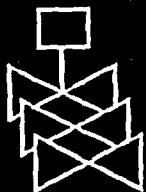
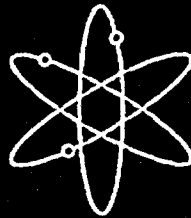


**TRISO-Coated Particle Fuel
Phenomenon Identification and
Ranking Tables (PIRTs) for
Fission Product Transport
Due to Manufacturing,
Operations, and Accidents**

Main Report

**U.S. Nuclear Regulatory Commission
Office of Nuclear Regulatory Research
Washington, DC 20555-0001**



**NUREG/CR-6844, Volume 1, has been
reproduced from the best available copy.**

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.

CONTENTS

	Page No.
Abstract	iii
Executive Summary	xiii
Foreword	xv
Acknowledgments	xvi
Acronyms and Abbreviations.....	xvii
1. INTRODUCTION.....	1-1
1.1. Need for Identification and Ranking	1-2
1.2. The PIRT Process.....	1-3
1.3. PIRT Process Application for the TRISO-Coated Particle Fuel PIRT	1-6
1.4. Report Organization	1-12
1.5. PIRT Panel Membership	1-14
1.6. References	1-14
2. TRISO-COATED FUEL PARTICLE PERFORMANCE	2-1
2.1. General Description of Coated Particle Fuel and Fuel Element	2-1
2.1.1. Operational Requirements.....	2-1
2.1.2. Basic Fuel Element.....	2-1
2.2. Design Function of Each Component	2-4
2.2.1. General	2-4
2.2.2. Kernel	2-4
2.2.3. Buffer Layer	2-13
2.2.4. Inner Pyrocarbon Layer.....	2-15
2.2.5. SiC Layer.....	2-18
2.2.6. Outer Pyrocarbon Layer	2-20
2.2.7. Fuel Element	2-23
2.3. Manufacturing	2-24
2.3.1. General	2-24
2.3.2. Kernel	2-26
2.3.3. Coating Particles	2-29
2.3.4. Fuel Element Manufacture	2-35
2.4. Normal Operation.....	2-41
2.4.1. General	2-41
2.4.2. Kernel	2-43
2.4.3. Buffer	2-44
2.4.4. IPyC Layer	2-46
2.4.5. SiC Layer.....	2-46
2.4.6. OPyC Layer.....	2-48
2.4.7. Fuel Element	2-49
2.5. Accident Conditions.....	2-51
2.5.1. Heatup Accident.....	2-52
2.5.2. Air and/or Water Intrusion Accident.....	2-61
2.5.3. Water Ingress Accident Phenomena	2-64
2.5.4. Air Ingress Accident Phenomena.....	2-74

2.5.5.	Reactivity Accident.....	2-84
2.6.	Summary of Fuel Failure Mechanisms	2-91
2.6.1.	Pressure Vessel Failure	2-91
2.6.2.	Irradiation-induced IPyC Cracking and Debonding.....	2-92
2.6.3.	Kernel Migration	2-92
2.6.4.	Fission Product/Coating Layer Chemical Interactions	2-93
2.6.5.	Matrix/OPyC Interaction.....	2-93
2.6.6.	As-Manufactured Defects	2-94
2.6.7.	SiC Thermal Decomposition.....	2-94
2.6.8.	Enhanced SiC Permeability and/or SiC Degradation.....	2-94
2.6.9.	Chemical Attack (Ingress Accidents).....	2-95
2.6.10.	Reactivity Insertion (Accident).....	2-95
2.7.	References	2-95
3.	FISSION PRODUCT TRANSPORT IN TRISO-COATED FUEL PARTICLES	3-1
3.1.	Introduction.....	3-1
3.2.	The Fuel Kernel.....	3-1
3.2.1.	Recoil	3-1
3.2.2.	Chemical Reaction at the Fuel Kernel Boundary.....	3-2
3.2.3.	Booth Diffusion.....	3-2
3.2.4.	Vaporization: Fission Product Chemical Form.....	3-6
3.3.	The Buffer Layer.....	3-7
3.3.1.	Thermal Behavior of the Buffer.....	3-8
3.3.2.	Fission Product Transport in a Porous Medium.....	3-11
3.3.3.	Thermal Diffusion	3-17
3.4.	The Inner and Outer Pyrocarbon Layers	3-20
3.4.1.	Gas Phase Fission Product Transport.....	3-21
3.4.2.	Metallic Fission Product Transport and Trapping.....	3-22
3.4.3.	Influence of PyC Structure on Transport in the Layer	3-25
3.5.	The SiC Layer	3-26
3.5.1.	Transport Mechanisms	3-26
3.5.2.	Grain Boundary Diffusion.....	3-28
3.5.3.	Influence of SiC Microstructure on Fission Product Transport	3-31
3.6.	A Simplified Integral Fission Product Transport Model.....	3-32
3.7.	Fission Product Transport in Failed Fuel Particles	3-37
3.7.1.	Short-lived Fission Gases.....	3-38
3.7.2.	Long-lived Fission Gases and Fission Metals.....	3-39
3.7.3.	Water and Air Ingress	3-40
3.8.	Fission Product Transport Factors.....	3-40
3.9.	Summary	3-41
3.10	References	3-42
4.	TRISO-COATED PARTICLE FUEL PHENOMENA IDENTIFICATION AND RANKING TABLES (PIRTS).....	4-1
5.	TRISO-COATED PARTICLE FUEL PIRT ANALYSIS AND SUMMARY.....	5-1
5.1.	General TRISO-Coated Particle Fuel PIRT Findings	5-1

5.2.	Manufacturing PIRT Analysis	5-7
5.3.	Operations PIRT Analysis.....	5-8
5.4.	Depressurization Heatup Accident PIRT Analysis	5-10
5.5	Reactivity Accident PIRT Analysis	5-12
5.6.	Depressurization Accident with Water Ingress PIRT Analysis	5-13
5.7.	Depressurization Accident with Air Ingress PIRT Analysis.....	5-15
5.8	Lesson Learned	5-18
	5.8.1. Development of PIRT Objectives	5-18
	5.8.2. PIRT Panel Size	5-18
	5.8.3. Documentation of Rationales	5-19

FIGURES

1-1	An example of a TRISO-coated particle fuel particle.....	1-1
1-2	PIRT Process	1-5
1-3	TRISO-coated particle fuel temperature transient for depressurized heatup scenario.....	1-8
2-1	Schematic of the four-layer particle design.....	2-2
2-2	Fuel element components.....	2-3
2-3	Three of many possible designs for a fuel element. The compact design can also be used as part of a pin in block design.....	2-4
2-4	Increase in particle pressure as a function of burnup for a UO ₂ kernel (representative of order of magnitude calculation)	2-6
2-5	Pressure vessel failure in HRB-8, Specimen 5 (UO ₂).....	2-7
2-6	Illustration of the Amoeba Effect. Carbon is transported from the hot side to the cool side.....	2-8
2-7	Oxide kernel fuel exhibiting the amoeba effect	2-9
2-8	High burnup kernel showing the loss of crystal structure and the development of large voids	2-10
2-9	Oxygen distribution in a UCO kernel	2-11
2-10	An example of a distorted Buffer Layer (HRB-21) (DOE-HTGR-100229)	2-14
2-11	Example of pyrocarbon layer failure (BISO fuel).....	2-16
2-12	CO oxidation of SiC (WAR UO ₂ kernel at ~1500°C in HRB-10).....	2-17
2-13	Qualitative stresses in coated particle layers for a moderate particle	2-19
2-14	Particles broken during irradiation due to matrix-particle interaction. Left - BISO particle / Right TRISO particle	2-21
2-15	Diagram of a coater (from ORNL-4324)	2-25
2-16	Flow diagram of external gelation kernel fabrication process	2-28
2-17	Flow diagram of the continuous coating process	2-30
2-18	SiC structure as a function of coater temperature	2-31
2-19	Performance of non-spherical particles.....	2-32
2-20	Illustration of the Admix fuel element forming process	2-36
2-21	Illustration of the injection method.....	2-37
2-22	Green fuel element bakeout process.....	2-39
2-23	Illustration of selected particle failure mechanisms during normal operations	2-42
2-24	Model calculation-pebble fractional release over its lifetime (IAEA TECHDOC-978)...	2-43
2-25	Kernel performance issues. Left-UO ₂ kernel that is moving up the temperature gradient. Right-UC ₂ kernel showing accumulation of rare earth fission products on cold side of the particle. Hot side is at the top of the photo	2-44
2-26	Failure in a BISO particle due to a missing buffer layer.....	2-45
2-27	Pd migration:70% burnup Pu kernel. FTE-13, PuO _{1.68} , 1150°C, Polarized light	2-48
2-28	Time versus temperature heatup accident curve considered by the PIRT panel.....	2-52
2-29	⁸⁵ Kr releases as a function of burnup and test temperature (IAEA TECHDOC-978)	2-53

2-30	Effective SiC thinning due to corrosion and decomposition. Comparison of frequency factors for failure (data from Goodin, 1898).....	2-57
2-31	Oxidation diagram for carbides of interest.....	2-57
2-32	Fission product release from a fuel sphere at 1600°C (IAEA TECDOC-978).....	2-59
2-33	⁸⁵ Kr release as a function of heating temperature (IAEA TECDOC-978)	2-59
2-34	An illustration of the chemical attack of a fuel element and fuel particles.....	2-63
2-35	⁸⁵ Kr release from a fuel sphere exposed to water vapor (AVR 92/7, type GLE-3, 9.2% FIMA) at 800C (IAEA TECDOC-978).....	2-65
2-36	Sphere particle failure fractions and 10 unbonded particles (1500°C line) heated in air (IAEA TECDOC-978).....	2-65
2-37	Exposure to water vapor causes the kernel to restructure and release much of its stored inventory. (from Meyers, DOE-HTGR-88486).....	2-66
2-38	Stored fission gas release versus water partial pressure for exposed kernels at 770°C for experiments HFR-B1 and HRB-17 (IAEA TECDOC-978).....	2-67
2-39	Oxidation of two similar fuel spheres in air. Top is from AVR 92/8, 9% FIMA, bottom is from AVR 92/22, 8.8% FIMA (IAEA TECDOC-978)	2-83
2-40	Particle failure rate versus pulse energy deposition (IAEA TECDOC-978)	2-85
3-1	Comparison of measured diffusivities of fission gases and some fission metals in UO ₂ kernels of coated particle fuel	3-3
3-2	Calculated fission product release from 500 micron UO ₂ kernel at 900 °C.....	3-5
3-3	Calculated fission product release from 500 micron UO ₂ kernel at 1200 °C.....	3-5
3-4	Influence of cyclic temperature in a pebble bed reactor on fission product release from a 500 micron UO ₂ kernel	3-6
3-5	Calculated effect of particle power on temperature gradient and temperature drop across the buffer layer of a standard 500-micron UO ₂ German particle.....	3-9
3-6	Different states of the buffer in coated particles following irradiation in the U.S.....	3-10
3-7	Calculated effective diffusivities for Knudsen and viscous diffusion.....	3-16
3-8	Calculated effect of thermal diffusion and irradiation on the distribution and transport of fission products in the coated particle	3-19
3-9	Measured fission product diffusivities in low temperature isotopic (LTI) PyC	3-21
3-10	Comparison of measured fission product diffusivities in PyC to permeability data (checkerboard box) Knudsen data, (black and white hatched box) and viscous (gray box) diffusion estimates.....	3-22
3-11	Calculated effects of trapping on apparent Cs diffusivity in PyC.....	3-24
3-12	Measured diffusion coefficients of Xe, Cs, Sr and Ag in SiC	3-27
3-13	Comparison of data for C and Si self-diffusion coefficient (hatched box) and Fe and Cr grain boundary diffusivities (gray box) with fission product diffusivities inferred from integral release measurements on coated particles	3-28
3-14	Schematic of grains and grain boundary	3-29
3-15	Influence of SiC microstructure on fission product transport	3-31
3-16	Calculated fractional release from a coated fuel particle during 1600 °C heating following a three-year irradiation at 1200 °C.....	3-33

3-17	Calculated release from a coated fuel particle during 1600 °C heating following a three-year ten-cycle PBR irradiation between 600 and 1200 °C.....	3-34
3-18	Calculated fuel temperature transient during a conduction cooldown.....	3-35
3-19	Calculated fractional diffusional release from TRISO coated particle during a conduction cooldown following a three-year ten-cycle PBR irradiation.....	3-35
3-20	Effect of segregation coefficient on fractional release during heating.....	3-37
3-21	Comparison of failed particle model (R/B) results	3-39

TABLES

1-1	Importance Ranks and Definitions	1-11
1-2	Knowledge Levels and Definitions	1-12
2-1	Oxygen Excess per Fission	2-6
2-2	Migration Factors	2-8
2-3	Order of Magnitude Estimates for CO Pressure.....	2-12
2-4	Typical German Kernel Specifications	2-13
2-5	Kernel Design Factors Identified By the PIRT Panel	2-13
2-6	Typical German Buffer Layer Specification.....	2-14
2-7	Buffer Layer Design Factors Identified By The PIRT Panel	2-15
2-8	Typical German IPyC Layer Specifications.....	2-17
2-9	IPyC Layer Design Factors Identified By The PIRT Panel	2-18
2-10	Typical German SiC Layer Specifications.....	2-20
2-11	SiC Layer Design Factors Identified By The PIRT Panel	2-20
2-12	Typical German OPyC Layer Specifications	2-22
2-13	OPyC Design Factors Identified By The PIRT Panel	2-22
2-14	Historic Reference German Fuel Element Specifications.....	2-24
2-15	Fuel Element Design Factors Identified By The PIRT Panel	2-24
2-16	Manufacturing Process Phenomena Identified By The PIRT Panel	2-27
2-17	Kernel Properties and QC Methods	2-28
2-18	Kernel Manufacturing Factors Identified By The PIRT Panel	2-29
2-19	Coating Layer Product Factors and Typical QC Methods	2-33
2-20	Manufacturing Layer Product Factors Identified by the PIRT Panel.....	2-34
2-21	Typical Fuel Element QC Methods.....	2-40
2-22	Fuel Element Manufacturing Factors Identified by the PIRT Panel	2-40
2-23	Kernel Operating Factors Identified By The PIRT Panel	2-45
2-24	Buffer Operating Factors Identified By The PIRT Panel.....	2-46
2-25	IPyC Operating Factors Identified By The PIRT Panel	2-47
2-26	SiC Operating Factors Identified By The PIRT Panel	2-48
2-27	OPyC Operating Factors Identified by The PIRT Panel	2-49
2-28	Fuel Element Operating Factors Identified By The PIRT Panel.....	2-50
2-29	Kernel Heatup Accident Factors Identified By The PIRT Panel	2-54
2-30	Buffer Layer Heatup Accident Factors Identified By The PIRT Panel	2-55
2-31	IPyC Layer Heatup Accident Factors Identified By The PIRT Panel.....	2-56
2-32	SiC Layer Heatup Accident Factors Identified By The PIRT Panel.....	2-58
2-33	Identified OPyC Heatup Accident Factors Identified By The PIRT Panel.....	2-60
2-34	Fuel Element Heatup Accident Factors Identified By The PIRT Panel.....	2-61
2-35	Kernel Water Ingress Accident Factors Identified By The PIRT Panel	2-68
2-36	Buffer Layer Water Ingress Accident Factors Identified By The PIRT Panel.....	2-69
2-37	IPyC Layer Water Ingress Accident Factors Identified By The PIRT Panel.....	2-70
2-38	SiC Layer Water Ingress Accident Factors Identified By The PIRT Panel	2-72

