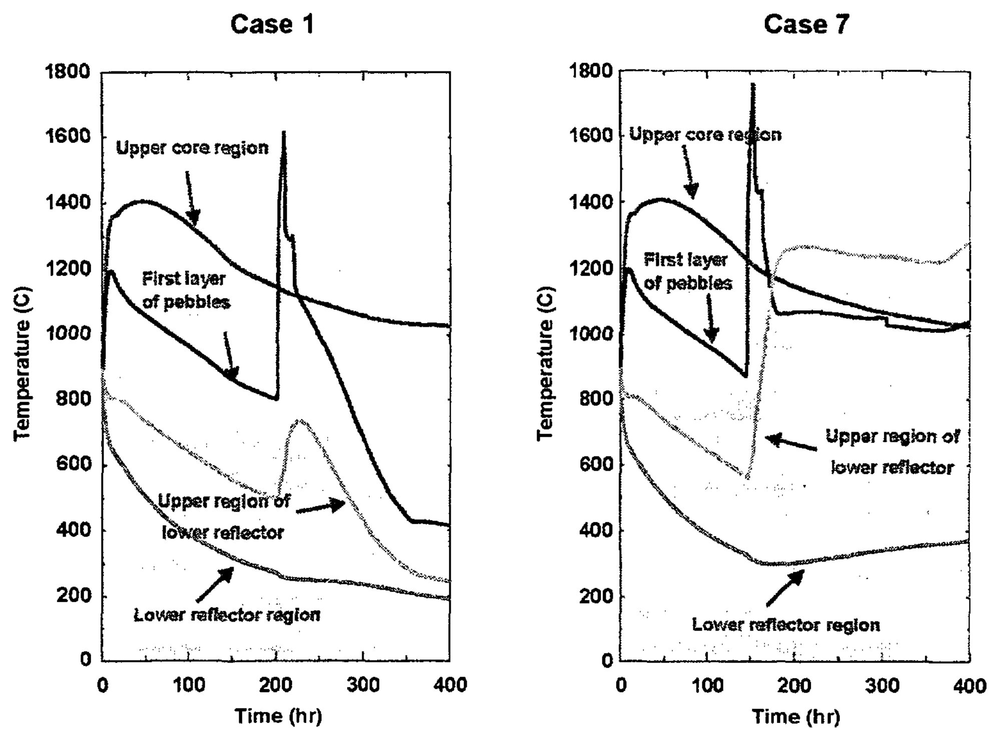


Figure G-24 Temperature history of the core and lower reflector region (Case 7)

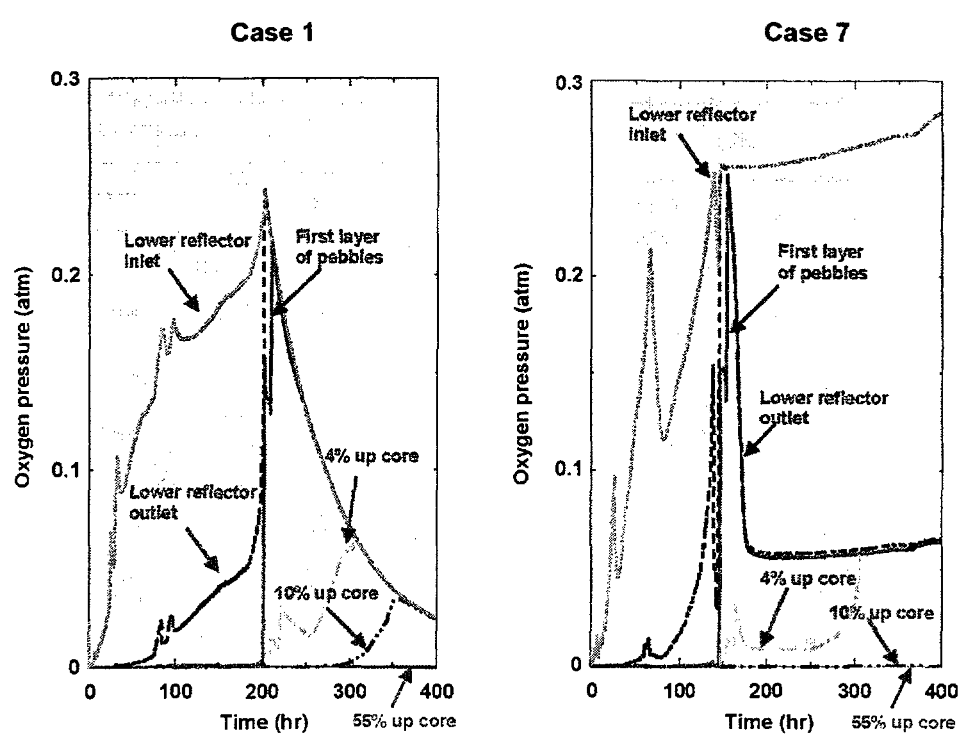


Figure G-25 Oxygen partial pressure history of the core and lower reflector region (Case 7)

the lower reflector at approximately 300 hours into the transient which indicates that the graphite in the pebbles in CV(008) has also been consumed by oxidation. The results presented in Figure G-25 indicates that no oxidation (at least out to 400 hours) is occurring above CV(014) which is located approximately 10% above the bottom of the core. At the end of 400 hours 1.5% of the fueled pebbles have been consumed.

G.8.8 Case 8 – All Factors Combined

Case 8 consists of a combination of all of the factors in the seven previous cases. This case is therefore considered to be extremely conservative or even excessively conservative. The temperature and partial pressure results for this case are presented in Figures 26 and 27 respectively. As in Case 3 the beginning of natural convection occurs at 22 hours. The temperature of the bottom layer of pebbles peaks at 1986°C and remains above 1600°C for 33 hours. However, as indicated in Figure G-27, the graphite in the bottom layer of pebbles is fully consumed by 26 hours (the partial pressure of oxygen increases to 0.2 atm which is the same as in the containment). The temperature plot of the first layer of pebbles shows the temperature continuing to decrease due to the assumption that a small radius of the pebble (r = 0.005m) cannot be oxidized.

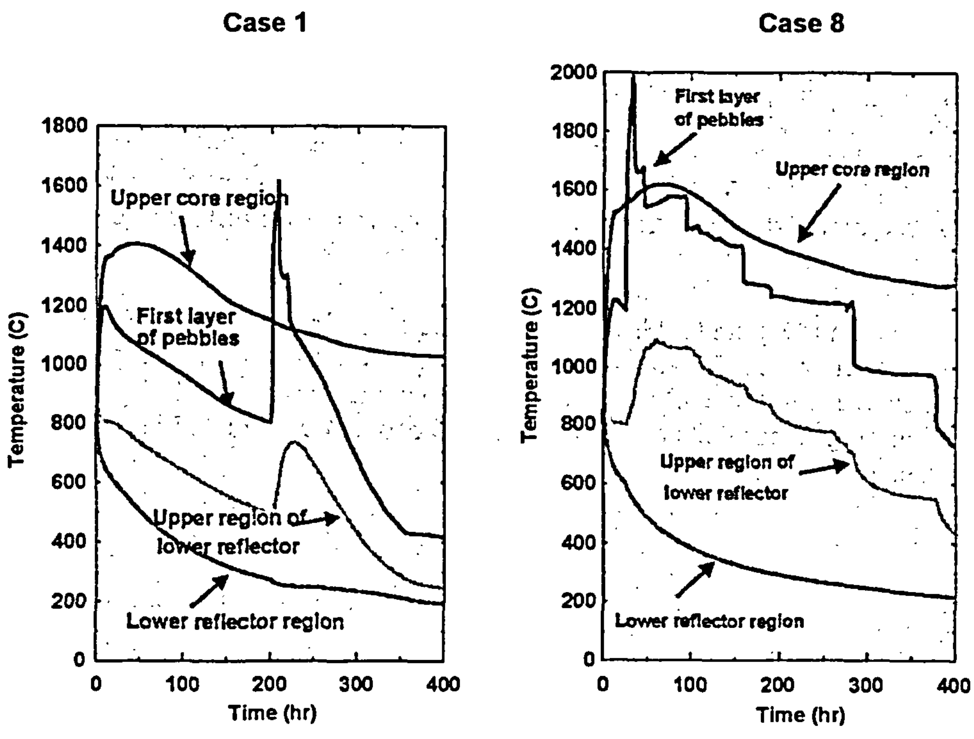


Figure G-26 Temperature history of the core and lower reflector region (Case 8)

This was necessary to eliminate any division by zero when the radius of the pebble goes to zero. The partial pressure results presented in Figure G-27 show that the pebbles in the layer 4% of the way up the core are consumed by 158 hours and the pebbles 10% up the core are consumed by

378 hours. This case indicates extremely severe graphite oxidation would be predicted if air ingress into the core occurs at very high core temperatures.