2-39	OPyC Layer Water Ingress Accident Factors Identified By The PIRT Panel	2-73
2-40	Fuel Element Water Ingress Accident Factors Identified By The PIRT Panel	2-74
2-41	Kernel Air Ingress Accident Factors Identified By The PIRT Panel	2-75
2-42	Buffer Layer Air Ingress Accident Factors Identified By The PIRT Panel	2-77
2-43	IPyC Layer Air Ingress Accident Factors Identified By The PIRT Panel	2-78
2-44	SiC Layer Air Ingress Accident Factors Identified By The PIRT Panel	2-79
2-45	OPyC Layer Air Ingress Accident Factors Identified By The PIRT Panel	2-80
2-46	Fuel Element Air Ingress Accident Factors Identified By The PIRT Panel	2-82
2-47	Kernel Reactivity Accident Factors Identified By The PIRT Panel	2-86
2-48	Buffer reactivity Accident Factors Identified By The PIRT Panel	2-87
2-49	IPyC Layer Reactivity Accident Factors Identified By The PIRT Panel	2-88
2-50	SiC Layer Reactivity Accident Factors Identified By The PIRT Panel	2-89
2-51	OPyC Layer Reactivity Accident Factors Identified By The PIRT Panel	2-90
2-52	Fuel Element Reactivity Insertion Factors Identified by the PIRT Panel	2-90
3-1	Calculated Temperature Drops Across Layers of a Coated Particle	3-9
3-2	Effects of Particle Power on Buffer in Coated Particle Fuel	3-11
3-3	Calculated Effect of Increased Temperature and Increased SiC Diffusivity on Fractional Diffusional Releases from TRISO Coated Particles	3-36
3-4	Fission Product Transport Phenomenon Identified by the PIRT Panel	3-41
4-1	TRISO-coated particle fuel Manufacturing Summary PIRT	4-3
4-2	TRISO-coated particle fuel Operations Summary PIRT	4-6
4-3	TRISO-coated particle fuel Depressurized Heatup Accident Summary PIRT	4-11
4-4	TRISO-coated particle fuel Reactivity Accident Summary PIRT	4-16
4-5	TRISO-coated particle fuel Depressurization Accident with Water Ingress Summary PIRT	4-21
4-6	TRISO-coated particle fuel Depressurization Accident with Air Ingress Summary PIRT	4-29
5-1	TRISO-coated particle fuel Factors, Characteristics, and Phenomena Ranked High	5-3
5-2	Significant Importance and Knowledge Level Statistics for Manufacturing	5-7
5-3	Significant Importance and Knowledge Level Statistics for Operations	5-8
5-4	Significant Importance and Knowledge Level Statistics for the Depressurization Heatup Accident	5-10
5-5	Significant Importance and Knowledge Level Statistics for the Reactivity Accident	5-12
5-6	Significant Importance and Knowledge Level Statistics for the Depressurization Accident With Water Ingress	5-14
5-7	Significant Importance and Knowledge Level Statistics for the Depressurization Accident With Air Ingress	5-16

EXECUTIVE SUMMARY

Most nuclear power reactors presently operating throughout the world are water-cooled. The core of these reactors consists of arrays of fuel bundles, each bundle containing a number of fuel pins. Each fuel pin contains a stack of cylindrical, ceramic UO₂ fuel pellets contained within a sheath of metallic cladding.

The fuel forms for gas-cooled reactors are very different. The TRISO-coated fuel particle is a spherical layered composite about 1 mm in diameter. It consists of a kernel of uranium dioxide surrounded by a porous graphite buffer layer. Surrounding the buffer layer are a layer of dense pyrolytic carbon, a SiC layer, and a dense outer pyrolytic carbon layer. These three isotropic layers are termed the TRISO coating. Thousands of these particles are combined with a matrix material and pressed into either spherical forms for pebble bed fuels or cylindrical or annular compacts for prismatic fuels.

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 has commissioned 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.

The objectives of the PIRT program on TRISO-coated particle fuel 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 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.

A three-member panel of experts developed the phenomena identification and ranking tables (PIRTs) presented in this document. The charter of this small PIRT panel was to develop TRISO-coated particle fuel PIRTs, i.e., structured PIRT tables and accompanying rationales. This report will be provided to international experts and other knowledgeable stakeholders for review and comment. The NRC will collect and compile the comments provided by the reviewers. The compiled peer review comments will be collected as a separate source of expert opinions on TRISO-coated particle fuel.

Six phenomena identification and ranking tables (PIRTs) were developed by the panel and are presented in this document. 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.

This report contains significant additional content.

The general PIRT process is described in Chapter 1 as well as a detailed discussion of the application of the general process for the TRISO-coated particle fuel PIRT program.

Chapter 2 presents an extensive discussion of the design function of each component of TRISO-coated particle fuel, i.e., the kernel, buffer layer, inner PyC layer, SiC layer, outer PyC layer, and the fuel element. Manufacturing practices, fuel particle performance throughout the operational life of the fuel and also under accident conditions, and fuel failure mechanisms are also discussed.

Chapter 3 presents a detailed discussion of fission product transport in TRISO-coated fuel particles in each component of TRISO-coated particle fuel. The physical processes comprising fission product transport are described, as are data and the potential analytical approaches to modeling fission product transport.

Summary PIRT tables for manufacturing, operations, depressurized heatup accident, reactivity accident, depressurization accident with water ingress, and depressurization accident with air ingress are provided in Chapter 4.

Chapter 5 presents an analysis and summary of the TRISO-coated particle fuel PIRTs. General technical findings from the TRISO-coated particle fuel PIRTs are presented. Analyses and summaries for each of the six PIRTs are also presented. A total of 327 factors, characteristics and phenomena were 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 of the three panel members. 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. The rationales are presented in Appendices A through F.

In addition to ranking importance, the panel members assessed the level of scientific knowledge and understanding of the factor, characteristic or phenomenon. Each panel member also prepared a written rationale supporting the knowledge level assigned to each highly ranked factor, characteristic, or phenomenon. The rationales for the knowledge level assessed by each panel member are also presented in Appendices A through F.

There were some factors, characteristics, or phenomena for which a consensus was not reached regarding importance or knowledge level. There were, for example, instances where two panel members assessed the importance as "High" and the remaining panel member ranked importance as "Medium" or "Low." There were also instances where importance was assessed as "High" by one panel member, "Medium" by the second panel member, and "Low" by the third panel member. Similar differences also arose in the assessment of knowledge level. The TRISO-coated particle fuel PIRT provides a comprehensive and current view of the significant phenomena that affect TRISO-coated particle fuel performance and fission. It is anticipated that the international peer review of the TRISO fuel PIRT report will provide additional insights and perspectives on the identified phenomena, as well as on the importance and the level of knowledge of these phenomena.

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)

Farouk Eltawila, Director
Division of Systems Analysis and Regulatory Effectiveness
Office of Nuclear Regulatory Research

ACKNOWLEDGMENTS

Several organizations and individuals were most supportive of the PIRT panel efforts. Although the PIRT panel maintained an independent and separate perspective, the panel acknowledges the contributions received from:

Frank Odar of the NRC's Office of Nuclear Regulatory Research, the project manager for the majority of the panel's efforts. We acknowledge his support and assistance.

Eugene Trager, Jr. of the NRC's Office of Nuclear Regulatory Research, the project manager for the completion of the panel's efforts.

Michael B. Rubin of the NRC's Office of Nuclear Regulatory Research, the project manager for the completion of this report and its publication as NUREG.

Stuart Rubin of the NRC's Office of Nuclear Regulatory Research, the technical project manager for the TRISO-coated particle fuel PIRT.

Robert Morris, the author of Chapter two of this report. Figures and photographs appearing in Chapter 2 were provided by Oak Ridge National Laboratory (ORNL). David Petti provided input for Section 2.6.

David Petti and Dana Powers, the authors of Chapter 3 of this report. Figures and photographs appearing in Chapter 3 were provided by Idaho National Engineering and Environmental Laboratory (INEEL).

Richard Moore and Brad Merrill (INEEL), the MELCOR air ingress calculations and text in Appendix G.

We acknowledge the permission received from the International Atomic Energy Association to include a number of their figures in this report.

ACRONYMS AND ABBREVIATIONS

Ag	silver
AVR	Arbeitsgemeinschaft Versuchreaktor
BAF	Bacon anisotropy factor
Ba	barium
BISO	BI ISOtropic
C	carbon
CFR	Code of Federal Regulations
Cr	chromium
CO	carbon monoxide
CO ₂	carbon dioxide
Cs	cesium
DG	draft regulatory guide
DOE	United States Department of Energy
FIMA	fissions of initial metal atoms
Fe	iron
HCl	hydrochloric acid
HEU	high enrichment uranium
HTGR	high temperature gas cooled reactor
HTR	high temperature reactor
HTTR	High Temperature Engineering Test Reactor
HRB	High Flux Isotope Reactor Removable Beryllium
IAEA	International Atomic Energy Agency
IGR	Impulse Graphite Reactor
INEEL	Idaho National Engineering and Environmental Laboratory
IPyC	inner pyrocarbon
j/gm	joules per gram
Kr	krypton
LEU	low enrichment uranium
LTI	low temperature isotropic
LWR	light water reactor
MeV	million electron-volts
MHTGR	Modular High Temperature Gas Reactor
Mo	molybdenum
Mpa	megapascal
MWe	megawatt electric
NPR	New Production Reactor
NRC	United States Nuclear Regulatory Commission
Ni	nickel
NUREG	Nuclear Regulatory Commission document
OPyC	outer pyrocarbon
ORNL	Oak Ridge National Laboratory
O/C	oxygen-to-carbon ratio
PBR	pebble bed reactor

Pd	palladium
PIRT	phenomena identification and ranking table
Pu	plutonium
Ru	ruthenium
Si	silicon
SiC	silicon carbide
SiO	silicon oxide
SiO₂	silicon dioxide
SNL	Sandia National Laboratories
Sr	strontium
T	temperature
Tc	technetium
TECDOC	technical document (IAEA)
THTR	Thorium High Temperature Reactor
TRISO	TRI ISOtropic
U	uranium
UO₂	uranium dioxide
UC₂	uranium carbide
UCO	uranium oxy-carbide
US	United States
UTS	ultimate tensile strength
Xe	xenon
Zr	zirconium

1. INTRODUCTION

Most nuclear reactors presently operating throughout the world are water-cooled. The reactor core consists of numerous fuel bundles, each bundle containing a number of fuel pins. Each fuel pin contains a stack of ceramic, cylindrical UO_2 fuel pellets. The fuel pellets are contained within a metallic sheath or cladding having an outside diameter of approximately 0.5-inches.

The fuel forms for gas-cooled reactors are very different. Tiny kernels of UO_2 fuel are encapsulated within several layers of pyrolytic carbon (PyC) and a single layer of silicon carbide (SiC) to create a fuel particle having a diameter of approximately 1-mm as shown in Fig. 1-2. This fuel is called TRISO-coated particle fuel. Thousands of these particles are combined with a matrix material and pressed into spheres for pebble bed fuels or cylindrical or annular compacts for prismatic fuels. TRISO-coated particle fuel particles are intended to stay intact and effectively retain and contain fission products during normal operation as well as during postulated accidents.

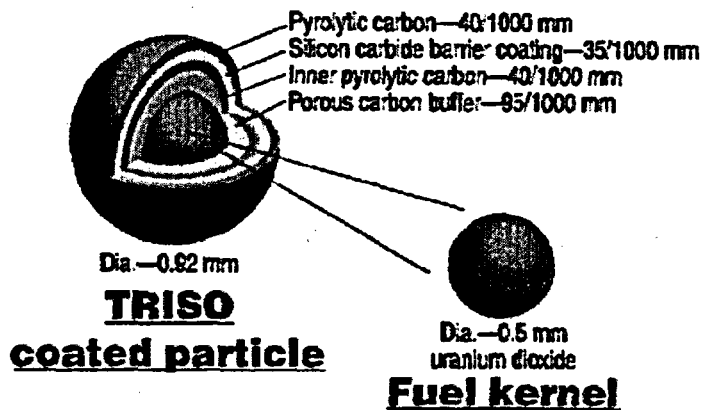


Figure 1-1 An example of a TRISO-coated particle fuel particle

TRISO-coated particle fuel has been used in several reactors in the past, e.g., the 330 MW(e) Ft. Saint Vrain reactor in the US and the 15 MW(e) AVR and 300 MW(e) THTR reactors in Germany. TRISO-coated particle fuel is being used in the 10 MW(t) HTR-10 research reactor in China and the 30 MW(t) HTTR research reactor in Japan. The HTR-10 has a pebble bed core and the HTTR uses a prismatic compact fuel form. The total numbers of reactor years of TRISO-coated particle fuel operating experience are few relative to water reactor fuel.

In anticipation of future licensing applications for gas-cooled reactors, the NRC seeks to fully understand the significant features of TRISO-coated particle fuel design, manufacture, operation and accident behavior. To address this objective, the NRC established a Phenomena Identification and Ranking Table (PIRT) panel to identify and rank the factors, characteristics, and phenomena associated with the life-cycle phases of TRISO-coated particle fuel.

The panel considered four TRISO-coated particle fuel life-cycle phases or conditions: (1) design, (2) manufacturing, (3) normal operation, and (4) accidents. Four accident

scenarios, namely depressurized heatup, reactivity insertion, intrusion of water vapor and intrusion of air were addressed. The panel identified the factors, characteristics and phenomena for each of the four life-cycle phases. The ranking portion of the PIRT process was completed for the manufacturing, normal operation, and accident life-cycle phases only.

1.1 Need for Identification and Ranking

The physical processes and phenomena that occur in nuclear reactors can be both complex and highly coupled. The ability to predict the behavior of nuclear reactors during normal operation as well as their response to accident conditions is of paramount importance. With predictability comes understanding. Both are required to ensure safe reactor operation.

Several fundamental elements form the basis for a safe design. First, the design itself is of paramount importance. An important recent trend in reactor design is the reliance on simplified, passive and/or inherent safety features to reduce the reliance on both active, complex hardware and systems and operator interventions. The ability to accurately predict the behavior of the design under operational and accident conditions using qualified analytical methods is essential.

Predictability, including an understanding of safety margins, is based upon both experiments in scaled component and integral facilities and calculations using analytical tools. It is not, however, feasible to build a full-scale test reactor and then expose that reactor to the aggressive conditions of all design basis accidents. Therefore, analyses based upon qualified analytical methods have become essential to confirming the safety basis for nuclear reactors. The development and qualification of transient and accident analysis methods is central to both designing and demonstrating the safety of a reactor design.

Recently, the NRC has issued a draft regulatory guide, DG-1120, for "Transient and Accident Analysis Methods" (Ref. 1-1). The regulatory guide articulates six basic principles of evaluation model development and assessment. The first principle is to "determine the requirements for the evaluation model." Central to this step is "identification of the . . . components, phenomena, physical processes, and parameters (hereafter collected under the general designation of 'phenomena') needed to evaluate event behavior relative to the figures of merit described in the Standard Review Plan and derived from the General Design Criteria in Appendix A to 10 CFR 50." This identification step is the first essential element of the Phenomena Identification and Ranking Table (PIRT) process. The second essential element is ranking each phenomenon relative to an evaluation criterion, also called a figure of merit. The ranking step is based upon the reality that plant behavior is not equally influenced by all processes and phenomena that occur during a transient or accident. The PIRT process reduces candidate phenomena to a manageable set by identifying and ranking the phenomena with respect to their influence on the figure of merit.

As stated in Ref. 1-1, the principal product of the process outlined above is a phenomena identification and ranking table. Evaluation model development and assessment should be based upon a credible PIRT. The PIRT should be used to determine the requirements for physical model development, scalability, validation, and sensitivities studies. Given

these importance statements, it is important to recognize that "the PIRT is not an end in itself, but is rather a "tool" to be used to guide and focus subsequent efforts.

1.2 The PIRT Process

The PIRT process has evolved from its initial development and application (Refs. 1-2 1-3, 1-4) to its description as a generalized process (Ref. 1-5). The PIRT process is deterministic; it is not risk-informed. A PIRT can be used to support several important decision-making processes. For example, the information can be used to support either the definition of requirements for related experiments and analytical tools or the adequacy and applicability of existing experiments and analytical tools. This information is important because it is neither cost effective nor required to assess each feature of an experiment or analytical tool in a uniform fashion. The PIRT methodology brings into focus the phenomena that dominate, while identifying all plausible effects to demonstrate completeness.

A simplified description of the PIRT process, as applied to the development of the PIRT for TRISO-coated particle fuel, is illustrated in Fig. 1-2 and described as follows.

Step 1: Define the issue that is driving the need, e.g., licensing, operational, or programmatic. The definition may evolve as a hierarchy starting with federal regulations and descending to a consideration of key physical processes.

Step 2: Define the specific objectives of the PIRT. The PIRT objectives are usually specified by the sponsoring agency. A clear statement of PIRT objectives is important because it defines the focus, content, and intended applications of the PIRT product. The PIRT objectives should include a description of the final products to be prepared.

Step 3: Define the hardware, equipment and scenario for which the PIRT is to be prepared. Generally, a specific hardware configuration and specific scenario are specified. Usually, but not always, the scenario is divided into phases. This is done because the importance of a phenomenon often varies during the course of a scenario. In addition, some system components may not be activated throughout the scenario. Experience obtained from previous PIRT efforts indicates that any consideration of multiple hardware configurations or scenarios impedes PIRT development. After the baseline PIRT is completed for the specified hardware and scenario, the applicability of the PIRT to related hardware configurations and scenarios can be assessed.

Step 4: Define the primary evaluation criterion. The primary evaluation criterion is the key figure of merit used to judge the relative importance of each phenomenon. It must, therefore, be identified before proceeding with the ranking portion of the PIRT effort. It is extremely important that all PIRT panel members come to a common and clear understanding of the primary evaluation criterion and how it will be used in the ranking effort. The characteristics of a well-defined evaluation criterion are that it is: (1) directly related to the issue(s) being addressed, (2) directly related to the phenomena expected to occur during the scenario, (3) easily comprehended, (4) explicit, and (5) measurable. The primary evaluation criterion is generally derived from regulatory requirements.

Step 5: Compile and review the contents of a database that captures the relevant experimental and analytical knowledge relative to the physical processes and hardware

for which the PIRT is being developed. Each panel member should review and become familiar with the information in the database.

Step 6: Identify all plausible phenomena i.e., PIRT elements. A primary objective of this step is completeness. In addition to preparing the list of phenomena, precise definitions of each phenomenon should be developed and made available to the PIRT panel to ensure that panel members have a common understanding of each phenomenon. In each PIRT effort, there is a phenomenological hierarchy beginning at the system level and proceeding in turn through the component level, local level, microscopic level, atomic levels and so on. Each PIRT panel must determine the appropriate phenomenological levels to include in its list of identified phenomena. Insights into the levels to be included can often be derived by considering the data needs for analytical methods and the level at which experimental data is collected. Usually, there is no need to proceed further down the phenomenological hierarchy than (a) the level at which physical processes modeled with analytical methods or (b) the level at which data, either direct or indirect, are acquired.

Step 7: Develop the importance ranking and rationale for each phenomenon. Importance is ranked relative to the primary evaluation criterion adopted in Step 4. Several ranking scales have been used in the past. However, consistent application of the scale is of equal importance as the specifics of the scale. A word-based scale, e.g., High, Medium or Low importance, has often been sufficient. Numerical scales, e.g., 1-5, have also been used. For example, an importance rank of 5 (equivalent to High in the word scale) might carry the explicit outcome that experimental simulations and analytical modeling with a high degree of accuracy are critical.

Step 8: Assess the level of knowledge regarding each phenomenon. This is a new step in the evolving PIRT process. It was not included, for example, in a recent generalized description of the PIRT process (Ref. 1-5). As with importance ranking, several scales have been used in the past. Again, a consistent application of the scale is of equal importance as the specifics of the scale. A word-based scale, e.g., Known, Partially Known or Unknown, has often been sufficient. A numerical scale, e.g., 1-5, which includes in its definitions a statement on uncertainty, has also been used. By explicitly addressing uncertainty due to a lack of knowledge, an observed defect of earlier PIRT efforts has been addressed, namely, the tendency of PIRT panel members to assign high importance to a phenomenon for which panel members concluded that there was significantly less than full knowledge and understanding.

A consistent outcome of PIRT efforts has been that phenomena found to be highly important relative to the primary evaluation criterion, but for which the knowledge level is insufficient, are carefully examined to determine if additional experimental or analytical efforts are warranted.

Step 9: Document the PIRT results. The primary objective of this step is to provide sufficient coverage and depth that a knowledgeable reader can understand what was done (process) and the outcomes (results). The essential results to be documented are the phenomena considered and their associated definitions, the importance of each

phenomena and associated rationale for the judgment of importance, the level of

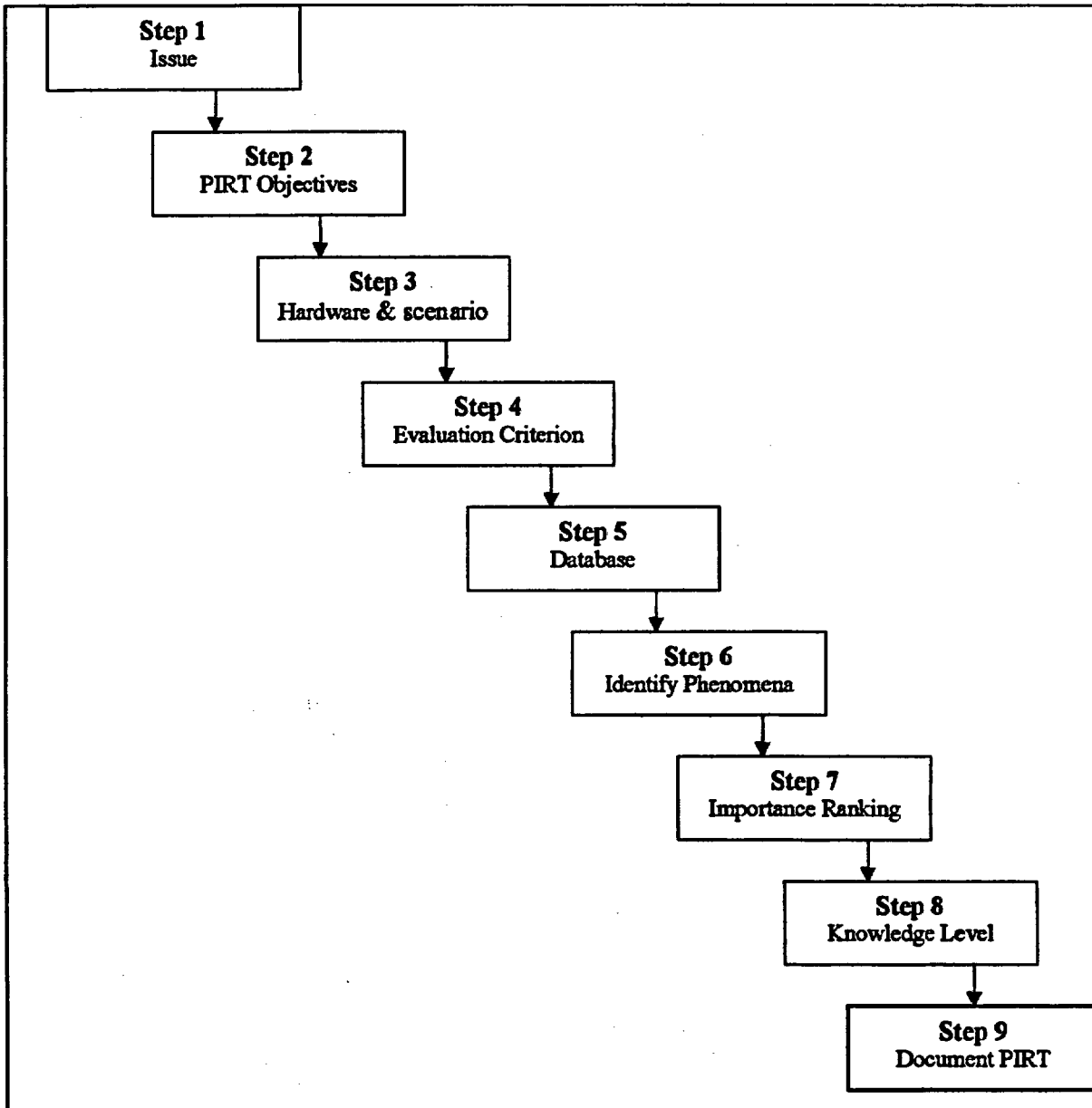


Figure 1-2 PIRT Process

knowledge or uncertainty regarding each phenomenon and associated rationale, and the results and rationales for any assessments of extended applicability for the baseline PIRT. Other information may be included as determined by the panel or requested by the sponsor. For the TRISO-coated particle fuel PIRT, the NRC requested that the panel members describe the research or other effort required to reach closure for a highly ranked phenomena for which only little or partial knowledge of the phenomenon was currently available.

As presented in Fig. 1-2, the PIRT process proceeds from start to end without iteration. In reality, however, the option to revisit any step is available and is often exercised during the PIRT development process.

1.3 PIRT Process Application for the TRISO-coated particle fuel PIRT

Although the PIRT process has been generalized, there are numerous details that must be addressed for each PIRT application. The initial PIRT application (Refs. 1-2 and 1-3) considered the response of a specific pressurized water reactor (PWR) design to a large-break loss of coolant accident. Such plants had been built and operated for a number of years and both the experimental and analytical databases for PWR designs were large. The current application focused on the TRISO-coated particle fuel particle and the fuel element within which the fuel particles are contained.

Numerous specific decisions were made during the development of the TRISO-coated particle fuel PIRT. These are summarized in the following for each PIRT process step described in Chapter 1.2.

Step 1 – Issue: In anticipation of future licensing applications for gas-cooled reactors, the NRC seeks to identify the significant features of TRISO-coated particle fuel design, manufacture, operation and accident behavior.

Step 2 - Objectives: The objectives of the PIRT for TRISO coated fuel particles were to (1) identify key attributes of HTGR fuel manufacture which may require regulatory oversight, (2) provide a valuable reference for the review of vendor HTGR fuel qualification plans and analytical methods, (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 HTGR 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 HTGR fuel safety analyses.

Objectives (1) through (4) are information and features included in the final PIRT report. Objectives (4) through (7) describe uses that will be made of the final PIRT report and the information provided therein.

The NRC requested that the TRISO-coated particle fuel PIRT panel identify the factors, characteristics, processes and phenomena, all of which are identified as phenomena for simplicity in the report, related to the design, manufacture, operation, and accident behavior of TRISO-coated particle fuel. The panel was asked to rank, with the exception of the design life-cycle phase, each phenomenon for importance relative to the evaluation criterion (figure of merit), assess the knowledge level for each phenomenon, and provide its rationale for both the importance and knowledge rankings. For those phenomena judged to be of high importance but not well understood, the panel was asked to describe the effort required to bring about closure, i.e., a sufficient level of knowledge regarding the phenomenon that it would be well understood.

Step 3 – Hardware & Scenario: For this step, there were significant variations relative to the generalized PIRT process. First, there are several forms of TRISO-coated particle fuel, with variations due to the kernel material, UO₂ or UCO; coating process as done, for

example, in either the U.S. or Germany; and fuel form, either a spherical pebble or prismatic compact. Second, there are currently two candidate commercial power reactor designs being developed for potential NRC licensing, e.g., the Pebble Bed Modular Reactor (PBMR), which utilizes spherical fuel elements and the Gas-Turbine Modular Helium Reactor (GT-MHR), which utilizes prismatic fuel elements. The experimental and analytical databases for these two reactors are limited but these reactors are the most likely candidates for early NRC licensing reviews. Given these factors, the NRC, after discussion with the panel, specified the following hardware and scenario conditions for the baseline TRISO-coated particle fuel PIRT.

- UO₂ fuel. This fuel was selected because the experimental and operational database for this fuel is much larger than for UCO fuel.
- The fuel production process is similar to the German process, while allowing needed production changes consistent with modern UO₂ fuel. There is more information on the reference German process than the US process, which involved more variability.
- The fuel form is a spherical “pebble.” As with the choice of UO₂ fuel, the database for pebbles is more extensive for this fuel form. Therefore, it was chosen as the fuel form for the baseline PIRT.
- Given the choice of pebble (spherical) fuel, the plant is considered to be a PBR and the operating conditions are consistent with that reactor type. There is one exception to this choice (see the description of the reactivity insertion scenario as described below)
- The panel did prepare incremental PIRTs relative to the baseline of UO₂ fuel produced by the German process and formed into pebbles. The panel identified and evaluated the importance rankings that would be altered for UCO fuel and prismatic fuel forms.

In a marked departure from highly plant- and scenario-specific specifications, the above specifications had a more general quality. The information needed to develop more detailed specifications were not available to the panel. Thus, the specifications were somewhat general but deemed sufficient to satisfy the NRC’s stated objectives.

Another innovation was the development of a PIRT for the manufacturing phase of the TRISO-coated particle fuel life cycle. Clearly, the approach taken for manufacturing was, of necessity, somewhat different than for the operation and accident scenarios. The panel undertook to identify and rank numerous manufacturing factors and characteristics and assess the knowledge level associated with each. Therefore, the manufacturing PIRT should be considered as an extension of the PIRT process in that identification and ranking are performed on factors and characteristics that are related to the manufacturing process rather than “phenomena” arising with the transition of the plant through physical states associated with operation or accidents.

A PIRT was developed for plant operation. However, consistent with the evolving nature of the TRISO-coated particle fuel and gas-reactor designs, the features of the operational phase were only generally specified. For example, the panel did not explicitly consider a

numeric burnup but did consider the fact that TRISO-coated particle fuel is taken to burnups higher than fuels in light water reactors.

Separate PIRT tables were prepared for four accident scenarios. With the exception of the air intrusion scenario, calculations for the remaining accident scenarios were not available. Therefore, the ranges of parameters occurring during the remaining accident scenarios were assumed. The accidents scenarios and a brief description follow.

Depressurized heatup scenario. Following a break in the reactor cooling system piping, the reactor depressurizes and heat is transferred from the core through the surrounding structures to the ground. This scenario has also been called the “conduction cooldown” scenario. All current reactor designs using TRISO-coated particle fuel are to be designed such that the fuel temperature will not exceed 1600 °C. This temperature is taken as a maximum allowable fuel temperature limit because the maximum accident fission product releases increase above this temperature. However, to address potential uncertainties and at the NRC’s direction, a time versus fuel temperature curve was defined in which the fuel temperature reaches 1800 °C. The fuel temperature transient used in the PIRT evaluation is presented as the dashed line in Fig. 1-3.

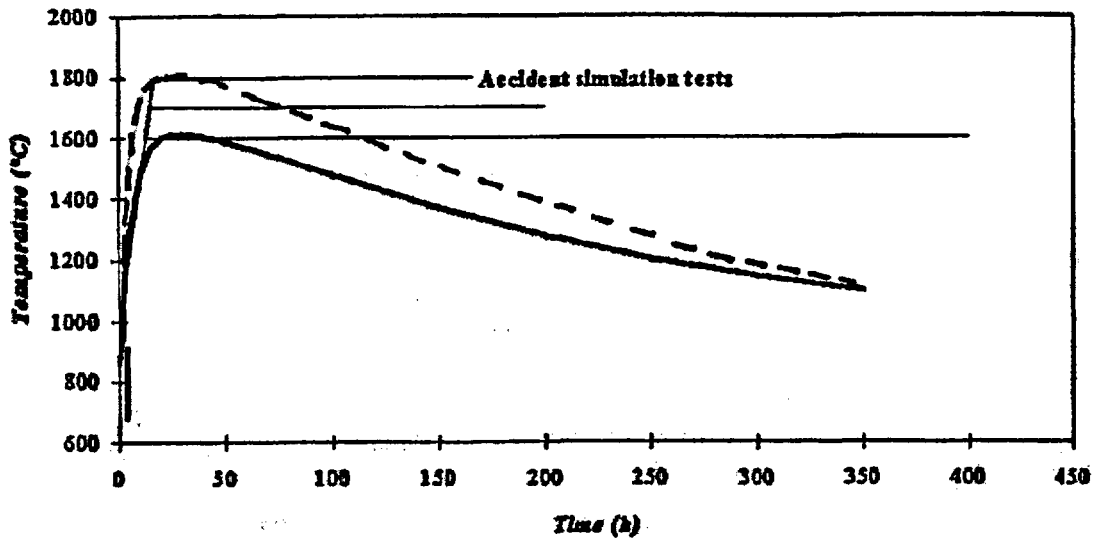


Figure 1-3 TRISO-coated particle fuel temperature transient for depressurized heatup scenario

- **Reactivity insertion scenario:** The potential reactivity additions for a pebble bed core undergoing a postulated control rod ejection accident are considered less challenging than for a prismatic reactor. For a pebble bed core, the reactivity accident would likely result in a fuel heatup event not dissimilar to the heatup event previously considered. Accordingly, the conditions arising from a potential reactivity scenario involving a postulated control rod ejection accident in a prismatic core design were selected as the basis for the postulated core conditions to develop the phenomena for this scenario and these conditions were applied to the pebble bed core.