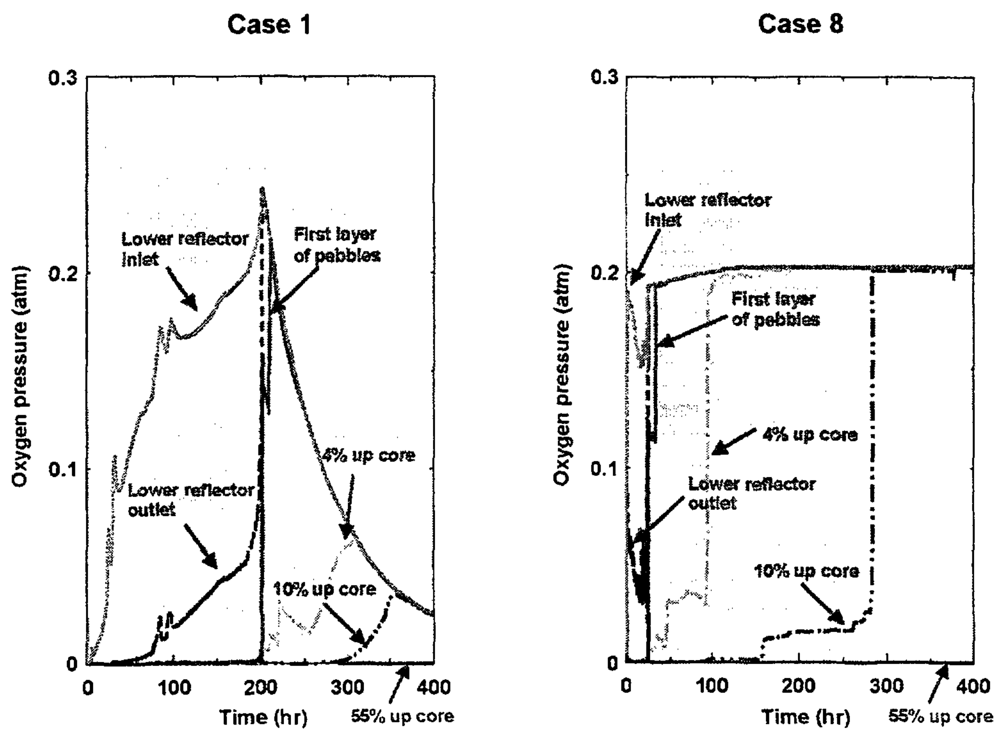


Figure G-27 Oxygen partial pressure history of the core and lower reflector region (Case 8)

The final figure present is Figure G-28, which shows the mass flow rates through the core for several of the sensitivity cases. The mass flow rates range from 0.1 kg/s to 0.125 kg/s except for the low core resistance case (Case 4) where the mass flow rate peaked at 0.22 kg/s. The onset of natural convection ranged from 22 hours for the upper head leak case to 225 hours for the low core flow resistance case.

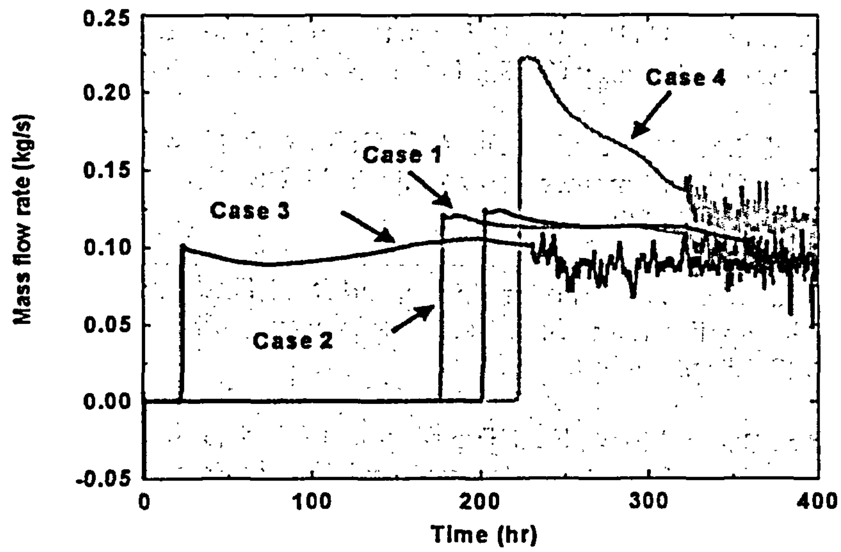


Figure G-28 Mass flow rate for Cases 1, 2, 3, and 4

G.9 Conclusions

The results of the scoping studies showed a remarkably consistent picture of the oxidation event:

1. Following depressurization, there is an incubation time associated with molecular diffusion of oxygen into the reactor. The incubation time ranged from 22 hours to 220 hours depending on assumptions related to the hydraulics of the system.

2. Very little oxidation occurs in the lower reflector region except for the upper head leak case (Case 3), the infinite containment case (Case 7), and Case 8 (combined case). Overall oxidation is limited to the lower 10% of the core. Partial pressures of oxygen in these regions range from 0.05 to 0.24 atm. Little or no oxidation occurs in the upper core region because of complete consumption of air with the exception of the case of infinite availability of air.

3. The amount of fuel at risk in the oxidation transient is limited. In all but the worse case scenario, the oxidized fuel pebbles experience temperature between 1600 and 1750°C for only 0.5 to 5 hours depending on the case.

4. The destruction of pebble matrix material and higher than normal temperatures allows the migration of fission products that were released during normal operation and the convection flow can act as a mechanism to transport these fission products out of the core. However, the potential source term is likely to be bounded by ≈ 10^{-4} normal operating fuel failure fraction since core temperatures do not exceed 1600°C for long periods of time.

G.10 References

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APPENDIX H

PANEL MEMBER DETAILED PIRT SUBMITTALS FOR TRISO FUEL DESIGN

The INEEL submittal is provided in Appendix H.1 (pages H-2 through H-24).
The ORNL submittal is provided in Appendix H.2 (pages H-25 through H-48).
The SNL submittal is provided in Appendix H.3 (pages H-49 through H-71).

Appendix H.1

Detailed PIRT Submittal by the INEEL Panel Member

D. A. Petti

TRISO Fuel PIRT: Design

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Design	Fuel Element	Specification of material properties
	Matrix material specification (common)	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	Level: 7	Remedy:
Rationale: The matrix material must provide protection for the coated particles during compaction or pressing of the pebble. Specifications for previous German and US are fairly well known. Specifications are placed on the properties of the pitch, and filler grades, matrix additives, filler crystallite sizes, and filler or shim particle sizes. The overall matrix composition is also generally specified. Unclear what the future material will be given a different supply of graphitic material.	Rationale: Knowledge is based heavily on experience from Ft. St. Vrain for US historical compacts and AVR and THTR for pebbles.	Closure Criterion:

Additional Discussion

See the following report for examples of specifications and rationale for historical US compacts

NP-MHTGR Fuel Product Specification Basis Report, CEGA-000396, June 1992

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Design	Fuel Element	Volume fraction of particles in fuel zone
	Particle packing fraction (common)	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 8	Remedy:
Rationale: Packing fraction differs in the pebble bed and prismatic gas reactors. In the pebble bed, the fuel pebble packing fraction is small (~ 10-15%). In prismatic design, the fuel compacts have packing fractions ranging from 35 to 50%. The packing fraction determines the power generated in the fuel element, which influences temperature gradients in the fuel element. Some fuel failure mechanisms and the transport of some fission products are strong functions of the temperature gradient across the fuel body.	Rationale: Irradiation performance of pebbles versus compacts has been linked to the level of acceleration in the irradiation and the power in the fuel body (which is sometimes translated into a power per particle). Generally, it is felt that the low packing fraction of particles in pebbles contributes to their superior performance. The higher packing fraction in prismatic fuel compacts can put the particles at greater risk for failure and fission product release under irradiation because of the impact on power generation in the fuel body and the induced temperature gradients. See reference below for details of irradiation performance review.	Closure Criterion:

Additional Discussion

See for example

D. A. Petti et al., "Key Differences in the Fabrication, Irradiation, and Safety Testing of U.S. and German TRISO-coated Particle Fuel and Their Implications on Fuel Performance," INEEL/EXT-02-00300, June 2002.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Design	Fuel Element	Unconfined heavy metal outside SiC layer (common)
	Unconfined heavy metal outside SiC layer (common)	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 9	Remedy:
Rationale: The unconfined heavy metal outside the SiC layer consists of the tramp uranium in the matrix material, any tramp uranium picked up by the particles in the coaters and fabrication process and any initially failed or defective particles produced during manufacture. Specifications limit the amount of unconfined heavy metal from both sources in the US; they are a combined specification in German pebble fuel.	Rationale: Burn leach testing is used as a QA technique to establish this value on each batch or lot of fuel produced.	Closure Criterion:

Additional Discussion

Values for the German and US fuel specification and values actually achieved in manufacture can be found in

D. A. Petti et al., "Key Differences in the Fabrication, Irradiation, and Safety Testing of U.S. and German TRISO-coated Particle Fuel and Their Implications on Fuel Performance," INEEL/EXT-02-00300, June 2002.

The technical basis for the US values can be found in

NP-MHTGR Fuel Product Specification Basis Report, CEGA-000396, June 1992

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Design	Fuel Element	The degree of homogeneity of the particles in the fuel element
	Particle distribution in fuel element	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	Level: 7	Remedy:
Rationale: Inhomogeneities can in principle lead to hot spots. There is a specification on homogeneity for compacts (see ref 1).	Rationale: The large overcoating in pebble fuel makes the particles tend to clump when the final matrix material is applied. The overcoating and final matrix material is applied in a rotating drum to ensure uniformity. In the compact fuel, graphite shim is added to the coated particles to ensure a uniform mixture in the mold before the liquid matrix material is injected.	Closure Criterion:

Additional Discussion

1. NP-MHTGR Fuel Product Specification Basis Report, CEGA-000396, June 1992

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Design	Fuel Element	Unfueled carbonaceous layer on outside of pebble
	Fuel free zone (Pebble)	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	Level: 7	Remedy:
Rationale: The fuel free zone in pebbles helps protect the fuel pebble from abrasion during its transit through the reactor. The fuel free zone absorbs any mechanical shock upon contact with other pebbles or metal and graphitic surfaces during transport of the pebble.	Rationale: The fuel free zone can hold up fission products. Diffusion of fission products in the matrix material has been measured. See reference below.	Closure Criterion:

Additional Discussion

IAEA, November 1997, *Fuel Performance and Fission Product Behaviour in Gas Cooled Reactors*, IAEA-TECDOC-978.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Design	Fuel Element	Layer on outside of outer PyC added after coating
	· Particle overcoat (pebble)	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 8	Remedy:
Rationale: The overcoating protects the particle during the creation of the pebble. The soft carbonaceous material helps cushion the particles during molding. This helps reduce the number of initially defective particles that would release fission products under normal and off-normal condittions	Rationale: The use of the overcoat reduces the number of particles that were broken during the manufacturing process.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Design	Outer PyC layer	Layer thickness and its standard deviation
	Thickness	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	Level: 8	Remedy:
Rationale: The OPyC layer is primarily used to provide a compressive stress to the SiC layer under irradiation. (The PyC layers shrinkage under fast neutron irradiation). The OPyC layer will retain fission gases but not fission metals like Cs, Ag and Pd. It plays a moderate role in the structural integrity of the particle based on recent fuel performance model assessments (see ref 1 below). The rationale for the thickness is found in ref 2 below.	Rationale: It's thickness and standard deviation are very well characterized in the fabrication process. Examples of typical specifications and values achieved during manufacturing are in reference 3 and 4 below.	Closure Criterion:

Additional Discussion

1. G. K. Miller et al., "Statistical Approach and Benchmarking for Modeling of Multi-dimensional Behavior in TRISO-coated Fuel Particles," J. Nuclear Materials, forthcoming

2. NP-MHTGR Fuel Product Specification Basis Report, CEGA-000396, June 1992

3. D. A. Petti et al., "Key Differences in the Fabrication, Irradiation, and Safety Testing of U.S. and German TRISO-coated Particle Fuel and Their Implications on Fuel Performance," INEEL/EXT-02-00300, June 2002.