- A power pulse occurs. This pulse is on the order of seconds, i.e., not milliseconds. A fraction of the TRISO-coated particle fuel particles fail. The kernel and buffer remain intact, as does the fuel element matrix, but the other layers are breached, i.e., the inner pyrolytic carbon (IPyC), silicon carbide (SiC) and outer pyrolytic carbon (OpyC). The remaining unfailed particles are considered to respond as in a heatup accident. For the purposes of the PIRT, the panel considered how fission product generation and transport would be affected for a rapidly failed particle.
- Depressurized heatup followed by water intrusion: The reactor is depressurized as in the conduction cooldown scenario. Water enters primary system and is vaporized but the amount of water vapor present is not sufficient to cool the core. The panel assumed 1% water vapor content in the core for the duration of the transient. Throughout the scenario, the core is assumed to be immersed in coolant having a composition of 1% water vapor and 99% helium. Carbon and steam react to produce reaction products. Some of these reaction products can also react with carbon. The panel did not consider phenomena associated with the interaction of these reaction products with carbon at high temperatures.
- Depressurized heatup followed by air intrusion: The reactor is depressurized as in the conduction cooldown scenario. The break location is assumed to be in the cross-over vessel between the reactor vessel and the power conversion system vessel. Initially, air can enter the primary system only by diffusion. Although this process proceeds slowly, sufficient air enters the primary system over time and moves to the core. When air reaches the core, natural circulation is initiated and the graphite structures in the flow path are exposed to increased flows of air. The results of this "base" scenario were analyzed using the MELCOR code. The results are presented in Appendix G. Sensitivity studies are also presented.

Step 4 – Evaluation Criterion: Each factor, characteristic, process or phenomenon was assessed relative to its importance to fission product release from the fuel or in a more licensing-specific term, the source term.

Step 5 – Database: The panel compiled and reviewed the contents of a database that captured the relevant experimental and analytical knowledge relative to the physical processes and hardware for which the PIRT was developed. Chapter 2 of this report, TRISO-Coated Fuel Particle Performance, describes the TRISO coated particle and fuel element; the design function of each part of the TRISO-coated particle fuel, e.g., kernel, buffer, pyrolytic carbon layers, silicon carbon layers, and fuel element; fabrication processes; fuel behavior during normal operation and fuel behavior during accident conditions. Chapter 3 discusses the potential phenomena responsible for the transport of fission products in TRISO-coated particle fuel. Finally, Appendices A-F present the individual panel member importance and knowledge rankings and rationales for each PIRT. Citations are provided for the importance and knowledge rankings for many of the more important phenomena.

Step 6 – Identify Phenomena: Over the course of the first TRISO-coated particle fuel PIRT panel meetings, the panel members first identified and then refined the phenomena lists. The "phenomena" definition for the manufacturing PIRT was broadened to include

manufacturing factors and characteristics. The “phenomena” identified for the operation and accident scenarios were those of the more typical PIRT. Precise definitions of each phenomenon were developed and made available to the PIRT panel to ensure that panel members had a common understanding of each phenomenon. The identified “phenomena” and associated definitions are presented in the summary PIRT tables found in Chapter 4 of this report.

Although the objective of the identification step is to identify all pertinent phenomena, it is necessary for the PIRT panel to determine how deep down into the phenomenological hierarchy levels to proceed. For example, no useful purpose is served by defining phenomena at the “microscopic” level when the PIRT is being developed for the system-wide response of a reactor to a large-break loss-of-coolant-accident. However, phenomena occurring at such levels may be appropriate when the PIRT is focusing on a TRISO-coated particle fuel kernel with a diameter of approximately 1-mm, said particle consisting of multiple thin layers of various materials. The phenomena identified in the TRISO-coated particle fuel PIRT tables (See Chapters 2 and 4) reflect the panel’s awareness of the need to be complete but at a level of phenomenological detail appropriate for the end practical use of the PIRT by the NRC.

The panel first identified elements of the design life-cycle phase. Importance of the design elements was ranked and the knowledge level assessed. The panel did not further discuss the results of their individual PIRT findings, as was done with the other PIRTs documented in this report. The PIRT findings of each panel member are provided in Appendix H.

Next, the panel applied the following conditions on the manufacturing, operations, and accident phenomena to be included in each PIRT.

Manufacturing PIRT

- Identify and rank the factors, specifications, material properties and manufacturing processes related to fuels manufactured per specification.
- Consider the importance of fuel defects beyond those permitted by the specifications as deemed necessary.

Operations PIRT

- Assume fuel manufacture meets specifications, i.e., “good” fuel. Such fuel can have defects at levels allowed by the specifications but no additional defects.
- Identify and rank the impacts of operation on good fuel properly operated to the time of the accident.
- Address fuel defects beyond that allowed by specification only in the manufacturing phase

Accident PIRTs (heatup, reactivity insertion, water and air intrusion)

- Assume fuel is manufacture meets specifications. Such fuel can have defects at levels allowed by the specifications but no additional defects.
- Assume the fuel is operated as specified by the operating specifications.
- Identify and rank the impacts of accidents on good fuel properly operated up to the time of the accident.
- Address fuel defects beyond that allowed by specification only in the manufacturing phase

The construct of the PIRT tables was aligned with the various physical features of a TRISO-coated particle fuel particle, i.e., the kernel, porous carbon buffer layer, inner pyrolytic carbon layer, silicon carbide layer, outer pyrolytic carbon layer, and fuel element. The phenomena list was essentially replicated for each layer for like life-cycle phases, e.g., operation and the accidents¹. As a consequence, the PIRT tables are large. Given the detailed PIRT information requested of the panel members, as documented in Appendices A-F, the effort required was very large.

Step 7 – Importance Ranking: The panel ranked each phenomenon in each table relative to the evaluation criterion, i.e., fission product release (See Step 4 of Chapter 1.4). A summary of the importance ranking assigned by each panel member (listed by institution) is found in Chapter 4. The rationale provided by each panel member for the importance ranking of each phenomenon is provided in the Appendices.

Each phenomenon was assigned an importance rank of “High,” “Medium,” or “Low.” The definitions associated with each of these importance ranks are shown in the following table.

Table 1-1 Importance Ranks and Definitions

Importance Rank	Definition
Low (L)	Small influence on primary evaluation criterion
Medium (M)	Moderate influence on primary evaluation criterion
High (H)	Controlling influence on primary evaluation criterion

Each PIRT panel is challenged by the need to apply consistent thought processes when evaluating the importance of each phenomenon. PIRT panels have found that expressing the importance ranking issue as a question proves helpful. The TRISO-coated particle fuel PIRT panel used this approach for the manufacturing PIRT. Following are selected

¹ One panel member expressed the following concern: “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 multi-component 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.”

questions formulated by the panel as consistency guides. The first question applies to specifications and the second to other factors and characteristics.

Question 1: Which of the specifications are most important with respect to manufacturing fuel that will successfully perform in the reactor under normal operations and accident conditions?

Question 2: Which of the material properties, factors, or processes are most important with respect to manufacturing fuel that will successfully perform in the reactor under normal operations and accident conditions?

Step 8 – Knowledge Level: Each panel member assessed the current knowledge level for each phenomenon in each PIRT table. The knowledge level for each phenomenon was assessed rather than the level of knowledge of the impact of each phenomenon on the Primary Evaluation Criterion. Numbers between 1 and 9 were assigned to reflect the knowledge level with the associated definitions shown in the following table. A summary of the knowledge ranking assigned by each panel member (listed by institution) is found in Chapter 4. The rationale provided by each panel member for the knowledge ranking of each phenomenon is provided in the Appendices.

Table 1-2 Knowledge Levels and Definitions

Knowledge Level	Definition
7-9	Known: Approximately 70%-100% of complete knowledge and understanding
4-6	Partially Known: 30%-70% of complete knowledge and understanding
1-3	Unknown: 0%-30% of complete knowledge and understanding

Step 9 – Documentation: This document represents the realization of the documentation step. The general PIRT process and its specific application to the TRISO-coated particle fuel PIRT effort are documented in Chapter 1. A description of TRISO design, manufacturing, operation and accident factors is presented in Chapter 2. Potential phenomena responsible for the transport of fission products in TRISO-coated particle fuel are presented in Chapter 3. Summary PIRT tables with the identified phenomena, importance ranks, and knowledge ranks are presented in Chapter 4. Analysis of the results and conclusions are presented in Chapter 5. The detailed PIRT panel member importance and knowledge findings and the rationales for each are presented in the appendices, as are brief biographies for each panel member.

1.4 Report Organization

The report is organized into five chapters and contains nine supporting appendices.

- Chapter 1, Introduction, provides an overview of the general PIRT process, identifies modifications to the general approach for the TRISO-coated particle fuel PIRTs, provides a brief description of the TRISO-coated particle fuel life-cycle phases and, where appropriate, the scenarios considered. The objectives of the PIRT effort are identified and the members of the TRISO-coated particle fuel PIRT panel are identified.

- Chapter 2, TRISO-Coated Fuel Particle Performance, describes the TRISO coated particle and fuel element; the design function of each part of the TRISO-coated particle fuel, e.g., kernel, buffer, pyrolytic carbon layers, silicon carbon layers, and fuel element; fabrication processes; fuel behavior during normal operation and fuel behavior during accident conditions.
- Chapter 3, Fission Product Transport in TRISO-Coated Particle Fuels, discusses the potential phenomena responsible for the transport of fission products in TRISO-coated particle fuel as a means of further understanding the identified phenomena.
- Chapter 4, TRISO-Coated Particle Fuel Phenomena Identification and Ranking Tables (PIRTs), contains the summary PIRTs for (1) manufacturing, (2) normal operation, (3) depressurization heatup accidents, (4) reactivity insertion accidents, and (5) depressurization heatup accidents with water intrusion, and (6) depressurization heatup accidents with air intrusion.
- Chapter 5, TRISO-Coated Particle Fuel PIRT Analysis and Summary, contains an analysis of the PIRT information and identifies the factors, characteristics and phenomena for which high importance and low knowledge level rankings were assigned by the panel members.

Important detailed and supporting information is presented in the appendices.

- Appendix A contains the individual panel member importance and knowledge rankings and rationales for the manufacturing phase.
- Appendix B contains the individual panel member importance and knowledge rankings and rationales for the operation phase.
- Appendix C contains the individual panel member importance and knowledge rankings and rationales for a depressurization heatup accident.
- Appendix D contains the individual panel member importance and knowledge rankings and rationales for a reactivity insertion accident.
- Appendix E contains the individual panel member importance and knowledge rankings and rationales for a depressurization heatup accident with water intrusion.
- Appendix F contains the individual panel member importance and knowledge rankings and rationales for a depressurization heatup accident with air intrusion.
- Appendix G contains the results of MELCOR calculations performed for the air-intrusion accident scenario.
- Appendix H contains the individual panel member submittals for the TRISO-coated particle fuel life-cycle design phase. Initial submittals were received from the panel members early in the TRISO-coated particle fuel PIRT effort and are included for completeness. The PIRT process was not taken to completion for the design phase.
- Appendix I contains brief biographies for each member of the TRISO-coated particle fuel PIRT panel.

1.5 PIRT Panel Membership

The participants in the TRISO-coated particle fuel PIRT Panel were:

Robert Morris, Oak Ridge National Laboratory

David A. Petti, Idaho National Engineering and Environmental Laboratory

Dana A. Powers, Sandia National Laboratories

A three-member PIRT panel was considered the minimum size for effective coverage of the phenomena and processes associated with the entire life cycle of TRISO-coated particle fuel, including operation and accident conditions. However, extensive experience with TRISO-coated particle fuels also exists within the international community. The NRC will, therefore, submit this TRISO-coated particle fuel PIRT report for review by a group of international experts and other knowledgeable stakeholders. The international participants will review the information developed during the present TRISO-coated particle fuel PIRT effort and provide comments. The NRC will collect and compile the comments provided by the reviewers. The compiled peer review comments will be collected as a separate source of expert opinions on TRISO-coated particle fuel.

1.6 References

- 1-1. Draft Regulatory Guide 1120, "Transient and Accident Analysis Methods" (December 2002).
- 1-2. "Quantifying Reactor Safety Margins: Application of CSAU to a LBLOCA," EG&G Idaho, Inc., NUREG/CR-5249 (1989).
- 1-3. "Quantifying Reactor Safety Margins: Application of CSAU to a LBLOCA," B. E. Boyack et al., Part 1: An overview of the CSAU Evaluation Methodology; G. E. Wilson et al., Part 2: Characterization of Important Contributors to Uncertainty; W. Wulff et al., Part 3: Assessment and Ranging Parameters; C. S. Lellouche et al., Part 4: Uncertainty Evaluation of Analysis Based on TRAC-PF1/MOD1; N. Zuber et al., Part 5: Evaluation of Scale-Up Capabilities of Best Estimate Codes; I. Catton et al., Part 6: A Physically Based Method of Estimating PWR LBLOCA PCT, Nuclear Engineering and Design 119 (1990).
- 1-4. Shaw, R. A., T. K. Larson, and R. K. Dimenna, "Development of a Phenomena Identification and Ranking Table (PIRT) for Thermal-Hydraulic Phenomena During a PWR LBLOCA," EG&G Idaho, Inc., NUREG/CR-5074 (1988).
- 1-5. Wilson, G. E., and B. E. Boyack, "The Role of the PIRT Process in Experiments, Code Development, and Code Applications Associated with Reactor Safety Analysis," Nuclear Engineering and Design 186, 2-37 (1998).

2. TRISO-COATED FUEL PARTICLE PERFORMANCE

2.1 General Description Of Coated Particle Fuel And Fuel Element

2.1.1 Operational Requirements

The contemporary goal of coated particle fuel and the associated fuel form is to allow high temperature reactor operation with very high fractional fuel particle integrity during normal operation and accidents and very low fission product release during normal operation and under accident conditions [2-1 to 2-7]. A secondary goal is high fuel burnup (>10% FIMA for pebble bed and >20% FIMA for prismatic core) to allow economic operation of the reactor system and good fissile material utilization. The core average exit temperatures currently in the range of 800°C to 950°C with peak fuel temperatures of 1200°C to 1250°C, which is higher than for LWRs. Long-term plans are to go to even higher core average exit temperature with burnups in the range of 20-25% FIMA, which is also higher than for LWRs.

Achieving these goals requires the use of different materials than commonly used in LWR fuel and a different core coolant environment. Unlike LWR fuels, the use of metallic materials is minimized and the coolant is an inert, single-phase gas (helium). Reliance instead is placed on ceramic materials, primarily carbon based materials such as graphite, pyrocarbon, and silicon carbide [2-8]. The properties of these materials also have shifted the fuel design away from an array of rods to graphite blocks with fuel compacts or fuel spheres. Also in contrast to LWRs, the coolant and the moderator are separate.

The philosophy of HTGR coated particle fuel is somewhat different than that of LWR fuel pellets and cladding. The fuel in an HTGR core is contained in billions of coated particles, each of which acts as its own containment. The small kernels of fuel are each coated with layers of carbon and silicon carbide. The resulting particle is designed to withstand the pressure of the generated fission gases and to form an essentially leak tight barrier to fission product release. While LWR fuel cladding performs this function on a larger scale during normal operating conditions, coated particle fuel also requires this high level of integrity under accident conditions. Thus, the fuel particle is required to stay intact with high reliability during both normal operation and accident conditions.

2.1.2 Basic Fuel Element

The fundamental component of the HTGR fuel element is the coated fuel particle. The particle is composed of a kernel of fuel and several coating layers, each of which has a specific function. For the purposes of this report, we will consider the traditional four-layer particle as illustrated in Fig. 2-1.

The HTGR kernel is either UO_2 or a two-phase mixture of UO_2 and UC_2 known as UCO. The diameter is about 500 microns for the pebble fuel kernels and about 350 and 500 microns for fissile and fertile kernels, respectively, in prismatic block fuel. Particles made from thorium and plutonium are also possible, but UO_2 and UCO are the materials of current interest for commercial power reactors. The UO_2 kernel has the most extensive civilian experience base, but the UCO kernel offers the ability to better control carbon

monoxide production and thus particle internal pressure buildup. This factor is important as the fuel is pushed to higher burnup and higher operating temperatures.