4. Bryan, M.F., 1992, *Evaluation of NP-MHTGR Performance Test Fuel Quality Control Data*, INEEL. Report EGG-NPR-10130.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Design	Outer PyC layer	Mass per unit volume
	Density	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 9	Remedy:
Rationale: The density of the OPyC layer is an important variable in describing the shrinkage of the layer. If the density is too high then the shrinkage is too great. If the density is too low then for US compacts, too much of the liquid matrix material can infiltrate the layer, causing it to fail under irradiation due to matrix shrinkage. Shrinkage rates as a function of temperature, density, and anisotropy are found in Ref. 1. The rationale for the specification for US compacts is found in Ref. 2.	Rationale: Density is easily measured and controlled during fabrication. See reference 3 and 4 for typical values.	Closure Criterion:

Additional Discussion

1. CEGA, 1993, *NP-MHTGR, Material Models of Pyrocarbon and Pyrolytic Silicon Carbide Report,* CEGA-002820.

2. NP-MHTGR Fuel Product Specification Basis Report, CEGA-000396, June 1992

3. D. A. Petti et al., "Key Differences in the Fabrication, Irradiation, and Safety Testing of U.S. and German TRISO-coated Particle Fuel and Their Implications on Fuel Performance," INEEL/EXT-02-00300, June 2002.

4. Bryan, M.F., 1992, *Evaluation of NP-MHTGR Performance Test Fuel Quality Control Data,* INEEL. Report EGG-NPR-10130.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Design	SiC Layer	Layer thickness and its standard deviation
	Thickness	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: II	Level: 9	Remedy:
Rationale: The thickness of the SiC layer is important in structural integrity of the particle (see ref 1) and determines the ability of fission products to escape the particle. (The thicker the layer, the harder it is for diffusing fission products to escape or "attacking" fission product like Pd to completely traverse the SiC layer under design service conditions.) Many fission product models scale with the thickness of the layer. (see ref 2) the basis for the thickness is found in ref 3.	Rationale: The thickness and standard deviation is measured routinely with high accuracy. (see references 4 and 5)	Closure Criterion:

Additional Discussion

1. G. K. Miller et al., "Statistical Approach and Benchmarking for Modeling of Multi-dimensional Behavior in TRISO-coated Fuel Particles," J. Nuclear Materials, forthcoming

2. R. C. Martin, "Compilation of Fuel Performance and Fission Product Transport Models and Database for MHTGR Design," ORNL/NPR-91/6, Oct. 1993.

3. NP-MHTGR Fuel Product Specification Basis Report, CEGA-000396, June 1992

4. D. A. Petti et al., "Key Differences in the Fabrication, Irradiation, and Safety Testing of U.S. and German TRISO-coated Particle Fuel and Their Implications on Fuel Performance," INEEL/EXT-02-00300, June 2002.

5. Bryan, M.F., 1992, *Evaluation of NP-MHTGR Performance Test Fuel Quality Control Data*, INEEL. Report EGG-NPR-10130.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Design	SiC Layer	Mass per unit volume
	Density	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 9	Remedy:
Rationale: Density is important to obtaining the proper strength of the SiC and ensuring there is not significant porosity that would allow fission products to be released. The diffusivity of metallic fission products is a function of the density. The technical basis for the density is found in Ref. 1.	Rationale: Density is measured routinely and is within specification. Coating temperature and MTS/H2 ratios are used to control the density during fabrication. Typical values are found in References 2 and 3.	Closure Criterion:

Additional Discussion

1. NP-MHTGR Fuel Product Specification Basis Report, CEGA-000396, June 1992

2. D. A. Petti et al., "Key Differences in the Fabrication, Irradiation, and Safety Testing of U.S. and German TRISO-coated Particle Fuel and Their Implications on Fuel Performance," INEEL/EXT-02-00300, June 2002.

3. Bryan, M.F., 1992, *Evaluation of NP-MHTGR Performance Test Fuel Quality Control Data*, INEEL. Report EGG-NPR-10130.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Design	Inner PyC layer	Layer thickness and its standard deviation
	Thickness	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 9	Remedy:
Rationale: The IPyC serves two major functions: (a) to protect the kernel from Cl attack during MTS decomposition during SiC layer formation and (b) to provide compression to the SiC layer during its shrinkage under irradiation. Both are very important. Mechanical modeling of the coated fuel particle suggests that the thickness is very important to the stress that could develop in the SiC layer were the IPyC to crack under irradiation (see references 1 and 2). The technical basis for the IPyC thickness for US fuel is found in Reference 3. In th NP-MHTR fuel, the thickness was set too high (~ 53 microns instead of the traditional 35 microns) to provide protection from Cl attack of the kernel. This had a deleterious effect on the overall in-pile performance under irradiation. (see ref. 4 and 5)	Rationale: The layer thickness is easy to characterize and meets specifications during manufacture (see Ref 5 and 6).	Closure Criterion:

Additional Discussion

1. G. K. Miller et al., "Statistical Approach and Benchmarking for Modeling of Multi-dimensional Behavior in TRISO-coated Fuel Particles," J. Nuclear Materials, forthcoming

2. Miller, G.K., et al., 2001, "Consideration of the Effects on Fuel Particle Behavior from Shrinkage Cracks in the Inner Pyrocarbon Layer," *Journal of Nuclear Materials*, Vol. 295, pp. 205-212.

3. NP-MHTGR Fuel Product Specification Basis Report, CEGA-000396, June 1992

4. D. A. Petti et al., "Key Differences in the Fabrication, Irradiation, and Safety Testing of U.S. and German TRISO-coated Particle Fuel and Their Implications on Fuel Performance," INEEL/EXT-02-00300, June 2002.

5. B. J. Leikind et al., "MHTGR TRISO-P Fuel Failure Evaluation Report," DOE-HTGR-90390, Oct. 1993.

6. Bryan, M.F., 1992, *Evaluation of NP-MHTGR Performance Test Fuel Quality Control Data*, INEEL. Report EGG-NPR-10130.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Design	Inner PyC layer	Mass per unit volume
	Density	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 9	Remedy:
Rationale: The density of the IPyC layer is an important variable in describing the shrinkage of the layer. If the density is too high then the shrinkage is too great. If the density is too low then the Cl from the MTS decomposition during CVD of the SiC layer can infiltrate the layer and attack the uranium kernel causing the production of uranium chloride. All of this can lead to excessive heavy metal dispersion in the TRISO coating. Shrinkage rates as a function of temperature, density, and anisotropy are found in Ref. 1. The rationale for the specification for US compacts is found in Ref. 2.	Rationale: Density is easily measured and controlled during fabrication. See reference 3 and 4 for typical values.	Closure Criterion:

Additional Discussion

1. CEGA, 1993, *NP-MHTGR, Material Models of Pyrocarbon and Pyrolytic Silicon Carbide Report,* CEGA-002820.

2. NP-MHTGR Fuel Product Specification Basis Report, CEGA-000396, June 1992

3. D. A. Petti et al., "Key Differences in the Fabrication, Irradiation, and Safety Testing of U.S. and German TRISO-coated Particle Fuel and Their Implications on Fuel Performance," INEEL/EXT-02-00300, June 2002.

4. Bryan, M.F., 1992, *Evaluation of NP-MHTGR Performance Test Fuel Quality Control Data,* INEEL. Report EGG-NPR-10130.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Design	Buffer Layer	Layer thickness and its standard deviation
	Thickness	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 9	Remedy:
Rationale: The buffer layer provides two functions: to accommodate fission recoils and fuel kernel swelling and to provide voidage to accommodate fission gas and CO (UO2 only) release from the kernel with burnup. Thus the buffer thickness and density determine the void volume and hence the pressure loading on the TRISO coating of the fuel particle. Because of its importance in pressure loading, there is a specification to limit the number of particles with very thin or missing buffers to limit pressure vessel failure of the particles. See reference 1 for technical basis for historic US fuel.	Rationale: The thickness is easily measured and is well within specification. See references 2 and 3 for typical values	Closure Criterion:

Additional Discussion

1. NP-MHTGR Fuel Product Specification Basis Report, CEGA-000396, June 1992

2. D. A. Petti et al., "Key Differences in the Fabrication, Irradiation, and Safety Testing of U.S. and German TRISO-coated Particle Fuel and Their Implications on Fuel Performance," INEEL/EXT-02-00300, June 2002.

3. Bryan, M.F., 1992, *Evaluation of NP-MHTGR Performance Test Fuel Quality Control Data*, INEEL. Report EGG-NPR-10130.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Design	Buffer Layer	Mass per unit volume
	Density	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 9	Remedy:
Rationale: The exact density of the buffer is not a critical parameter. Given its function (i.e., to accommodate fission recoils and fuel kernel swelling and to provide voidage to accommodate fission gas and CO (UO_2 only) release from the kernel with burnup) a low-density material is required. It is usually about 50% theoretical density but in principal could probably be somewhat more or less and still be accommodated in the design. The technical basis is found in Ref. 1	Rationale: Well known and measured. See reference 2 and 3 for typical values.	Closure Criterion:

Additional Discussion

1. NP-MHTGR Fuel Product Specification Basis Report, CEGA-000396, June 1992

2. D. A. Petti et al., "Key Differences in the Fabrication, Irradiation, and Safety Testing of U.S. and German TRISO-coated Particle Fuel and Their Implications on Fuel Performance," INEEL/EXT-02-00300, June 2002.

3. Bryan, M.F., 1992, *Evaluation of NP-MHTGR Performance Test Fuel Quality Control Data*, INEEL. Report EGG-NPR-10130.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Design	Kernel	Design diameter with standard deviation
	Diameter	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	Level: 7	Remedy:
Rationale: Different kernel diameters have been used historically. Small kernels have been specified for HEU systems with larger kernels for LEU systems. Fertile particles also have a different size. (In most recent actinide burning scenarios of MHTGRs, the kernel size is set to optimize self shielding of the fuel) The size determines the moles of fission gases produced and the number of moles of non-gaseous fission products produced. Structurally, the size of the kernel has less importance than other factors in the stress developed in the coatings. The buffer volume is sized to accommodate changes in kernel size	Rationale: There has never been any definitive proof that satisfactory performance depends on the size of the kernel. Different size kernels have been made to appropriate specifications.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Design	Kernel	Mass per unit volume
	Density	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 9	Remedy:
Rationale: The density of the kernel is less important from a performance standpoint, especially for fuel that will be irradiated to high burnup. High density kernels will initially retain fission gases and non-gaseous fission products better than low density kernels. However, the high burnups proposed for current designs will essentially destroy the structure of the kernel making the density less important in terms of fission product release. In the US both high and low density (so called WAR kernels) were tested. (see ref 1). The rationale for the kernels used in the NP-MHTGR is found in reference 2.	Rationale: Kernels made with sol-gel process are typically 95% theoretical density. The density is easily controlled and measured to be within the given specifications. Typical values are found in references 1 and 3.	Closure Criterion:

Additional Discussion

1. D. A. Petti et al., "Key Differences in the Fabrication, Irradiation, and Safety Testing of U.S. and German TRISO-coated Particle Fuel and Their Implications on Fuel Performance," INEEL/EXT-02-00300, June 2002

2. NP-MHTGR Fuel Product Specification Basis Report, CEGA-000396, June 1992

3. Bryan, M.F., 1992, *Evaluation of NP-MHTGR Performance Test Fuel Quality Control Data*, INEEL. Report EGG-NPR-10130.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Design	Kernel	Maximum and minimum axis lengths of particles
	Sphericity (max/min diameter)	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	Level: 7	Remedy:
Rationale: The lack of sphericity in particles has been looked at as a cause for particle failure (and hence fission product release). Structural calculations suggest that the effect is moderate for typical sphericities encountered in fabrication. (see ref 1). Tabling techniques are used to separate the most out of round particles both the kernel stage and the final coated product stage. (see ref 2) in addition, there are numerous photomicrographs of irradiated fuel with slight asphericity that have remained intact following irradiation and/or accident heating tests.	Rationale: Sphericity is measured during fabrication and techniques are used (tabling) to remove out of spec kernels. See reference 2 for values of as-manufactured sphericities.	Closure Criterion:

Additional Discussion

1. G. K. Miller and D.C. Wadsworth, "Treating Asphericity in Fuel Particle Pressure Vessel Modeling," Journal of Nuclear Materials, Vol. 211, pp 57-69, 1994.
2. D. A. Petti et al., "Key Differences in the Fabrication, Irradiation, and Safety Testing of U.S. and German TRISO-coated Particle Fuel and Their Implications on Fuel Performance," INEEL/EXT-02-00300, June 2002

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Design	Kernel	Oxygen to uranium atomic ratio for UO_2 fuel
	Stoichiometry: Uranium to oxygen	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 8	Remedy:
Rationale: The O/U ratio determines the oxygen potential in the fuel, which in turn determines the chemical forms and mobility of key fission products in the fuel. See ref. 1	Rationale: The value is measured and specifications are used to ensure an acceptable O/U ratio. Typical values for German UO_2 are found in reference 2.	Closure Criterion:

Additional Discussion

1. D. Olander, "Fundamental Aspects of Nuclear Reactor Fuel Elements," ID-26711-P1, 1976.

2. Gontard, R., and H. Nabielek, 1990, *Performance Evaluation of Modern HTR TRISO Fuels*, HTA-IB-05/90.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Design	Kernel	Oxygen:carbon:uranium ratio for UCO
	Stoichiometry: Uranium to carbon and uranium to oxygen	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 6	Remedy: Measurements of oxide and carbide phases must be performed at the particle level to ensure that the values at a particle level are acceptable relative to the batch average specification values currently in use.
Rationale: The O/U and C/U ratios determine the stoichiometry of UCO fuel. The purpose of UCO fuel is to add enough UC_2 to prevent formation of CO during operation. The UC_2 acts as a buffer to prevent any free oxygen released during fission from reacting with carbon in the buffer to produce CO. If too much UC_2 is added then rare earth fission products will form carbides that are too mobile under off-normal conditions. There is a specification to ensure the proper amount of oxygen and carbon in the kernel to get the fission product chemistry correct. The overall theory is discussed in References 1 and 2. The technical basis for the specification is found in reference 3.	Rationale: The values are measured on a batch basis. There is some concern that at the individual particle level the ratios could be different but would still meet the batch average values. (For example, you could mix in appropriate proportions UO_2 kernels and UC_2 kernels and still meet the specification but the performance would be unacceptable.) At the high burnups envisioned for GT-MHR, an oxide-rich particle or a carbide rich particle could fail under either irradiation or high temperature accident conditions. Typical specification values are found in Reference 4 and 5. Information on particle specific values from studies conducted during the NPR program is found in Reference 6.	Closure Criterion:

Additional Discussion

1. Homan, F.J., et al., 1977, "Stoichiometric Effects on Performance of High-Temperature Gas-Cooled Reactor Fuels from the U-C-O System," *Nuclear Technology,* Vol. 35, pp. 428-441.
2. McCardell, R.K., et al., 1992, *NP-MHTGR Fuel Development Program Plan.* Idaho National Engineering Laboratory, Report EGG-NPR-8971 (Revision C).
3. NP-MHTGR Fuel Product Specification Basis Report, CEGA-000396, June 1992
4. Bryan, M.F., 1992, *Evaluation of NP-MHTGR Performance Test Fuel Quality Control Data,* INEEL. Report EGG-NPR-10130.

5. D. A. Petti et al., "Key Differences in the Fabrication, Irradiation, and Safety Testing of U.S. and German TRISO-coated Particle Fuel and Their Implications on Fuel Performance," INEEL/EXT-02-00300, June 2002
6. Saurwein, J., and L. Shilling, September 1993, *Final Report – Testing of As-manufactured NPR-PTF, German, and U.S. Historical Fuel*, General Atomics, Issue/Release Summary, Doc. No. 910647 N/C.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Design	Kernel	Elemental constituents and amounts other than design
	Purity	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	Level: 7	Remedy:
Rationale: Impurities in the kernel can potentially migrate during irradiation and pose a threat to the SiC. There are certain elements that can reduce SiC chemically, especially the transition elements. The rationale behind the impurity limits for US fuel is found in reference 1. (Note impurities from other parts of the fabrication process may be more important).	Rationale: The elemental limits have been established and are easy to control in fabrication. These elements have not been found to be a serious problem related to particle failure and fission product release from this fuel. Values of the limits and manufacturing values are found in Reference 2 and 3.	Closure Criterion:

Additional Discussion

1. NP-MHTGR Fuel Product Specification Basis Report, CEGA-000396, June 1992
2. Bryan, M.F., 1992, *Evaluation of NP-MHTGR Performance Test Fuel Quality Control Data*, INEEL. Report EGG-NPR-10130.
3. D. A. Petti et al., "Key Differences in the Fabrication, Irradiation, and Safety Testing of U.S. and German TRISO-coated Particle Fuel and Their Implications on Fuel Performance," INEEL/EXT-02-00300, June 2002

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Design	Kernel	Weight fraction U-235 in total uranium
	Enrichment	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 9	Remedy:
Rationale: Enrichment is very well known in the particles. It determines the ultimate burnup that can be achieved given reactor constraints relative to reactivity etc. The enrichment determines the fission rate, which is of secondary importance in some fission gas release models at low temperature. (see Reference 1). However this effect is rather small compared to the effects of burnup and temperature on fission gas release	Rationale: Is easily measured and meets the specification with high precision.	Closure Criterion:

Additional Discussion

W. K. Terry (editor) "Modular Pebble-Bed Reactor Project: Laboratory Directed Research and Development Program FY-2001 Annual Report," INEEL/EXT-2001-1623, December 2001.

Appendix H.2

Detailed PIRT Submittal by the ORNL Panel Member

R. Morris

TRISO Fuel PIRT: Design

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Design	Fuel Element	Specification of material properties
	Matrix material specification (common)	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 7	Remedy: Investigate the key aspects of fuel element formation and irradiation behavior if new materials and methods are introduced.
Rationale: The matrix binds the particles together and serves as a structural and heat transfer medium. Many carbon materials dimensionally change under processing and unirradiation and these changes can affect the fuel performance. In addition, impurities and fuel element processing can damage particles.	Rationale: Scores of fuel compacts and pebbles have been made with generally good results, especially in the case of pebbles. However, in some cases a switch in the matrix material from petroleum pitch to thermosetting resin is under consideration. Less is known about this resin in the case of compacts, although no deleterious behavior is anticipated.	Closure Criterion: Generate data that shows fuel particles are not damaged by the resin during fuel element formation and satisfactory irradiation performance results.

Additional Discussion

The German pebble bed technology has used a thermosetting resin for pebble fabrication while the US has used a petroleum pitch. Early experience at GA has shown that if a resin is substituted for pitch in the injected molded compact the particle matrix bond is too strong and coatings can be damaged as the matrix shrinks during subsequent processing. This interaction does not take place in the pebble because of the lower amounts of binder material. The US examined the compacting issue in the 1990's and will revisit this issue during the upcoming work on the GT-MHR. Thermosetting resins have some process advantages. Modest changes to the compacting process are expected to resolve this issue.

For a past comparison (1984) of German and US fuel systems see:

Review of Pebble Bed HTGR Fuel and Graphite Technology for Potential Application in the US, GA Document Number 907634.

For a description of the German fuel system see:

Status of Qualification of High-Temperature Reactor Fuel Element Spheres, Nuclear Technology, W. Heit, et. al., 69 (1985), page 44.