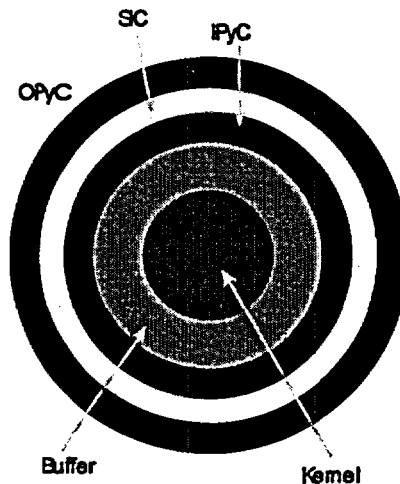


Figure 2-1 Schematic of the four-layer particle design

The HTGR kernel is either UO_2 or a two-phase mixture of UO_2 and UC_2 known as UCO. The diameter is about 500 microns for the pebble fuel kernels and about 350 and 500 microns for fissile and fertile kernels, respectively, in prismatic block fuel. Particles made from thorium and plutonium are also possible, but UO_2 and UCO are the materials of current interest for commercial power reactors. The UO_2 kernel has the most extensive experience base, but the UCO kernel offers the ability to better control carbon monoxide production and thus particle pressure. This factor is important as the fuel is pushed to higher burnup and higher operating temperatures.

The buffer layer is a low-density porous carbon layer that acts as an expansion space to collect the released gases. The gases are generated as a result of (1) fission and (2) chemical reactions between the carbon buffer layer and oxygen liberated from the UO_2 . The inner pyrocarbon (IPyC) layer provides a smooth surface for the silicon carbide layer to be deposited and also shields the kernel from chlorine released during fabrication. It also plays a role in the mechanical stress distribution within the particle. The silicon carbide (SiC) layer is the major fission product barrier and plays an important structural function. Finally, the outer pyrocarbon (OPyC) layer isolates the SiC layer from the matrix that binds the particles together and provides a compressive force on the SiC. These layer functions will be described in more detail in the following sections. As described in Chapter 1.0, the particles are aggregated in a matrix material to form a fuel element for the reactor core.

The reader may wonder why suspending and binding the particles in a fuel form is necessary and why it wouldn't be acceptable to pour them into a tube or a hole in a block. Two reasons preclude this approach. – particle heat transfer and mismatches between their thermal expansions.

Close packed particles would have limited contact area and a considerable amount of void space, thus the contact heat transfer would be modest. The flow impedance of very small closely packed particles would be too high, thus limiting the heat that can be removed by convection. These two effects would limit the effective heat transfer from a loose bed of small particles.

The second reason for combining particles in a fixed matrix material, differences in the thermal expansion of the particles and holder, is more limiting. Loosely packed particles would have a tendency to settle under vibration or temperature cycling. Settling would generally be irreversible and the application of significant forces would not reverse it. As the particles heat up and are subject to normal reactor system flow-induced vibrations, the particles would settle into a new, more closely packed configuration. This might be acceptable if the particles and their holder had the same thermal expansion and only modest temperature gradients, but this is generally not the case. Temperature cycling after the particles settle would result in differential expansion between the particles and the holder. Since the settling cannot be reversed by force, large compression forces would build up in the particles that could damage the particles or rupture the holder.

A practical approach to this problem is to suspend and bind the particles with a thermal-mechanically compatible medium [2-1 through 2-4, 2-9]. Figure 2-2 shows the basic concept. The fuel particles are fixed within a matrix of graphite powder and binder and may be encased within a non-fuelled layer depending on the application. In practice two basic fuel element forms have evolved.

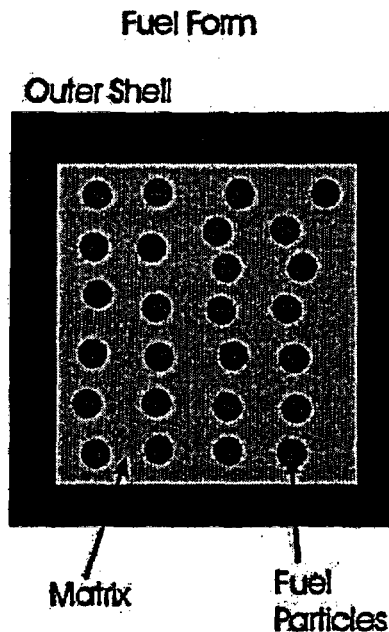


Figure 2-2 Fuel element components

The first involves fuel particles suspended in a matrix in the shape of a sphere surrounded by an outer unfueled layer of matrix material (i.e. a fuel "pebble"). This fuel form is used by the pebble bed type reactor designs. It must be sufficiently tough so that it can be

dropped repeatedly several meters onto a bed of pebbles without breaking. The fuel pebbles are typically 6 cm in diameter and contain about 15,000 fuel particles. The second design is a cylindrical fuel compact design that can be stacked and inserted into a graphite block. This form may be solid or annular in configuration. Each compact contains about 10,000 particles. See Fig. 2-3 for the designs. Over the years other designs such as a complex fuel block molded from particles have been considered, but these are currently not of interest [2-9]. The details of fuel element fabrication will be covered in later sections of this chapter.

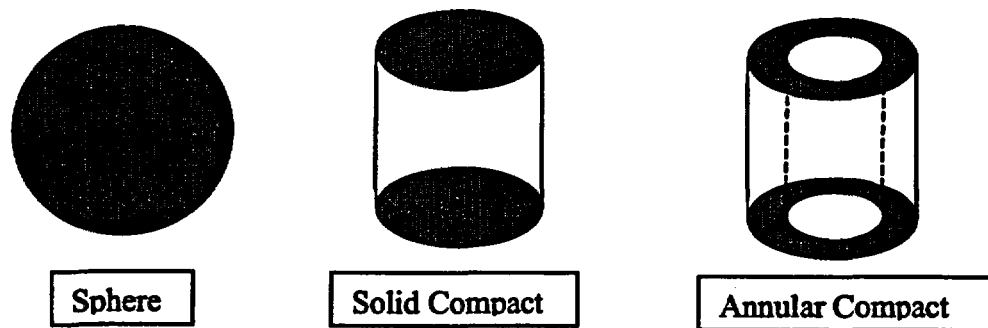


Figure 2-3 Three of many possible designs for a fuel element. The compact design can also be used as part of a pin in block design

2.2 Design Function of Each Component

2.2.1 General

Each component of the fuel particle and fuel element has specific functions, specific material needs and specific challenges. A description of each component and its design considerations is followed by its relevant phenomena in the PIRT Table.

2.2.2 Kernel

The kernel contains the nuclear fuel and its composition controls the basic chemistry of the particle environment. Contemporary design focuses on controlling the oxygen potential of the particles either by limiting burnup or by tailoring the kernel composition [2-8]. There are two reasons for this. The first is to tie up the oxygen liberated by fissioning the U in UO_2 so that it cannot react with the carbon buffer layer and form CO. CO production can greatly increase the particle pressure and increase its failure likelihood [2-6, 2-8, 2-10, 2-11]. In addition, in the presence of a thermal gradient, CO can result in migration of the kernel away from its centered position [2-8]. The second is to make ensure that the rare earth elements are oxidized and thus immobilized so they do not migrate to the SiC and react with it.

Summarizing, the basic functions of the kernel are to:

- 1) Control particle internal pressure and migration potential by holding down CO production.
- 2) Tie up rare earths as oxides to limit their migration to the coating.
- 3) Produce the desired power.

The fission gases and volatile fission products are largely contained by the coatings. However, fission gas retention by the kernel is important at the low to moderate burnup levels (less than about 20%) [2-22]. Up to this burnup and at normal operating temperatures, the kernel provides significant holdup (~50%, see Chapter 3) of the fission gases krypton and xenon as well as volatile species such as iodine and cesium. This retention aids in controlling particle pressure and is important for exposed kernels, as it greatly reduces the amount of fission products that are released to reactor internal components. Significant retention of some isotopes can even occur as accident temperatures are approached.

As the kernel burnup increases, its ability to retain fission gases and volatile fission products can decrease, especially at the higher temperatures. Designers often assume high release levels (up to 100%) of fission gases (very high burnup, ~70% FIMA) at end of life or for accident conditions. This is different from LWR fuel (normal operating temperatures) where fuel fission gas retention is considered important (retention levels ~95%) and secondary gases such as CO are not important.

An important design consideration for the kernel is the oxygen potential [2-8]. Its importance comes about from the fact that the fission products from a fissioned uranium atom have an oxygen combining ability less than that of the original U, thus oxygen is available in the system to combine with other elements. Table 2-1 illustrates the available oxygen ratio for several actinides assuming the metal oxides do not become super stoichiometric. Note that the oxygen to metal ratio is not the same as oxygen potential. The ratio simply looks at the number of oxygen and metal atoms in the system and allows one to determine whether or not oxygen is likely to be available for chemical reactions. The oxygen potential is determined by the amount of oxygen in the system and the affinity of particular elements for it. The oxygen potential determines which elements are successful in competing for the oxygen and which are not.

The fission products, carbon, and uranium all compete for oxygen in this closed system and the system oxygen potential determines which elements are oxidized and which are not for a limited amount of oxygen. The oxygen potential, μ_{O_2} is defined as:

$$\mu_{O_2} [kcal / mol] = RT \ln(P_{O_2} [atm])$$

where R is the gas constant, T is the absolute temperature, and P_{O_2} is partial pressure of oxygen. In pure UO_2 fuel (our reference case), the oxygen potential increases as a function of burnup and results in the production of CO. This CO increases the pressure in the particle. Figure 2-4 illustrates how particle pressure can be affected as burnup increases.

Table 2-1 Oxygen Excess per Fission

Isotope	O/F
U-233	0.092
U-235	0.132
Pu-239	0.623
Pu-241	0.599

$2C + (O_2) = 2(CO)$	UO ₂ Burnup	T (K)	P _{co} (atm)
		Low	1300
	($\mu_{O_2} = -100$ kcal/mol)	1600	5
	High	1300	580
	($\mu_{O_2} = -75$ kcal/mol)	1600	1300

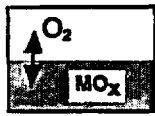


Fig. 2-4 Increase in particle pressure as a function of burnup for a UO₂ kernel (representative order of magnitude calculation)

Particle pressure translates directly into coating stresses [2-13 to 2-18]. This can be illustrated with a simple model. If it is assumed that the SiC layer carries the entire internal pressure load, the stress, σ , in the layer is approximately:

$$\sigma = \frac{rP}{2t}$$

where r is the radius, P is the pressure, and t is the layer thickness. If the stress in the SiC layer is greater than its ultimate tensile strength (UTS) the layer will fail. The total gas pressure in the particle is the sum of the CO gas pressure and the released fission gases:

$$P_{Total} = P_{Kr} + P_{Xe} + P_{CO}$$

The stress equation can be solved for P and, with an UTS of SiC of 350MPa, an SiC thickness of 35 μ m, and an SiC layer radius of 310 μ m, one gets:

$$P_{Max} = \frac{UTS_{SiC} 2t}{r} = 790 atm$$

This scoping calculation tells the designer that the particle internal pressure needs to be limited to a few hundred atmospheres to prevent overpressure failure of the SiC. Factors

such as uneven coating thickness, thin coatings, non-spherical shapes, and less than expected material properties would reduce this pressure considerably.

A more sophisticated analysis for both oxygen potential and layer stress would be required for actual particle design work. To summarize, for UO_2 fuel:

- 1) The krypton and xenon pressure depend on burnup, kernel gas retention, and free volume (buffer). The kernel gas retention diminishes with burnup and is often assumed to be nil for accidents. For the 10% FIMA burnup fuel kernel gas retention is fairly high at normal temperatures, likely in the 50% FIMA or more range for fission gases.
- 2) CO pressure depends only on oxygen potential and temperature. Oxygen comes from fissioning the U in UO_2 and carbon comes from the buffer.
- 3) The oxygen potential depends on UO_2 burnup.

Figure 2-5 shows a SiC layer overpressure failure (known in the literature as *pressure vessel failure*). For particles designed and operated within specifications, this failure is not commonly seen.

Carbon monoxide is involved in another particle damage phenomena known as the *Amoeba Effect* [2-8]. This phenomenon involves in the transfer of carbon from one side of the kernel to another in the presence of a temperature gradient and results from the differing equilibrium between CO and CO_2 at different temperatures.

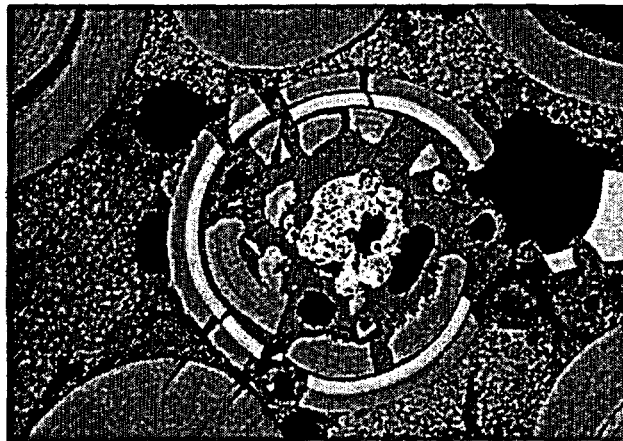


Figure 2-5 Pressure vessel failure in HRB-8, Specimen 5 (UO_2)

This effect can also occur in UC_2 , but is due to solid-state carbon transport rather than CO/CO_2 [2-12]. The greatest effect is with UO_2 .

The net effect of this carbon transport is to gradually push the kernel in the direction of increasing temperature, across the kernel so that the kernel moves toward the SiC layer and damage the layer. This is clearly undesirable. Figure 2-6 illustrates the action.

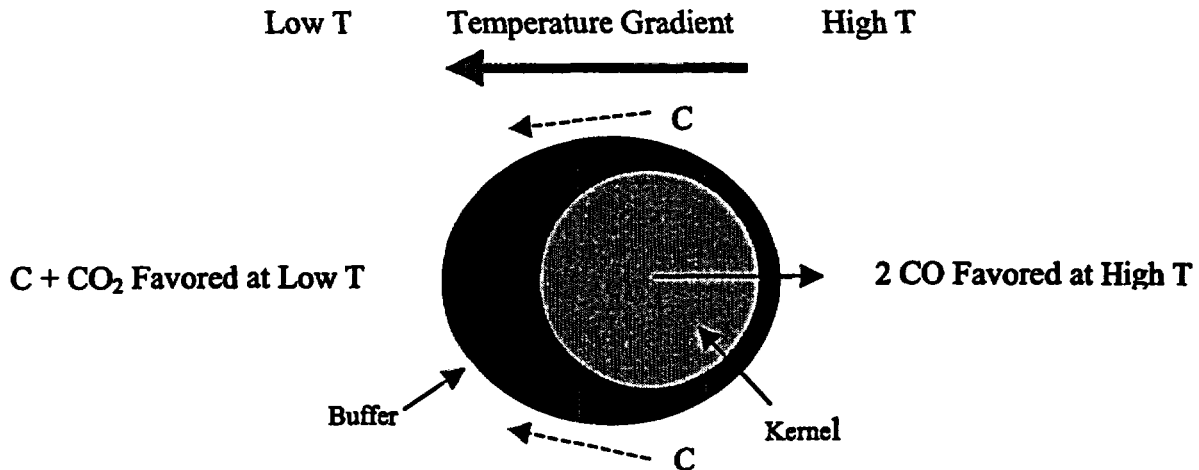


Figure 2-6 Illustration of the Amoeba Effect. Carbon is transported from the hot side to the cool side

An expression for the movement of the kernel is:

$$\Delta x = KMC \frac{1}{T^2} \frac{dT}{dx} t$$

where Δx is the kernel movement in meters, t is the time in seconds, T is the temperature ($^{\circ}\text{K}$), and KMC is the migration factor. Typical migration factors are shown in Table 2-2.