Spherical Fuel Elements for Advanced HTR Manufacture and Qualification by Irradiation Testing, A. W. Mehner, et.al., Journal of Nuclear Materials, 171 (1990), pages 1-18.

Long Time Experience with the Development of HTR fuel Elements in Germany, Nuclear Engineering and Design, H. Nickel, et. al., 217 (2002), pages 141-151.

A recent reference (1994) containing much useful background material on the subject of fuel element fabrication is:

Fuel Compact Design Basis Report, DOE-GT-MHR-100212.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Design	Fuel Element	Volume fraction of particles in fuel zone
	Particle packing fraction (common)	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 7	Remedy: None required at present unless radical changes are made in the process
Rationale: This parameter helps determine the heat production of a fuel element and particle damage during fabrication is more likely at the higher particle loading.	Rationale: This parameter has been investigated to a fair extent over the years. Higher packing fractions (>35%) can result in greater particle breakage if the admixture method is used, limiting the choice to the injection method.	Closure Criterion: Satisfactory irradiation and accident performance.

Additional Discussion

Over the years, two main methods have been used for fabricating fuel elements. The first involved the use of a binder with high filler content. The particles were overcoated with a mixture of binder/filler and then pressed together with additional binder/filler (admixture compaction) to form the green fuel element. This method has advantages with respect to element shrinkage during both sequent process and irradiation. A disadvantage is that it is limited to a particle packing fraction of about 35%. An injection method can be used to achieve a higher packing fraction of about 60%. The particles and any shim are placed into a mold and a hot fluid pitch is injected under pressure into the mold. The disadvantage is that the pitch mixture has a lower filler content and the compact matrix has a higher shrinkage, which tends to show up as mircocracks and increased matrix porosity.

Volume packing fraction differences are a direct result of the smaller volume fraction available for fuel in the prismatic designs versus the pebble designs. Higher reactivity fuel such as plutonium may reduce the required packing fraction and allow the admix process to be used for the GT-MHR.

For excellent source of background material (some 15 different fuel element methods have been used) on the subject see:

Fuel Compact Design Basis Report, DOE-GT-MHR-100212

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Design	Fuel Element	Unconfined heavy metal outside SiC layer (common)
	Unconfined heavy metal outside SiC layer (common)	.

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: II	Level: 8	Remedy: None
Rationale: Unconfined heavy metal results in fission products in the primary circuit and potential for releases under accident conditions as well as possible maintenance concerns.	Rationale: Tests are available (burn-leach, HCl-leach, carbon analysis, TRIGA irradiation) that can detect low levels of U contamination. These tests are routinely done during fabrication.	Closure Criterion: None

Additional Discussion

Unconfined heavy metal can come from several sources. Some sources are: defective particles, particles broken during green fuel element fabrication, particles damaged during heat treatment of the green fuel element, and matrix/resin U impurities. Some of this U can be removed from fuel elements by leaching with hot HCl.

For a general discussion of the fuel fabrication and SiC defect issues see:

Nuclear Technology, Volume 35, Number 2, 1977 (entire issue is devoted to coated particle fuels)

TRISO Fuel Particle Coating Design Basis, DOE-GT-MHR-100225, 1994

Fuel Compact Design Basis Report, DOE-GT-MHR-100212, 1994

Data Support Document: Operating Procedures for SiC Defect Detection, DOE-HTGR-88359, 1991

An Assessment of the Methods for Determining Defect or Failure Fractions in HTGR Coated Particle Fuels and Their Relationship to Particle Microstructure, DOE-HTGR-88260, 1989

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Design	Fuel Element	The degree of homogeneity of the particles in the fuel element
	Particle distribution in fuel element	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 8	Remedy: None
Rationale: Inhomogeneous particle distribution within fuel elements can result in hot spots and possible fuel damage. Also, particles touching each other could result in damage.	Rationale: Fuel particle distribution can and has been investigated by X-ray scans, sectioning, plane-by-plane deconsolidation, and gamma scanning. Inhomogeneous packing and clustering is fairly easy to see.	Closure Criterion: None

Additional Discussion

For compact type elements uranium fuel homogeneity can be determined by gamma counting both halves of a fuel compact at the green stage. The relative spectrums or counts can be compared to each other and the relative loading determined. Similar methods can be used for other fuel types. Sectioning provides information, but is destructive. Uranium shows up well against the carbon background for X-ray analysis. Since there have been considerable developments both in gamma spectrometry and X-rays analysis, it is likely that an evaluation of the two techniques will be done before a new fuel facility is built.

For historical (1988) general QA issues see:

MHTGR Fuel Manufacturing Quality Assurance Plan, DOE-HTGR-88091

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Design	Fuel Element	Unfueled carbonaceous layer on outside of pebble
	Fuel free zone (Pebble)	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 8	Remedy: None
Rationale: The fuel pebble requires a fairly strong outer layer to shield the inner-fueled region from damage as the pebble is dropped several meters during its transient into the reactor.	Rationale: The Germans have studied this layer extensively and have had few failures with their high quality material.	Closure Criterion: None

Additional Discussion

The pebble is unique in that it is required to withstand being dropped from a height of several meters. Now only does it need a hard outer layer to withstand this impact, the outer layer must be tightly bound to the fuelled region to insure integrity of the pebble and good heat transfer throughout the life of the pebble.

For a description of pebble fabrication history see:

Fuel Compact Design Basis Report, DOE-GT-MHR-100212, 1994

For a description of the German pebble manufacturing process see:

Fuel Elements for the High Temperature Pebble Bed Reactor, L. Wolf, et. al., Nuclear Engineering and Design, 34, (1975), pages 93-108

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Design	Fuel Element	Layer on outside of outer PyC added after coating
	Particle overcoat (pebble)	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 7	Remedy: None for the German process. However, if overcoating is applied to compact type fuel elements, testing is warranted.
Rationale: This layer helps protect the particle during fuel element fabrication by slightly deforming, provides a spacing function, and integrates the particle into the matrix material.	Rationale: The Germans have developed an overcoating process that works very well for their pebbles. Also, other international efforts have achieved good results. US attempts to overcoat particles did not fair well.	Closure Criterion: None for the German process, but irradiation testing would be required for other fuel element types.

Additional Discussion

The particle overcoating process is really a part of the admix process for making fuel elements. It has been tried in conjunction with the US injection process, but fatal design problems lead to irradiation failure. High particle packing fractions favor the injection process.

For overcoating and fuel element fabrication see:

Fuel Compact Design Basis Report, DOE-GT-MHR-100212, 1994

For a description of the US problems that arose from an overcoating process see:

MHTGR TRISO-P Fuel Failure Evaluation Report, DOE-HTGR-90390, 1993

It is likely that the overcoating process will not be used for injection-molded fuel (compacts). Improvements in the injection process promise to resolve the historical difficulties.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Design	Outer PyC layer	Layer thickness and its standard deviation
	Thickness	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 8	Remedy: None needed for these dimensional parameters
Rationale: This layer performs a structural function during irradiation by placing a compressive force on the SiC layer.	Rationale: The layer thickness and its standard deviation can be fairly easily measured. The major uncertainties are in the material properties.	Closure Criterion: None.

Additional Discussion

According to the fuel models, the outer PyC functions as an important load-bearing component of the fuel particle. The major uncertainties associated with the layer come from material properties and not dimensional uncertainties.

Over the years there have been many, many papers and models published for HTGR fuel performance. A simple model to gain a conceptual understanding is:

Considerations Pertaining to the Achievement of High Burn-ups in HTR Fuel, D.G. Martin, Nuclear Engineering and Design, 213 (2002), pages 241-258

Also see (useful primer, but dated on fission product release):

Coated-Particle Fuels, T.G. Godfrey, et. al., ORNL-4324, 1968

A very short list of historical model references is:

A Mathematical Model for Calculating Stresses in a Pyrocarbon and Silicon Carbide Coated Fuel Particle, J. KAAE, Journal of Nuclear Materials, 29 (1969), page 249

Evaluation of High Temperature Gas Cooled Reactor Fuel Particle Coating Failure Models and Data, Tokar, NUREG-0111

An Explicit Solution for Stresses in Pyrocarbon-Coated Fuel Particles, Stevens, D.W., Nuclear Technology, 10, page 301

Improvement of a Method for Predicting Failure Rates of Coated Particles During Irradiation, Bongartz, K., Nuclear Technology, 35, page 379

A Mathematical Model for Calculating Stresses in a Four-Layer Carbon-Silicon-Carbide-Coated Fuel Particle, Kaae, J.L., Journal of Nuclear Materials, 32, (1969), page 322.

The Mechanical Design of TRISO-Coated Particle Fuels for the Large HTGR, T.D. Gulden, et. al., Nuclear Technology, 16 (1972), pages 100-109.

The modeling field is becoming active again and recent efforts are to employ much more complex structural and chemical models. Consult the researchers in the field for the most up to date models and theories.

A relatively recent design manual (these specifications may or may not be used in future fuel fabrication) by General Atomics is:

TRISO Fuel Particle Coating Design Basis, DOE-GT-MHR-100225

A recent review on the performance of pyrocarbon and its effect on fuel performance is:

Key Differences in the Fabrication, Irradiation and Safety Testing of U.S. and German TRISO-coated Particle Fuel and Their Implications on Fuel Performance, D.A. Petti, et. al., Nuclear Engineering and Design, 222 (2003) 281-297.
All these references tend to point to material properties and their uncertainties as the major issues.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Design	Outer PyC layer	Mass per unit volume
	Density	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 6	Remedy: Investigate pyrocarbon properties as a function of irradiation performance. Investigate new methods of characterizing pyrocarbon.
Rationale: The density of the PyC layer is connected to its material properties so it is important to control it.	Rationale: One can measure density fairly well, but the implications of the measurement are not clear. The PyC dimensionally changes under irradiation and this property is connected to the density among other things. Density can also affect the permeability of the coating. Connecting measurable material properties to pyrocarbon irradiation performance has been difficult and no foolproof method has been found to date.	Closure Criterion: A method or process for verifying pyrocarbon behavior under irradiation. (The German fuel has a defined process.)

Additional Discussion

The pyrocarbon layers have been the most difficult to characterize. The goal of relating measurable properties to irradiation performance has remained elusive leaving process conditions as part of the fuel QA. Density is one parameter, but so are others such as rate of material deposition in the coater. Density alone is not a complete enough specification for design.

For a general review of pyrocarbon fabrication see:

Nuclear Technology, Volume 35, Number 2, 1977 (entire issue is devoted to coated particle fuels)

For an evaluation of US and German pyrocarbons see:
Key Differences in the Fabrication, Irradiation and Safety Testing of U.S. and German TRISO-coated Particle Fuel and Their Implications on Fuel Performance, D.A. Petti, et. al Nuclear Engineering and Design, 222 (2003) 281-297.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Design	SiC Layer Thickness	Layer thickness and its standard deviation

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 8	Remedy: None needed for these dimensional parameters
Rationale: This layer performs a structural function during irradiation and acts as the major fission product barrier.	Rationale: The layer thickness and its standard deviation can be fairly easily measured. The major uncertainties are in the material properties.	Closure Criterion: None

Additional Discussion

The major issues with SiC are material properties rather than dimensions. The manufacturing QA has reached the point that missing and grossly out of specification material is extremely rare. See the pyrocarbon entries for model references and a discussion of past US problems.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Design	SiC Layer	Mass per unit volume
	Density	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 6	Remedy: Investigate SiC properties as a function of irradiation performance. Investigate new methods of characterizing SiC.
Rationale: The density of the SiC layer is connected to its material properties so it is important to control it.	Rationale: The density measurement is fairly well defined, but it is not sufficient to characterize the material. Density may affect the permeability of the coating to fission products. Connecting measurable material properties to irradiation performance has been difficult and no foolproof method has been found to date.	Closure Criterion: A method or process for verifying SiC behavior under irradiation and accident conditions. (The German fuel has a process.)

Additional Discussion

The density and the grain structure of the SiC help determine the fission product retention ability of this layer. Deposition rates and temperatures determine the final product. See the entries on pyrocarbon for references on design models.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Design	Inner PyC layer	Layer thickness and its standard deviation
	Thickness	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 8	Remedy: None needed for these dimensional parameters
Rationale: This layer performs a structural function during irradiation by placing a compressive force on the SiC layer. The layer also shields the fuel kernel from HCl during fabrication.	Rationale: The layer thickness and its standard deviation can be fairly easily measured. The major uncertainties are in the material properties.	Closure Criterion: None

Additional Discussion

The design models and past US results have shown that the IPyC layer is structurally important. Counter to intuition, too thick of a layer can increase the failure probability by increasing the stresses in the IPyC and those transmitted to the SiC, especially if the layer cracks. See the model references in the pyrocarbon entry, but also see:

MHTGR TRISO-P Fuel Failure Evaluation Report, DOE-HTGR-90390, 1993

for some of the issues that arise from a too thick IPyC

Since the IPyC shields the kernel from the HCl produced during SiC coating, a trade off condition is encountered. Thinner, higher porosity IPyC may be desirable for irradiation performance, but thicker, less porous IPyC is desired to limit the attack of the kernel from the HCl. In addition, the reactivity of the kernel is an issue as well.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Design	Inner PyC layer	Mass per unit volume
	Density	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 6	Remedy: Investigate pyrocarbon properties as a function of irradiation performance. Determine the tradeoff between irradiation behavior and kernel attack. Investigate new methods of characterizing pyrocarbon.
Rationale: The density of the PyC layer is connected to its material properties so it is important to control it.	Rationale: One can measure density fairly well, but the implications of the measurement are not clear. The PyC dimensionally changes under irradiation and this property is connected to the density among other things. Density can also affect the permeability of the coating to HCl and thus attack of the kernel during SiC coating. Connecting measurable material properties to pyrocarbon irradiation performance has been difficult and no foolproof method has been found to date.	Closure Criterion: A method or process for verifying satisfactory IPyC behavior under coating and irradiation.

Additional Discussion

See the previous entry for some of the issues relating to IPyC and the design tradeoffs. Also contact researchers as this issue is again under active investigation.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Design	Buffer Layer	Layer thickness and its standard deviation
	Thickness	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 8	Remedy: None needed for these dimensional parameters
Rationale: This layer attenuates recoils and provides a collection volume for the released gases	Rationale: The layer thickness and its standard deviation can be fairly easily measured.	Closure Criterion: None

Additional Discussion

The buffer layer has not been a subject of great controversy.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Design	Buffer Layer Density	Mass per unit volume

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 7	Remedy: Performance is not a major issue.
Rationale: The density of the PyC layer is connected to its material properties so it is important to control it. In particular, one wants to control void volume.	Rationale: The PyC dimensionally changes under irradiation and this property is connected to the density among other things. This layer has minimal structural properties so it is less of an issue than the inner and outer pyrocarbons. At present, void volume has not been an issue.	Closure Criterion: None

Additional Discussion

Density and microstructure affects irradiation performance. Great structural integrity is not required of the buffer layer, but minimal cracking is desired to limit kernel extrusion.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Design	Kernel	Design diameter with standard deviation
	Diameter	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 8	Remedy: None required for these dimensional measurements
Rationale: The diameter of the kernel affects the power generated and the gas production in a fuel particle. Off-sized kernels may affect coating behavior.	Rationale: Kernel diameters are fairly easy to measure and a considerable experience base exists in their manufacture.	Closure Criterion: None

Additional Discussion

Considerable experience exists in the manufacturing and measurement of kernels. Diameter measurement is not a major issue with fuel performance.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Design	Kernel Density	Mass per unit volume

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 8	Remedy: None required for this measurement
Rationale: The kernel density affects the power generated, the gas production, and perhaps the reactivity with HCl	Rationale: Kernel densities are fairly easy to measure and a considerable experience base exists in their manufacture	Closure Criterion: None

Additional Discussion

Measuring kernel density is not a major issue, but related items may be. One issue is reactivity to HCl liberated during SiC deposition. Kernels that are sensitive to HCl may require that the designer use thicker and/or less porous IPyC. This compromise could result in a less robust particle design unless a way to limit kernel reactivity is found.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Design	Kernel	Maximum and minimum axis lengths of particles
	Sphericity (max/min diameter)	

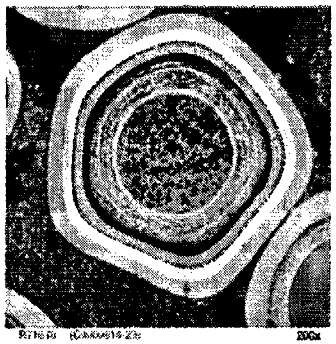
Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	Level: 8	Remedy: None
Rationale: The kernels need to be fairly round to be easily handled and free flowing during processing, but no serious irradiation effects have been noted for slightly out-of-round particles.	Rationale: There is a considerable experience base with kernel fabrication and inspection. Simple methods are available to remove deformed particles.	Closure Criterion: None

Additional Discussion

Detailed structural studies have reviewed the issue of non-spherical particles:

Treating Asphericity in Fuel Particles Pressure Vessel Modeling, G.K. Miller, D.C. Wadsworth, Journal of Nuclear Materials, 211 (1994), pages 57-69

Some additional problems could be forthcoming for seriously deformed particles, but in practice modest deviations seem to cause no serious problems. See photos at right. Current QC methods limit particles to those that are quite round and the odd shapes are no longer a problem.



Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Design	Kernel	Oxygen to uranium atomic ratio for UO_2 fuel
	Stoichiometry: Uranium to oxygen	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	Level: 8	Remedy: None
Rationale: The stoichiometry affects the amount of oxygen available for release and thus the particle gas pressure. The stoichiometry of UO_2 is not a big issue as radical changes are unlikely.	Rationale: Stoichiometry is not a problem for UO_2 and a great deal of experience is available for its production.	Closure Criterion: None

Additional Discussion

There is a great deal of experience with UO_2 fuels and controlling the stoichiometry within the desired limits is not considered to be a problem. Large deviations are not a problem.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Design	Kernel	Oxygen:carbon:uranium ratio for UCO
	Stoichiometry: Uranium to carbon and uranium to oxygen	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 6	Remedy: Investigate the production methods for UCO to assure they produce the desired product
Rationale: The stoichiometry affects the amount of oxygen available for release and thus the particle gas pressure. The stoichiometry of UO_2 is not a big issue, but it matters greatly for UCO.	Rationale: Stoichiometry is a more difficult problem for UCO as the material is harder to produce. Less experience is available for UCO large-scale production.	Closure Criterion: Satisfactory production of UCO.

Additional Discussion

UCO is a two-phase material that is much more difficult to make than UO_2. Significant deviations in the O/C ratio are important because the purpose of the material is to control the oxygen potential within the particle. Modest changes in the ratio can result in considerably more CO pressure in the kernel and the designer must bear in mind the implications for his fuel design.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Design	Kernel	Elemental constituents and amounts other than design
	Purity	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 9	Remedy: None
Rationale: Impurities can affect the neutronic behavior of the kernel and, in larger amounts, the chemical behavior of the kernel fabrication process.	Rationale: Chemical analysis of fuel is well developed.	Closure Criterion: None

Additional Discussion

Uranium handling and chemical analysis is well-understood process. The sources of the impurities may not be known, but their presence can be detected.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Design	Kernel	Weight fraction U-235 in total uranium
	Enrichment	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 9	Remedy: None
Rationale: The enrichment determined the nuclear properties of the kernel	Rationale: The methods of analyzing isotopic compositions are well developed	Closure Criterion: None

Additional Discussion

There is a considerable amount of experience in the isotopic analysis of uranium and it is not an issue.

Appendix H.3

Detailed PIRT Submittal by the SNL Panel Member

D. A. Powers

TRISO Fuel PIRT: Design

We have two peculiar situations in this section. The first of these unusual situations is that it is not possible now to produce fuel that reliably meets the reactor designer's own specifications. Though design specifications may exist, they are for fuel that will not be used in a power reactor. We don't know what it will take to produce fuel that reliably meets design requirements and must assume that changes to the current design will have to be done. Right now many, are operating in the belief that some relatively small changes in process have to be made to meet the standard set some 20 years ago by "German" fuel that itself cannot now be made. Such small changes may not be enough and it may be necessary to make radical changes in the design of the fuel to achieve the sought after level of reliability. We have to assume that eventually this level of reliability will be reached. When it is, the specifications for the fuel will be known with great accuracy. These specifications will most likely be in the form of tolerance ranges that really will not be especially useful for those predicting the performance of fuel in the reactor including fission product release during normal operations, upset conditions and during accidents.