Table 2-2 Migration Factors

Typical KMC at 1300 $^{\circ}\text{K}$ ($\text{m}^2\text{K/s}$)	
LEU UCO	9×10^{-13}
LEU UO ₂	6×10^{-11}
UC ₂ (Solid state diffusion)	9×10^{-13}

Particle failure is assumed to occur when the kernel touches the SiC layer. Examples of the Amoeba Effect are shown in Fig. 2-7.

The amoeba effect was a concern for the large (1000 MWe) HTGR designs using UC₂ and UO₂ kernels. Kernels with UCO significantly reduce this effect because CO production is minimized (see below) and solid-state carbon transport through the UCO is very low. Even at higher fuel operation temperatures, the modular prismatic designs that utilize UCO fuel are not expected to be significantly impacted by amoeba effect failures. Pebble bed reactors are also not expected to be significantly impacted by the amoeba effect because these reactors have small temperature gradients.

Thus, UO₂ fuel has been proposed as the fuel of choice in reactor systems with low temperature gradients and burnups in the range of 10%. This kernel type has had extensive testing under the conditions of interest for the modular steam cycle reactors and it is currently planned for direct cycle gas turbine systems (pebble bed).

Relative Thermal stability of HTGR Candidate Recycle Oxide Fuel Kernels Irradiated in HRB-7. Time-average temperature, 1200-1220EC; thermal gradient, 1000-1030EC/cm; fast fluence, $6 \times 10^{21} \text{ n/cm}^2$.

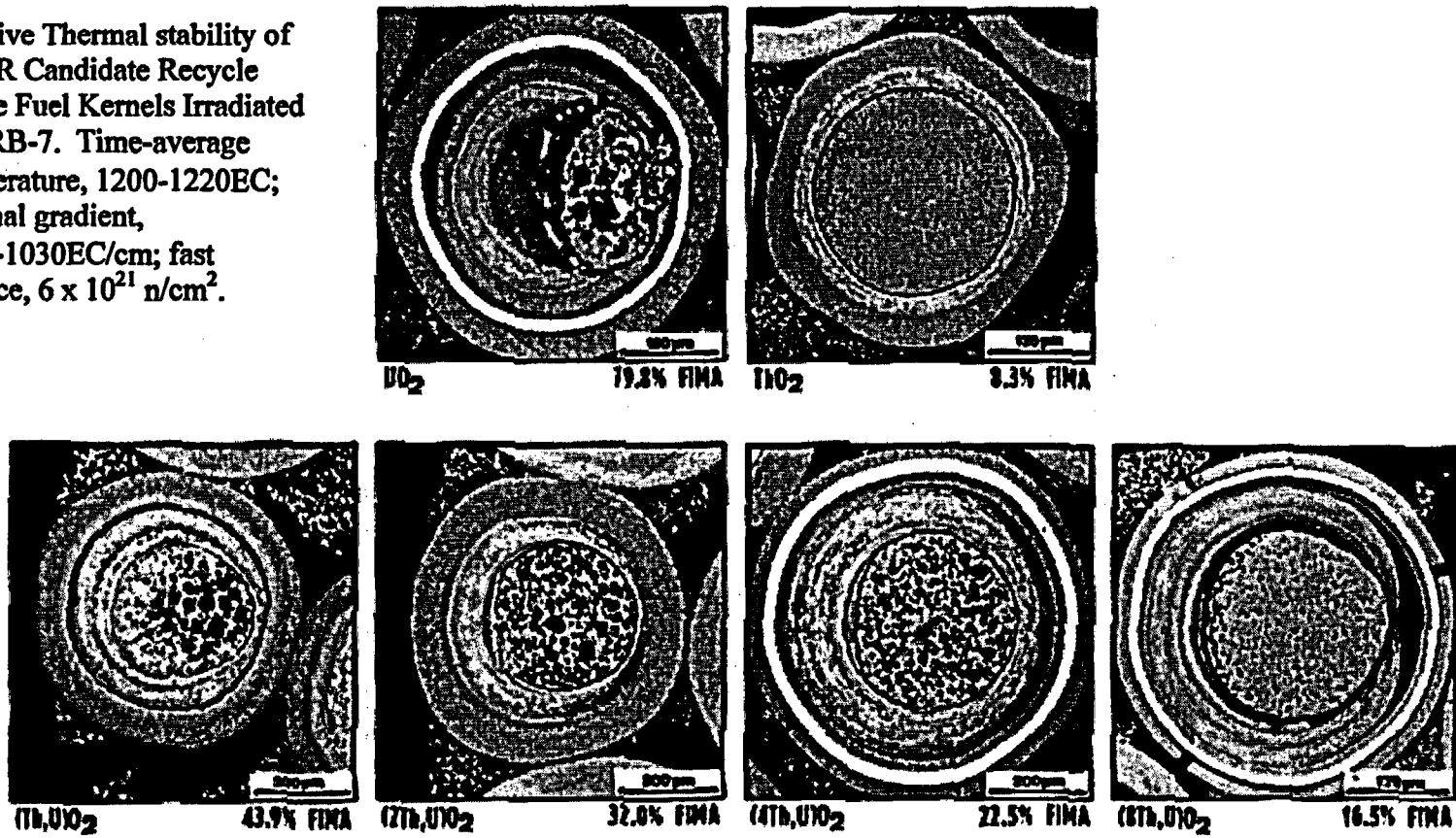
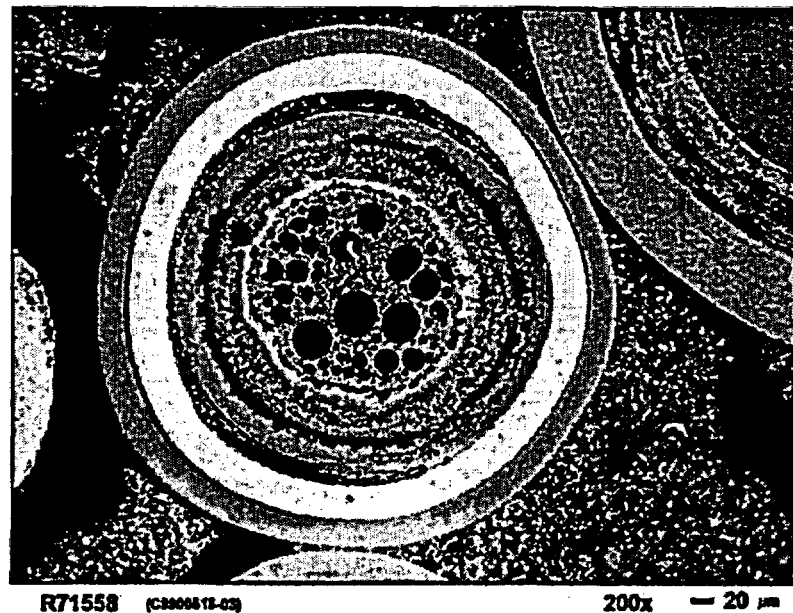


Figure 2-7 Oxide kernel fuel exhibiting the amoeba effect

Some reactor concepts have higher temperature gradients and greater fuel burnup needs and these reactors may not choose to use the UO_2 based fuel. The prismatic core GT-MHR is likely to have fuel burnups in the range of ~20% FIMA. Thus, there is interest in fuels that can achieve higher burnups without changing kernel migration or elevated internal pressures associated with CO.

Unlike lower burnup LWR fuel, the particle fuel designer cannot depend on the crystal structure of the kernel to contain a high percentage of fission gases and volatile fission products in high burnup fuel (>50%), especially under accident conditions. The relatively uniform kernel structure deteriorates with burnup and the kernel coatings must be relied upon for containing the mobile fission products. However, the kernel retains the refractory non-mobile compounds. A high burnup kernel is shown in Fig. 2-8. The figure shows a highly sub-stoichiometric plutonium dioxide kernel that limits CO problems by reducing the amount of oxygen initially available (note: it is not possible to fabricate highly sub-stoichiometric UO_2). At high burnup the kernel structure becomes highly voided.



FTE-13, $\text{PuO}_{1.68}$ Kernel, 1150°C ave, 2.2×10^{25} fluence, 70% BU

Figure 2-8 High burnup kernel showing the loss of crystal structure and the development of large voids

To avoid the problems associated with CO production, three approaches are possible. The first is to make a sub-stoichiometric kernel and thus limit the amount of oxygen available for CO production. This is possible with plutonium, but not with uranium. A second approach is to include a “getter” material in or near the kernel to absorb the released oxygen and make it unavailable for CO production. This approach has been

used, but involves greater complexity in particle production [2-40]. The third approach is to make a two-phase kernel consisting of both carbide and oxide phases.

The two-phase approach, known as UCO, allows the released oxygen from the oxide phase to oxidize the carbide phase at the expense of CO production [2-8]. This approach works because the oxidation energy of uranium is much lower than that of carbon. However, sufficient oxygen must be available to oxidize the rare earth elements, as the carbide forms of some rare earth elements are mobile and can migrate to the SiC and damage it. Figure 2-9 is a diagram of the process.

The two phases, UC_2 and UO_2 , interact in the following way. As oxygen is liberated, it first oxidizes the UC_2 and rare earth elements because they have the greatest affinity for oxygen. Once they have been oxidized, oxygen is available for some of the elements with less affinity, such as Sr, Eu, Zr, and Ba, which were limited to carbide form earlier. Finally, only at the end of life is there enough oxygen for CO production. The goal is to balance this final CO production point with the need to oxidize the rare earths.

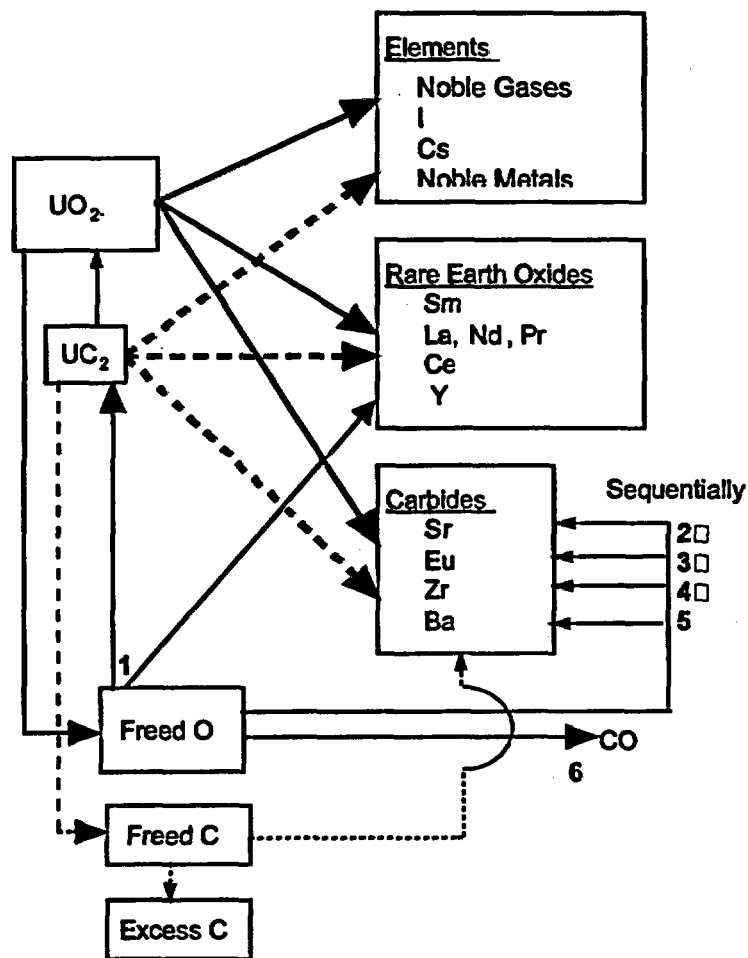


Figure 2-9 Oxygen distribution in a UCO kernel

The additional challenge of the UCO kernel is that it involves a more complex fabrication process and cesium, which can attack the SiC, may be more mobile (based on thermochemical calculations). Table 2-3 shows estimates for CO pressure. As seen from the calculations, UCO results in lower CO pressures for the higher burnups (>10%).

Table 2-3 Order of Magnitude Estimates for CO Pressure

T(°K)	Fuel	CO Pressure (atm)
1300	UCO	~0
	Low BU UO ₂	1
	High BU UO ₂	580
1600	UCO	~0
	Low BU UO ₂	5
	High BU UO ₂	1270

UCO kernels have had much less irradiation testing than UO₂ kernels and an important research objective is to further explore UCO behavior and performance limits.

To summarize, for higher burnup applications (>10% FIMA) it is important to control CO production (pressure) while still keeping the rare earth elements oxidized to limit their migration out of the kernel. The two-phase UCO kernel design is intended to provide these attributes without kernel migration so CO pressure problems can be avoided.

Kernel shape and density also have an impact on particle behavior. A manufacturing objective is to have a fairly round kernel so that the resulting coated particle departs little from sphericity [2-19]. The degree of sphericity effects the stress distribution in the coating. Significant departures from sphericity can result in high local stress in the coating layers. The density affects the amount of fissile material available in the particle, but it may also affect the degree to which the kernel can retain fission products (at least at lower burnup) and its reactivity with chlorine during the coating process (discussed later).

Unlike LWR fuel pellets, the kernel is at essentially a constant temperature and its behavior is more like that of "single crystal" release at low burnup; at high burnup the characteristic UO₂ structure is destroyed. In general, oxygen and carbon are used to form refractory compounds and the coatings are relied upon to hold the more volatile compounds.

Specifications for kernels are somewhat different than for LWR fuel pellets. The reader may note that there is less concern with grain structure or size and little mention of pores or complex structure. Table 2-4 lists a past kernel specification for typical German (pebble) fuel [2-2].

Table 2-4 Typical German Kernel Specification

Material	UO ₂
Enrichment, wt%	9.82
Sphericity	< 1.058
Diameter, μm	509 ± 9.7
Density, g/cm ³	10.81 ± 0.048

2.2.2.1 Kernel Design Factors Identified By The PIRT Panel

Table 2-5 lists the important kernel design factors and their rationales. Both items discussed in the previous section and items of general interest are included.

Table 2-5 Kernel Design Factors Identified By The PIRT Panel

Kernel Design Factor	Rationale
Diameter	Power generation and fission product production
Density	Power generation and fission products, fabrication reactivity with chlorine (perhaps), and may impact fission product retention at low burnups
Sphericity	Effects the coating uniformity (stress distribution in coating layers)
Stoichiometry: Uranium to oxygen (UO ₂ kernel)	CO production
Stoichiometry: Uranium to carbon and uranium to oxygen (UCO kernel)	CO production and oxidation of rare earths
Purity	General chemical and nuclear behavior (poisons)
Enrichment	General nuclear behavior and power production

2.2.3 Buffer Layer

The buffer layer surrounds the kernel and performs three main functions [2-6, 2-13 to 2-18, 2-25 to 2-27]:

- 1) **Fission Product Recoil Attenuation.** When uranium fissions, the resulting fission products are ejected at high velocity and are slowed down and stopped by the nearby material. Dense materials such as UO₂ and LWR fuel cladding limit the range of these recoils to roughly 10 microns. However, in low-density materials like carbon, the range of these recoils can be longer and they can cause significant local damage to the area they impact. The thickness of the dense outer layers in coated particle fuel is comparable to the recoil range. The buffer layer captures fission-produced recoils originating on the surface of the kernel and shields the IPyC from recoil damage.
- 2) **Void Volume.** The porous buffer layer provides the free volume for gas generation and expansion necessary to control the particle pressure.
- 3) **Sacrificial layer.** The buffer layer can distort to accommodate kernel swelling.

The thickness of the buffer layer affects the particle internal pressure. Too thin a buffer or a missing buffer layer will cause increased internal pressure, which can cause the particle to fail before the design burnup is reached.

The thermal conductivity of the buffer is not as high as the other coatings and too thick a buffer can raise kernel temperatures (somewhat) and thereby limit fuel core power density. Thus, the buffer thickness (already the thickest layer) is limited by pressure and heat transfer. The buffer layer is not required for particle strength, but it must be able to hold the kernel away from the IPyC.

Fast flux and recoils can cause shrinkage and cracking of the buffer layer. While not desirable, a certain amount of shrinkage and cracking is acceptable. However, a line of sight path from the kernel to the IPyC may expose the IPyC to serious recoil damage [2-28]. Figure 2-10 shows a particle with a distorted buffer layer. This particle did not perform well for other reasons (note the cracked OPyC and IPyC).