The second peculiarity is most of the items listed below will be needed for the prediction of fission product release. But, it is not the specification values of these quantities that are needed except for gross exploratory calculations. What will be needed for realistic calculations and likely to be needed for regulatory processes involving advanced reactor is what actually gets manufactured and the way these quantities evolve during operations for the most part and during accidents in a few cases. In most cases there will be distributions of the values that are needed.

Consequently, the 'design' values for the quantities discussed below are just not very important. These same questions need to be addressed for the manufactured materials. The answers here, then, are nearly always, "The design specifications really are not very important. The design specifications will eventually be known rather well, but they are still nearly irrelevant."

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Design	Fuel Element	Specification of material properties
	Matrix material specification (common)	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level 8	Remedy: No need for remediation
Rationale: The analysis of anticipated fuel behavior during operations upset conditions and accidents requires that the materials and their properties be known. What is needed is not the design specifications of the materials. What is needed is the nature of the materials of the actual fuel and how this nature has evolved during operations	Rationale: The level of knowledge now of the material specifications is not high. It will be by the time fuel is ready to be added to the reactor.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Design	Fuel Element	Volume fraction of particles in fuel zone
	Particle packing fraction (common)	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 8	Remedy: No need for remediation
Rationale: The particle packing fraction will be an important quantity for the analysis of fuel behavior under conditions of operations, upsets or accidents. It is, however, not the design packing fraction that is of interest. It is the packing fraction of the fuel that is actually produced and installed in the reactor	Rationale: Though the design packing fraction cannot be specified with any definitiveness now, it will be specified quite well by the time the fuel is ready to be incorporated into the reactor. The specification will not be a number. It will be a range of packing fractions which will not be very useful of analysis of fuel performance. What will be needed is the actual distribution of packing fractions that actually go into the reactor	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Design	Fuel Element	Unconfined heavy metal outside SiC layer (common)
	Unconfined heavy metal outside SiC layer (common)	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 8	Remedy: No need for remediation
Rationale: The design specification of this quantity is not of any importance. What is important is what is the heavy metal contamination outside the SiC layer in material that is actually introduced into the reactor	Rationale: It will be very easy to provide a specification for this quantity. It will be rather more difficult to ascertain that this specification has been met. The specification will most likely be a range and what will needed for the analysis of fuel performance will be the distribution of values within this range – again, not the design specification, but the actual distribution for fuel going into the reactor.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Design	Fuel Element	The degree of homogeneity of the particles in the fuel element
	Particle distribution in fuel element	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 5	Remedy: No need for remediation except there will very much be a need to develop techniques to measure the homogeneity of the particle distribution in fuel compacts that are actually produced
Rationale: This will be a quite important quantity for the estimation of local neutronic behavior in compacts as well as understanding of the thermal environment for the particles both during operations and during accident or upset conditions. But, the design specification is not what is important. It is the actual homogeneity of fuel in the reactor that is important	Rationale: It is unlikely that a very high level of knowledge of the distribution will ever be generated. Rather some idealized approximate description of the distribution of particles in a fuel compact will be generated and used as a specification	Closure Criterion: What is really needed here is some description of what exactly needs to be measured and how well. This probably requires some careful neutronic analysis and some careful heat transfer analysis.

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Design	Fuel Element	Unfueled carbonaceous layer on outside of pebble
	Fuel free zone (Pebble)	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 8	Remedy: No need for remediation
Rationale: The unfueled carbonaceous layer could have a significant impact on the estimation of temperatures and fission product releases from the fuel. But, the layer of interest is that actually produced in fuel in the reactor and not the design specification of this layer	Rationale: Presumably the fuel design specifications will provide a range for the carboneceous layer – perhaps as a set of bounds which will not be of great use for the prediction of fission product release. Detailed knowledge of this specification is not know available because there is not an acceptable fuel that can be routinely and reliably produced	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Design	Fuel Element	Layer on outside of outer PyC added after coating
	Particle overcoat (pebble)	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 8	Remedy :no need for remediation
Rationale: This outer layer has some importance in fuel behavior. The design specification is inconsequential. What is important is what is done on fuel actually in the reactor	Rationale: Presumably, once an acceptable fuel can be produced reliably and routinely this specification will be provided. Without doubt, the specification will be in a form of limited utility for analysis of fuel performance.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Design	Outer PyC layer	Layer thickness and its standard deviation
	Thickness	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 8	Remedy: no need for remediation
Rationale: The outer PyC layer thickness will be of some importance for the analysis of fission product release as well as for estimation of local temperatures and temperature gradients. The specification, pe se, is not important. What actually gets produced is important and the evolution of this layer thickness and integrity with time will be important	Rationale: Because an adequate fuel cannot now be produced, there is little knowledge of this thickness nor of its standard deviation. But eventually when reliable fuel can be produced this layer thickness will be specified well, one presumes.	Closure Criterion: What is really needed is an agreed upon reliable method for measuring the layer thickness and its standard deviation in fuel that is manufactured. And also to monitor how it evolves under the operating conditions of the reactor which will not be uniform – that is, it will not be spatially uniform and certainly no temporally uniform. Even locally the system will be in thermal gradient and not in a uniform temperature.

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Design	Outer PyC layer	Mass per unit volume
	Density	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 8	Remedy no need for remediation:
Rationale: The density of the outer PyC layer will be modestly important for estimating fission product transport and for the calculation of temperatures in local regions. Again, the specification will not be of any importance. What will be important is what the distribution of densities that actually exist in the fuel . This is beyond even what is manufactured since this density will evolve during operations.	Rationale: One can safely assume that once some method for manufacture of reliable fuel is available this specification will be known well.	Closure Criterion: There will be a very significant need to have a way to measure the density of the outer PyC layer in manufactured fuel and predict how it evolves in the environment of the reactor during operations.

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Design	SiC Layer	Layer thickness and its standard deviation
	Thickness	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 8	Remedy no need for remediation:
Rationale: See discussion above for the outer PyC layer since it applies as well for this layer	Rationale: See discussion above for the outer PyC layer since it applies as well for this layer	Closure Criterion: See discussion above for the outer PyC layer since it applies as well for this layer

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Design	SiC Layer	Mass per unit volume
	Density	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 8	Remedy: No need for remediation
Rationale: See discussion above for the outer PyC layer since it applies as well for this layer	Rationale: See discussion above for the outer PyC layer since it applies as well for this layer	Closure Criterion See discussion above for the outer PyC layer since it applies as well for this layer:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Design	Inner PyC layer	Layer thickness and its standard deviation
	Thickness	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 8	Remedy :No need for remediation
Rationale: See discussion above for the outer PyC layer since it applies as well for this layer	Rationale: See discussion above for the outer PyC layer since it applies as well for this layer	Closure Criterion: See discussion above for the outer PyC layer since it applies as well for this layer

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Design	Inner PyC layer	Mass per unit volume
	Density	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 8	Remedy: No need for remediation
Rationale: See discussion above for the outer PyC layer since it applies as well for this layer	Rationale: See discussion above for the outer PyC layer since it applies as well for this layer	Closure Criterion: See discussion above for the outer PyC layer since it applies as well for this layer

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Design	Buffer Layer Thickness	Layer thickness and its standard deviation

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 8	Remedy: No need for remediation
Rationale: See discussion above for the outer PyC layer since it applies as well for this layer	Rationale: See discussion above for the outer PyC layer since it applies as well for this layer	Closure Criterion: See discussion above for the outer PyC layer since it applies as well for this layer

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Design	Buffer Layer	Mass per unit volume
	Density	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 8	Remedy No need for remediation:
Rationale: See discussion above for the outer PyC layer since it applies as well for this layer	Rationale: See discussion above for the outer PyC layer since it applies as well for this layer	Closure Criterion: See discussion above for the outer PyC layer since it applies as well for this layer

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Design	Kernel	Design diameter with standard deviation
	Diameter	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 8	Remedy No need for remediation:
Rationale: The bounding design specification of kernel diameters will have no importance in the estimation of fuel performance and fission product release. What will be needed is what actually goes into the reactor fuel and how these kernels evolve in geometry under the conditions of thermal gradients thermal cycling and intense irradiation when adjacent to a reactive material like carbon.	Rationale: Currently reliable fuel cannot be produced. Once presumes that current thoughts on kernel design will evolve in the effort to produce reliable fuel. So one has to admit that the current specification for the kernel diameter is not well known. But, once reliable fuel can be made, the specification of the kernel diameter will be known well. It will likely be a range. For analysis of fuel performance what will be needed is not the specification but what actually goes into the reactor cast in the form of a continuous probability distribution	Closure Criterion: There is a need for a reliable technique to measure what is actually in the fuel and to monitor how the kernel geometry evolves under the conditions of irradiation, thermal gradients and thermal cycling while in contact with a reactive material like carbon.