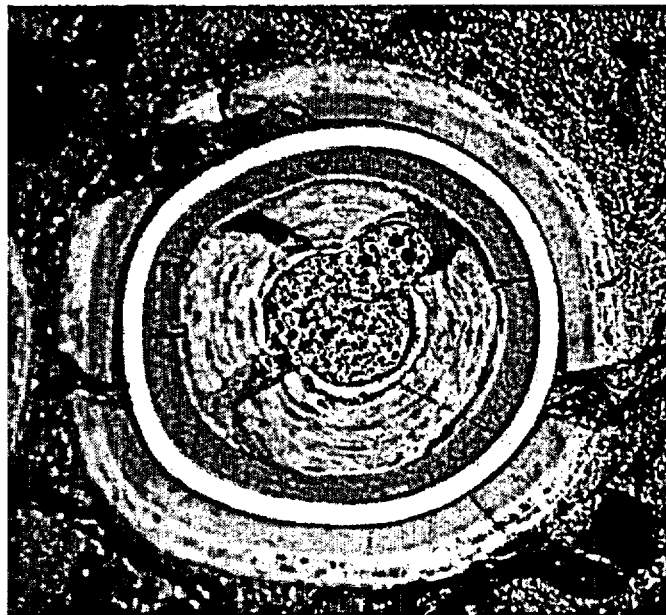


Figure 2-10 An example of a distorted buffer layer (HRB-21). (DOE-HTGR-100229)

It should be noted that the reference German pebble fuel did not exhibit buffer layer distortion under irradiation conditions. This may be because of different material properties and less challenging irradiation conditions [2-27]. The properties of coatings are currently a research topic.

The specifications for the buffer layer are shown in Table 2-6 (German fuel) [2-2]. These specifications are used in conjunction with process specifications; the layer generally has both process and product specifications.

Table 2-6 Typical German Buffer Layer Specification

Material	Carbon
Thickness, μm	100 ± 12.4
Density, g/cm^3	1.02 ± 0.01

2.2.3.1 Buffer Layer Design Factors Identified By The PIRT Panel

Table 2-7 details important buffer layer design factors and their rationale.

Table 2-7 Buffer Layer Design Factors Identified By The PIRT Panel

Buffer Design Factor	Rationale
Thickness	Void volume for gases, recoil attenuation, and distortion to accommodate kernel swelling. Also, the buffer affects the thermal impedance.
Density	

2.2.4 Inner Pyrocarbon Layer

The inner pyrocarbon layer (IPyC) is a higher density carbon layer deposited on the buffer layer [2-6, 2-13 to 2-18, 2-25 to 2-27]. It serves several functions:

- 1) It protects the kernel from chlorine (in the form of HCl) liberated during SiC deposition. Without the IPyC layer, chlorine would easily migrate through the buffer layer to the kernel, react with the uranium and produce volatile chlorides. These chlorides would then transport the uranium out of the kernel and contaminate the coatings. During operation, fissioning of this uranium contamination would then damage the layers. Fissioning outside of the kernel would also lead to increased fission product transport and releases from the particle.
- 2) It provides a smooth surface for SiC deposition (the buffer layer is too porous).
- 3) It delays transport of fission products to the SiC layer. The IPyC layer retains gases well and effectively isolates the SiC from CO, which can attack the SiC at higher temperatures. The layer does not effectively retain metals.
- 4) It can help maintain the SiC layer in compression. Depending on the IPyC/SiC layer bonding, the IPyC can place compressive forces on the SiC due to irradiation-induced shrinkage of the IPyC.

Good irradiation behavior requires that the pyrocarbon layer exhibit similar dimensional changes in the longitudinal and latitudinal directions for the fast fluence of interest [2-6, 2-8, 2-13, 2-25 to 2-27]. That is, it is desired that the carbon layer material and physical properties be anisotropic. This can be achieved by ensuring that the deposited carbon has a random rather than a preferred macroscopic crystal orientation. A measurement of anisotropy is known as the Bacon Anisotropy Factor (BAF). A BAF of 1 is completely isotropic, greater than 1 implies increasing crystal orientation. In practice, measurement techniques used to determine BAF have in some cases been inaccurate. In such cases the measured BAF has not correlated with irradiation performance as well as expected. This is an area of current research.

For the IPyC, there are six material and physical properties of interest to the designer of coated fuel particles:

- 1) Density
- 2) Permeability
- 3) Anisotropy
- 4) Creep
- 5) Shrinkage
- 6) Strength

These properties cannot be independently specified and two sets of conflicts are of particular designer interest. The first set is anisotropy and permeability. Some believe that a BAF of less than about 1.05 is necessary for good irradiation performance, with a BAF in the range of 1.02-1.05 as the desired target. However, permeability (in our case the transport of HCl to the kernel during SiC layer coating) tends to be less with a higher BAF (at least for past US fabrication experience; past German fabrication experience may have been somewhat better in this area). Thus, the designer has to balance irradiation stability and coating contamination. The situation can be made better or worst by the chlorine reactivity of the kernel.

Increased IPyC thickness would not resolve this problem as thicker IPyC can result in higher irradiation induced stresses in the IPyC and greater failure probabilities for the particle. Figure 2-10, previously shown, is an example of poor pyrocarbon performance. Both the inner and outer pyrocarbon layers failed by shrinkage-induced cracks. Figure 2-11 shows another pyrocarbon failure. This particle is an earlier design that lacked a SiC layer (buffer and OPyC only).

The other potential tradeoff is between IPyC shrinkage and IPyC creep. The fast flux causes shrinkage of the IPyC (influenced also by BAF), which is relieved by IPyC creep. The latter is a function of temperature. The designer has to minimize the rate of SiC stress increase caused by both particle pressure and pyrocarbon shrinkage due to fast flux with stress reduction by creep [2-13].

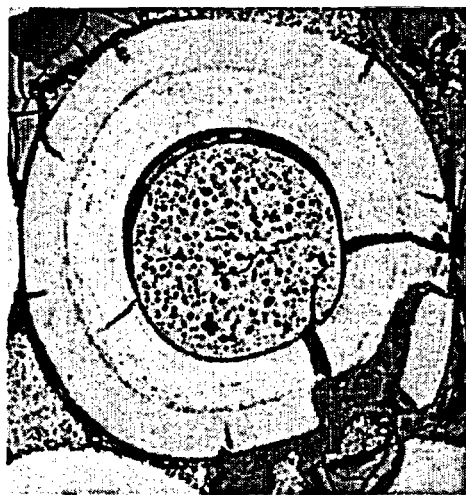


Figure 2-11 Example of pyrocarbon layer failure (BISO fuel)

Detailed modeling with accurate and manufacturing specific material properties is necessary to understand and optimize the tradeoffs in the particle design. The historical TRISO-coated particle design and fabrication process are an empirical solution to this problem for the design core environmental conditions.

The thermal properties of the (relatively thin and dense) IPyC are generally not as important as those of the buffer layer or the kernel. A more significant performance concern is IPyC radial cracking. Cracks (or debonding) in the IPyC can act as stress risers and induce locally high tensile stresses in the SiC layer if the between layer bond is strong [2-27, 2-29, 2-30]. Such cracks can also allow CO exposure to oxidize the SiC at high temperatures [2-31]. Figure 2-12 is an example of an IPyC crack that allowed CO to attack the SiC layer. Such attack occurs at elevated temperatures. Thus, this particle failure mode could be important in regions of power peaking.

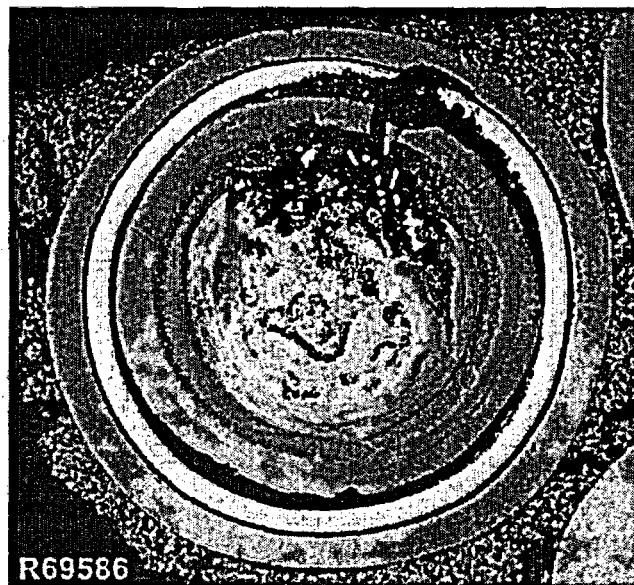


Figure 2-12 CO oxidation of SiC (WAR UO₂ kernel at ~1500°C in HRB-10)

The past German product specifications for the IPyC layer are shown in Table 2-8 [2-2]. These product specifications are used in conjunction with manufacturing process specifications. The process specifications are used to control the other properties such as IPyC crystalline structure. PyC quality assurance will continue to require a process specification until such time that additional measured product parameters can be developed, measured, and controlled to ensure good irradiation performance.

Table 2-8 Typical German IPyC Layer Specifications

Material	Carbon
Thickness, μm	39 ± 3.9
Density, g/cm^3	1.92 ± 0.007
BAF	1.043

In summary, the IPyC plays three major roles. It protects the kernel from Cl attack during SiC layer processing, provides structural stability, and retain gases. Dimensional stability is important as cracking can lead to particle failure.

2.2.4.1 IPyC Layer Design Factors Identified By The PIRT Panel

Table 2-9 details important IPyC layer design factors and their rationale.

Table 2-9 IPyC Layer Design Factors Identified By The PIRT Panel

IPyC Design Factor	Rationale
Thickness	Structural properties of the IPyC, gas retention, and control of possible HCl attack of kernel during fabrication
Density	Indirectly determines material properties. In particular, one is interested in radiation stability. Note that process specifications may also be needed to characterize this layer.
Anisotropy	The crystalline structure determines the irradiation stability of the layer.

2.2.5 SiC Layer

The SiC layer is the primary fission product barrier in the coated particle. It was the major innovation that took the pyrocarbon-coated particle to its high level of fission product retention performance. The SiC layer has two major functions [2-6, 2-13 to 2-18, 2-25 to 2-27]:

- 1) Provides structural support to accommodate internal gas pressure.
- 2) It is the primary fission product barrier. It retains gases and metallics (except silver), but is subject to attack from palladium and rare earth elements.

For design purposes, the strength of the SiC is important as well as the strength distribution. For very low particle failure rates, the tails of the SiC strength distribution become important. In addition, SiC density, grain size and grain orientation as well as the trace amounts of free silicon in the layer are thought to be important. However, conclusive evidence connecting these properties to particle irradiation performance is lacking [2-8, 2-32 to 2-36].

The interaction of strains between the pyrocarbon layers and the SiC layer are important to SiC layer failure [2-13, 2-27, 2-29, 2-30]. Figure 2-13 shows the qualitative model stresses in a particle. Stress in the PyC layers is driven by gas pressure and irradiation induced shrinkage; it is relieved by irradiation-induced creep [2-13]. Both shrinkage and creep are temperature dependant. Stress in the SiC layer is driven by particle pressure and the relative stress distributions between the layers, which depend on material properties and layer bonding strengths. Two important points are made in this figure:

- 1) The particle should be designed so that the pyrocarbons keep the SiC in compression for as long as possible.
- 2) Failure of a pyrocarbon layer will change the stress distributions and will change the SiC stress from compression to tension at a lower burnup. Since the SiC is a brittle material, the particle designers seek to keep the pyrocarbon layers intact over the design burnup.

For design purposes, intact SiC is assumed to retain all fission products at normal operating temperatures except for silver, which has a high release rate above 1100°C.

As the operating temperatures increase (>1250°C) fission product attack of the SiC becomes more likely. The major concerns are the lanthanides (even at lower temperatures) and palladium. Design of the kernel can retain the lanthanides as oxides, but palladium (noble metal) cannot be tied up and migrates (diffuses) to the SiC at the higher temperatures where it attacks the layer. This behavior effectively limits the normal operating temperatures (below ~1300°C) [2-8, 2-35 to 2-36].

At accident temperatures, above ~1600-1800°C, fission product release quickly increases. Above about 2000°C, thermal decomposition of SiC is a dominant failure mechanism.

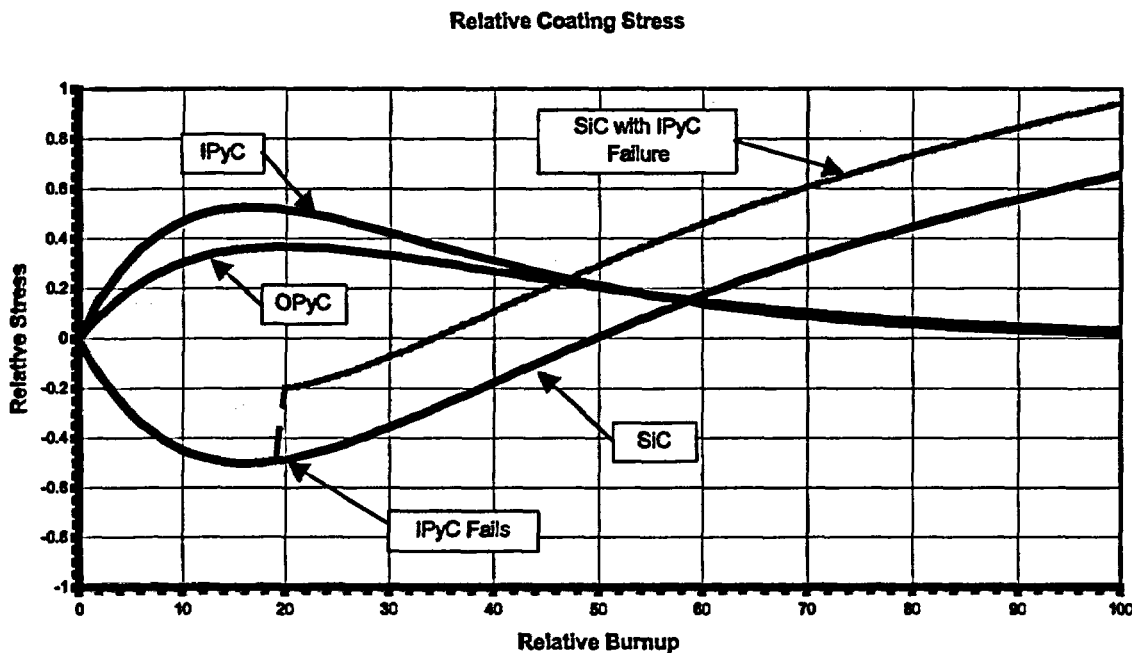


Figure 2-13 Qualitative stresses in coated particle layers for a model particle. (Assumes weak bonding between the IPyC and SiC – strong bonding may create local stress risers in the SiC)

However, above about 1600°C decomposition effects in the SiC such as the development of porosity are noted, implying that thermal decomposition mechanisms are active. At the assumed particle temperature limit, ~1600°C, diffusion of fission products begins to

increase (over normal operating values) and limits the time at temperature [2-6, 2-21 to 2-24].

To summarize, the designer tries to keep the SiC layer in compression during most of the irradiation and limits the operating and accident temperature to control SiC layer corrosion and decomposition.

The past German specifications for the SiC layer are shown in Table 2-10 [2-2]. These product specifications were used in conjunction with manufacturing process specifications. The process specifications are used to envelope the other properties such as SiC microstructure. The specifications for the SiC layer for contemporary HTGR particle fuel may include grain size and orientation as well as strength and strength distribution. This is an area of current research and the relevance of these items is being studied.

Table 2-10 Typical German SiC Layer Specifications

Material	SiC
Thickness, μm	35 ± 1.9
Density, g/cm^3	3.20 ± 0.007
Fraction Defective, (mean value)	7.7×10^{-6}

2.2.5.1 SiC Layer Design Factors Identified By The PIRT Panel

Table 2-11 details important SiC layer design factors and their rationale.