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	*Definition*
Design	Kernel	Mass per unit volume
	Density	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 7	Remedy No need for remediation:
Rationale: The initial fuel density will affect its performance during reactor operations. But what is needed is not the density specification. The need is for the density of fuel that actually goes into the reactor	Rationale: Not known well now, but will be known well once fuel can be reliably produced	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Design	Kernel	Maximum and minimum axis lengths of particles
	Sphericity (max/min diameter)	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 3	Remedy: No need for remediation
Rationale: Lack of sphericity of the kernel is very important since it can make the codes used for predicting diffusive process like fission product release and heat transfer complicated. The design specification on this quantity is inconsequential. What is needed is information on the lack of sphericity of the fuel that goes into the reactor and how it evolves with operation.	Rationale: This probably is not getting a great deal of attention from those designing specifications for fuel	Closure Criterion: What will be very much needed is an agreed upon way to measure the deviation from sphericity both in fuel that goes into the reactor and in fuel as it evolves within the reactor

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Design	Kernel	Oxygen to uranium atomic ratio for UO_2 fuel
	Stoichiometry: Uranium to oxygen	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 5	Remedy: No remediation needed
Rationale: The stoichiometry of fuel affects the diffusion of fission products through that fuel. It also affects the potential for the fuel to react with the carbon. The design specification is not important and probably won't characterize the fuel very well. What will be needed is the O to M ratio for fuel that actually goes into the reactor and a model of how this O to M ratio varies during operation in light of internal buffering by the MoO2/Mo equilibrium as well as reaction with the carbon adjacent to the fuel kernel.	Rationale: control of O to M ratios in urania based fuels has reached sufficient sophistication that fairly tight specifications can be imposed	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Design	Kernel	Oxygen:carbon:uranium ratio for UCO
	Stoichiometry: Uranium to carbon and uranium to oxygen	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level:3	Remedy Need models of the UOC system :
Rationale: The phase relations in the U-O-C system are not known well enough to predict with certainty how sensitive fuel behavior is to the precise stoichiometry	Rationale: Current knowledge of the U_O_C system even at the thermodynamic level is at best rudimentary. There is limited understanding of the effects of non-stoichiometry and the effects of irradiation in a thermal gradient on non-equilibrium phase separation. Transport properties of non-stoichiometric materials in the U-O-C system remain largely unexplored.	Closure Criterion: We are going to have to have predictive modeling of both the thermodynamics of the U-O-C system and the transport properties of materials in this system to have specifications of composition of fuel. Existing modeling is not at all encouraging because of the complexities of non-stoichiometry

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Design	Kernel	Elemental constituents and amounts other than design
	Purity	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 8	Remedy: No remediation needed
Rationale: The effects of impurities on the behavior of urania-based fuels have been relatively well established for conventional reactor fuels. Though important levels of impurities such as chloride and some metal oxides such as iron oxide can drastically affect behavior, the fluorite structure is amazingly forgiving for most commonly encountered levels of impurity. Where the material is unforgiving is gas generation such as the reaction during operation of carbon impurities with the oxide to form CO that pressurizes the cladding. In the case of the SiC 'pressure vessel' for coated particle fuel, this may not be a concern since the reaction with buffer carbon will occur regardless of the purity of the fuel. Still chloride contamination will be a concern as will iron oxide contamination.	Rationale: The specification of urania purity to avoid deleterious fuel behavior has been established by experience with conventional fuel behavior. Experience with the urania in coated particle fuel is, of course quite limited, but, still, there should be no problem providing a specification that will remove this issue from consideration in the analysis of fuel performance and fission product release during normal operations, upset conditions and accidents.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Design	Kernel Enrichment	Weight fraction U-235 in total uranium

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 9	Remedy: No need for remediation
Rationale: The enrichment of the fuel does not normally enter into the analysis of most severe reactor accidents except that it may affect the fission product inventory. Enrichment will affect reactivity insertion accident analysis from the point of susceptibility and energy input during the accident. The energy input will, of course, affect the fission product release associated with the event in a fairly complicated, and not too strong a way. Enrichment of the fuel also determines the extent of burnup of the fuel. As burnup gets high , the fuel kernel geometry and integrity gets degraded very badly to the point it will be difficult to identify a kernel at burnups in excess of about to GWd/t. This makes the usual approaches to analysis of fission product release exceptionally difficult. This kind of distortion of the kernel from idealized spherical symmetry is very likely to happen as a consequence of the kernel being in a thermal gradient during operations and reacting with the adjacent carbon, so it is an issue that the modelers of fission product release are going to have to confront for a variety of reasons.	Rationale: Presumably the reactor design will specify rather exactly what the enrichment of the fuel will be.	Closure Criterion:

Additional Discussion

APPENDIX I

MEMBERS OF TRISO FUEL PIRT PANEL

Robert N. Morris

R. N. Morris received his Bachelor of Science degree in Electrical Engineering from Wayne State University in 1978, his Masters Degree in 1979 from the Georgia Institute of Technology and continued on to receive his Ph. D. in Nuclear Engineering from the Georgia Institute of Technology in 1984. His research efforts were in the field of fusion energy and computational plasma physics. The Oak Ridge National Laboratory has employed Robert Morris since the spring of 1984 and his job experience has included a wide variety of tasks from plasma physics computational modeling to nuclear fuel post irradiation examination (PIE). Past work has included computational and theoretical analysis of the Advanced Toroidal Facility and other three dimensional magnetic fusion candidate configurations. Topics included stellarator magnetic configurations, neutral beam heating, and plasma equilibrium and stability. Recent work has concentrated on irradiated fuel examination, irradiated capsule measurements, and High Temperature Gas-Cooled Reactor (HTGR) fuel accident behavior. This experience has included both HTGR program (New Production Reactor, Civilian HTGR, and Gas Turbine Modular High Temperature Gas-Cooled Reactor (GT-MHR)) and Mixed Oxide (MOX) LWR (Fissile Materials Deposition Program (FMDP)) irradiated fuel examinations and analysis. He has authored and co-authored over 60 technical reports, proceedings, and journal articles.

Current work is focused on participation in the FMDP, both the LWR MOX fuel and the Russian Federation GT-MHR program. Domestic work is involved in the post irradiation examination of LWR MOX test fuel containing weapons grade plutonium and the Russian effort is technical support of coated particle fuel development, also containing weapons grade plutonium. He is also currently involved with the Advanced Gas-Cooled Reactor program in the areas of coated particle fuel PIE planning and fuel accident behavior.

David A. Petti

Dr. Petti is currently an Engineering Fellow in the Advanced Nuclear Energy Directorate at the Idaho National Engineering and Environmental Laboratory. He has fifteen years of experience at the INEEL where he has worked in programs that have dealt with issues related to nuclear materials, nuclear safety, and radiological source term behavior in high temperature applications.

Dr. Petti is currently a Principal Investigator for gas cooled reactor research at INEEL. related to coated particle fuel modeling and material properties development. He is an INEEL technical lead for Advanced Gas Reactor Fuel Qualification and Development Program focusing on irradiation testing and fuel modeling. He was recently named Chief Scientific Investigator for the United States by the DOE to participate in IAEA Coordinated Research Program on Coated Particle Fuel Technology. He has directed and been personally involved in INEEL research related to reactor safety issues for gas cooled reactors..

Dr. Petti was also heavily involved in the development of SiC-coated gas reactor fuel and targets for the New Production Modular High Temperature Gas Reactor (NP-MHTGR). His areas of responsibility included the technical development and execution of the fuel and fission product development qualification program, the development of the technical bases for irradiation and safety testing required to support the NP-MHTGR tritium target demonstration and qualification program and the modeling of TRISO-coated particle fuel and targets, and the radiological source term for the NP-MHTGR. He has served on technical committees for the Department of Energy. He has received a number of awards including two Literary Awards from the Materials Science and Technology Division of the American Nuclear Society. He is the author or co-author of more than 50 technical publications.

Dana A. Powers

D. A. Powers received his Bachelor of Science degree in chemistry from the California Institute of Technology in 1970. He received a Ph.D. degree in Chemistry, Chemical Engineering and Economics in 1975 from the California Institute of Technology. His research for this degree program included magnetic properties of basic iron compounds, catalyst characterization and the rational pricing of innovative products. In 1974, Powers joined Sandia National Laboratories where he worked in the Chemical Metallurgy Division. His principal research interests were in high temperature and aggressive chemical processes. In 1981, he became the supervisor of the Reactor Safety Research Division and conducted analytic and experimental studies of severe reactor accident phenomena in fast reactor and light water reactors. These studies included examinations of core debris interactions with concrete, sodium interactions with structural materials, fission product chemistry under reactor accident conditions, aerosol physics, and high temperature melt interactions with coolant. In 1991, Powers became the acting Manager of the Nuclear Safety Department at Sandia that was involved in the study of fission reactor accident risks and the development of plasma-facing components for fusion reactors. Powers has also worked on the Systems Engineering for recovery and processing of defense nuclear wastes and has developed computer models for predicting worker risks in Department of Energy nuclear facilities. Dr. Powers was promoted to Senior Scientist at Sandia in 1997. Dr. Powers is the author of 103 technical publications.

From 1988 to 1991, Dr. Powers served as a member of the Department of Energy's Advisory Committee on Nuclear Facility Safety (ACNFS). In 1994, he was appointed to the Advisory Committee on Reactor Safeguards (ACRS) for the U.S. Nuclear Regulatory Commission. He was Vice Chairman of the ACRS in 1997 and 1998. He was elected Chairman in 1999 and 2000. In 2001, Dr. Powers received the Distinguished Service Award from the US Nuclear Regulatory Commission. Dr. Powers has served on committees for the National Research Council involved with the safety of Department of Energy facilities and the nuclear safety of reactors in the former Soviet Union. He has been an instructor for courses on reactor safety and accident management held by the International Atomic Energy Agency in several countries.

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M. B. Rubin, NRC Project Manager

11. ABSTRACT (200 words or less)

TRISO-coated particle fuel is to be used in the next generation of gas-cooled reactors. In anticipation of future licensing applications for gas-cooled reactors, the United States Nuclear Regulatory Commission (NRC) seeks to fully understand the significant features of TRISO-coated particle fuel design, manufacture, and operation, as well as behavior during accidents. The objectives of the TRISO Phenomena Identification and Ranking Table (PIRT) program are to (1) identify key attributes of gas-cooled reactor fuel manufacture which may require regulatory oversight, (2) provide a valuable reference for the review of vendor fuel qualification plans, (3) provide insights for developing plans for fuel safety margin testing, (4) assist in defining test data needs for the development of fuel performance and fission product transport models, (5) inform decisions regarding the development of NRC's independent reactor fuel performance code and fission product transport modules, (6) support the development of NRC's independent models for source term calculations, and (7) provide insights for the review of vendor fuel safety analyses. To support those objectives, the NRC commissioned a PIRT panel to identify and rank the factors, characteristics, and phenomena associated with TRISO-coated particle fuel. PIRTs were developed for (1) Manufacturing, (2) Operations, (3) a Depressurized Heatup Accident, (4) a Reactivity Accident, (5) a Depressurization Accident with Water Ingress, and (6) a Depressurization Accident with Air Ingress.

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