Table 2-11 SiC Layer Design Factors Identified By The PIRT Panel

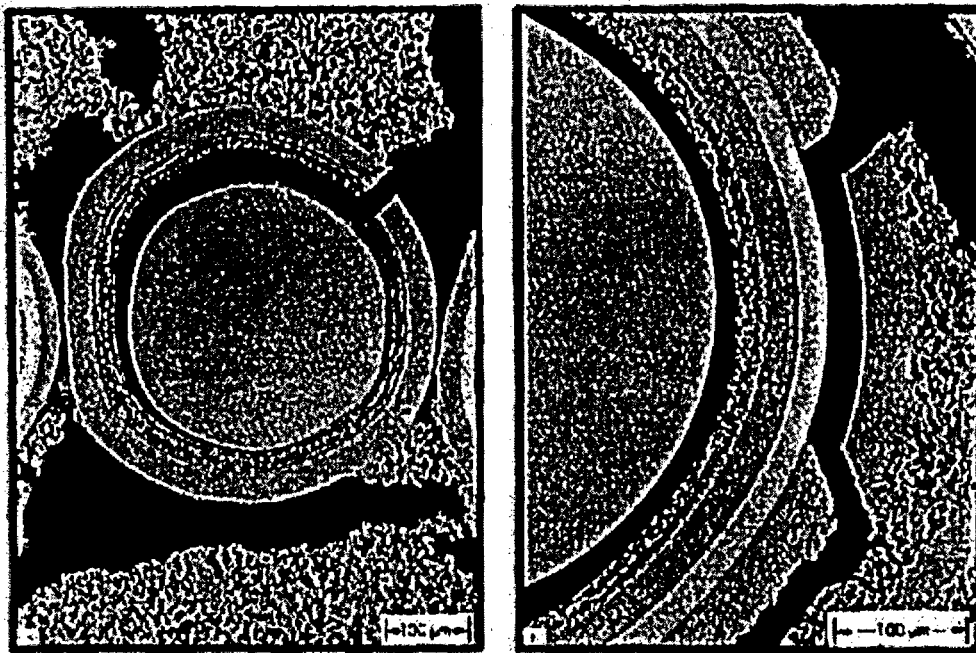
SiC Layer Design Factor	Rationale
Thickness	Determines the strength of the layer. Distribution of thickness is also important.
Density	Indirectly determines material properties. Desire high density and small grain size.
Fraction with defective SiC layers	The number of initially defective particles is an upper limit on fuel performance and impacts fabrication effort/cost.

2.2.6 Outer Pyrocarbon Layer

The outer pyrocarbon layer (OPyC) is the final layer on the coated particle and is the layer that binds the particle to the fuel form [2-6, 2-8, 2-9, 2-13 to 2-18, 2-25 to 2-27]. Many of the performance factors associated with the OPyC are similar to those of the IPyC, especially irradiation stability, but there are differences. The OPyC:

- 1) Protects the SiC during fuel particle handling prior to fuel element fabrication.
- 2) Provides a bonding surface for the matrix material.
- 3) Compresses the SiC during irradiation.
- 4) Acts as a final barrier to gaseous fission product release.
- 5) Provides some isolation of the SiC from external chemical reactions.

The six material properties of importance to the IPyC are important to the OPyC. Permeability of the OPyC is also important and is related to the intrusion of matrix material into the pores of the coating. If the OPyC were too permeable, it could result in too strong a bond between the OPyC and the fuel element matrix material. This could fail a coating as the materials differentially shrink from irradiation exposure. This is illustrated in Fig. 2-14.



This

strong bonding was a cause of fuel particle failures for past US made fuel and lead to the
 Figure 2-14 Particles Broken During Irradiation Due to Matrix-Particle Interaction.
 Carbonized in graphite tube. Irradiated to 3.6×10^{21} n/cm² ($E > 0.18$ MeV) at 940-1145°C. Left - BISO particle / Right TRISO particle

introduction of additives to the matrix binder to control the bonding strength. The contemporary US approach is to replace the fuel element injection fabrication approach (requires the thinner resin) with a new process that does not require the thinner resins and their resultant bonding concerns. The former and later fuel element fabrication methods are detailed in later sections.

The irradiation shrinkage and creep of the OPyC play similar roles as were outlined for the IPyC. The properties of interest to the OPyC are similar to those of the IPyC with the exception of permeation, which is important to matrix bonding rather than chlorine transport to the kernel.

The past German specifications for the OPyC layer are shown in Table 2-12 [2-2]. These product specifications were used in conjunction with process specifications. The process specifications are used to envelope the other important properties. OPyC quality assurance will continue to require a process specification until such time that additional measured parameters can be developed, measured, and controlled to guarantee good irradiation performance.

Table 2-12 Typical German OPyC Layer Specifications

Material	Carbon
Thickness, μm	39 ± 3.6
Density, g/cm^3	1.92 ± 0.02
BAF	1.028

2.2.6.1 OPyC Layer Design Factors Identified By The PIRT Panel

Table 2-13 details important OPyC layer design factors and their rationale. They are similar to those identified for the IPyC.

Table 2-13 OPyC Design Factors Identified By The PIRT Panel

OPyC Layer Design Factor	Rationale
Thickness	Strength of the OPyC and gas retention if the SiC fails.
Density	Indirectly determines material properties. In particular, one is interested in radiation stability. Note that process specifications may be needed to characterize this layer. Also, bonding between the layer and the matrix must be controlled.
Anisotropy	The crystalline structure determines the irradiation stability of the layer.

2.2.7 Fuel Element

The fuel element provides a fixed uniformly random distribution of fuel particles and matrix material with good irradiation and thermal properties [2-2 to 2-4, 2-6, 2-9]. It satisfies several needs:

- 1) Allows the fuel to be handled and placed in the reactor without damage to the particles.
- 2) Stabilizes the particles so they do not shift or move relative to the matrix.
- 3) Provides a good heat transfer medium from the particles to the reactor environment.
- 4) In the cases of pebbles, isolates the particles from impacts.

Generally, two fuel forms are considered:

- 1) Fuel compacts in graphite prismatic blocks. The cylindrical fuel compacts are approximately 2" long by ½" diameter (US design).
- 2) Fuel pebbles. Spheres 6 cm in diameter (Germany, China, South Africa).

Pebble fuel is the reference case for this PIRT.

The fuel form is selected on the basis of reactor fuel cycle, thermal considerations, particle loading requirements, and whether or not it must be removed from a "block" at end of life. Also, the number of particles broken during fuel element fabrication can be a consideration.

The number of broken particles along with the tramp uranium in the matrix material determines the quality of the fuel as both release fission products into the primary system.

The power produced by a fuel element depends in part on the number of particles; however, more particles per element (particle loading) can lead to increased particle damage during fabrication. This is a fundamental trade-off that can greatly influence the integrity of the element by limiting fabrication choices (described later). Power distribution can be skewed by an inhomogeneous distribution of particles within the element. This distribution must be controlled within designer limits.

The fuel element can be made by placing particles (and shim) in a mold and injecting matrix material to form a unit or by coating the particles with a thin soft layer of matrix material and forming the overcoated particles into shape under pressure. For pebble fuel an unfueled layer of matrix material is added to the outside of the fueled zone to protect the fuel particles from fuel element impacts associated with on line refueling and from pebble contact with other pebbles or walls during pebble flow through the core. This will be described in greater detail in the fabrication section. At this point, the designer is interested in the shape, heat transfer properties, damaged particle fraction, and any impurities in the matrix that may cause problems.

Table 2-14 lists some key German design specifications for their past pebble fuel elements [2-2].

Table 2-14 Historic Reference German Fuel Element Specifications

Outer Diameter, mm	60.0
Fuel-free shell thickness, mm	5.0
Uranium loading, grams per element	7.0 to 10
²³⁵ U enrichment, %	8 to 9.7
Free uranium fraction	6×10^{-5}

2.2.7.1 Fuel Element Design Factors Identified By The PIRT Panel

Table 2-15 details the important fuel element design factors and their rationale.

Table 2-15 Fuel Element Design Factors Identified By The PIRT Panel

Fuel Element Design Factor	Rationale
Matrix material specification	The matrix material binds the fuel particles in a uniformly random distribution and contributes to the fuel element properties.
Particle packing fraction	This parameter determines in part the nuclear and thermal power properties of the fuel element. Particle damage during manufacture is more likely at higher packing fractions.
Unconfined heavy metal outside SiC layer	Unconfined heavy metal results in fission products in the primary circuit and the potential for releases during off-normal conditions.
Particle distribution in fuel element	Inhomogeneous particle distribution within fuel elements can result in hot spots.
Particle overcoat	This layer protects the particle during fuel element fabrication by deforming, providing a particle-to-particle spacing function, and integrating the particle into the matrix.
Fuel free zone (Pebble)	The fuel pebble requires a fairly strong outer layer to protect the inner-fueled region from damage as the pebble must be repeatedly dropped several meters into the pebble bed core.

2.3 Manufacturing

2.3.1 General

The kernel coating layers are added in a fluidized bed coater. The coating process is statistical and results in a distribution of attributes. The goal is to control the process so that the distribution meets the demanding manufacturing specifications and the process is predictable. A simplified diagram of a coater is shown in Fig. 2-15.

The coating chamber consists of a graphite tube that is maintained at the desired temperature by electrical heating. A fluidizing gas is introduced to the chamber by a gas distribution nozzle at the bottom. The flow rate of the fluidizing gas is enough to levitate and randomly circulate the bed of particles, but not so much as to eject particles out of the top of the coater chamber, which could result in coating defects. Separate coating gases are introduced and gas ratios automatically changed and controlled to produce the desired coating [2-8, 2-25 to 2-27, 2-37]. Hydrocarbon gases are pyrolytically decomposed into carbon and hydrogen for the application of the buffer, IPyC, and OPyC layers.

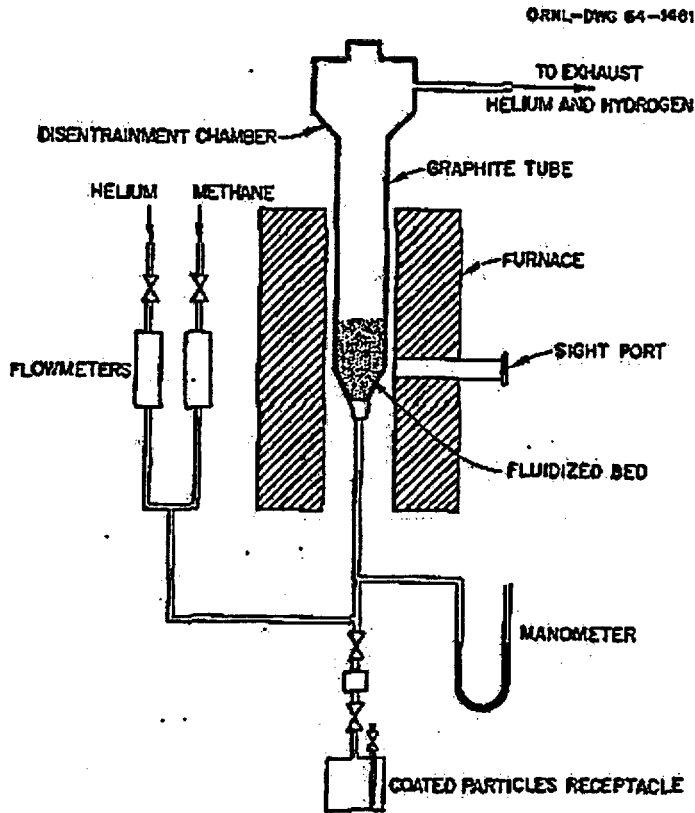


Figure 2-15 Diagram of a coater (from ORNL-4324)

During the coating process the bed of particles is agitated continuously by the levitation (fluidizing) gas and each particle is coated over time with about the same amount of material. Since heat transfer rates are very high in a fluidized bed, thermal gradients are generally very low within the bed. Temperatures can be monitored with optical pyrometers or thermocouples through access ports. When the desired coating run has been completed, the flow is reverted to pure fluidizing gas and reduced until the particles drop to the bottom.

Important variables in the design of the coater are the shape of the inlet nozzle and cone or "frit" at the inlet to the reaction chamber. The gas flow distribution angle affects the refluxing action of the fluidized bed, the tendency of soot plugging, and the gas flow distribution. The exact influence of all these factors combined with the operating parameters is not well understood and some experimentation is necessary with each coater design to make particles within specifications. The temperatures, sources gases, and coating deposition rates are particularly important and determine the coating properties. Also, during manufacture of a coated particle lot the diameter and mass of the particles increase, but compensating the flow rate for this fact has not always been done, although it appears to be necessary to assure uniformity of coating properties.

Coaters have been operated in either of two ways: continuous or interrupted. In a continuous coating process the coating layers are put on one right after another by changing the feed gases, flow rates, and temperatures as a function of time. That is, the particles are not removed from the coater after each layer is completed. This method has the advantage that there are no interruptions to introduce defects into the coatings or the way the coatings adhere to each other. The disadvantage is that defective particles cannot be removed or problems identified until the process is complete. However, particles can be siphoned off the bed for sampling after a layer is added. Interrupted coating empties the coater after a layer has been applied and allows a layer-by-layer inspection of a batch, but the extra handling can introduce problems of its own such as impurities and coating damage.

The typical feed gases are argon, hydrogen, acetylene, propylene, and methyltrichlorosilane (for the SiC). The coating rate effects PyC anisotropy, with low rates, 1-4 micron/min, favoring high BAF, and high rates, 4-10 micron/min, favoring low BAF [2-8, 2-25, 2-27]. A tradeoff between porosity and density occurs in PyC coating and optimizing the tradeoff in these properties to some degree may be necessary. To date, process knowledge generally has been necessary to characterize a coating, as measured product characteristics alone were not found to be sufficient to assure good irradiation performance.

2.3.1.1 Manufacturing Process Phenomenon Identified By The PIRT Panel

Table 2-16 lists factors identified by the PIRT panel for coated particle manufacturing.

2.3.2 Kernel

The kernel is made by an ammonia-based gel-precipitation process, referred to as either "internal" or "external" gelation. Briefly, for internal gelation, uranium is dissolved in nitric acid and mixed with urea (and carbon for a UCO kernel). The mixture is then chilled and mixed with hexamethylene (HMTA) to form a broth. This broth is only stable at low temperatures (~0°C) and is kept chilled. The broth is then pulsed through needle orifices to form droplets that fall into a heated column of immiscible liquid. The rise in temperature causes internal ammonia production and the droplet to gel. The resulting spheres sink to the bottom of the column, are removed, and are then washed in ammonium hydroxide to remove ammonium nitrate and dried.

Table 2-16 Manufacturing Process Phenomena Identified By The PIRT Panel

Manufacturing Factor	Rationale
Layer coating process specifications: Gases (levitation gas and coating gas)	The gases used in the coater directly influence the quality of the layer and the operation of the coater.
Layer coating process specifications: Ratio of gases	The gas mixtures affect the layer properties and production rate.
Layer coating process specifications: Temperature	The properties of the coating layer are dependant on the coater temperature.
Layer coating process specifications: Coating rate	The microstructure of the coating layer is influenced by the coating rate.
Layer coating process specifications: Pressure	Pressure affects reaction rates. (The coaters are generally operated at atmospheric pressure.)
Layer coating process specifications: Coater size	Coater size effects the distribution of layer properties.
Layer coating process	Continuous versus interrupted coating may affect coating layer interface properties.
Process control	Controlling the process is important. Coating product measurements may not be sufficient to guarantee good irradiation performance.
Product control	Coatings must meet designer specifications.

An external gelation process can also be used. This process also induces gelation with ammonia, but the source of the ammonia is external to the droplet. A somewhat different broth is prepared and pulsed through needle orifices, but this time the droplets fall through an ammonia vapor phase and then into an ammonium hydroxide containing aqueous column to induce the gelling. They are then washed and dried. The external process is used for the reference Pebble fuel [2-1 to 2-3, 2-25].

The dried spheres are calcined and sintered in a hydrogen atmosphere to remove the excess oxygen. If they are UCO kernels, they are next sintered in an argon or argon/CO atmosphere to adjust the O/C ratio for a UCO kernel.

The kernels are then screened for size and tumbled to eliminate the non-round and odd shapes. They are inspected for size, size distribution, density, and stoichiometry. Figure 2-16 is a flow diagram of the external gelation process (reference for this PIRT).

Table 2-17 outlines important properties and likely quality control methods [2-1 to 2-4, 2-38, 2-39].

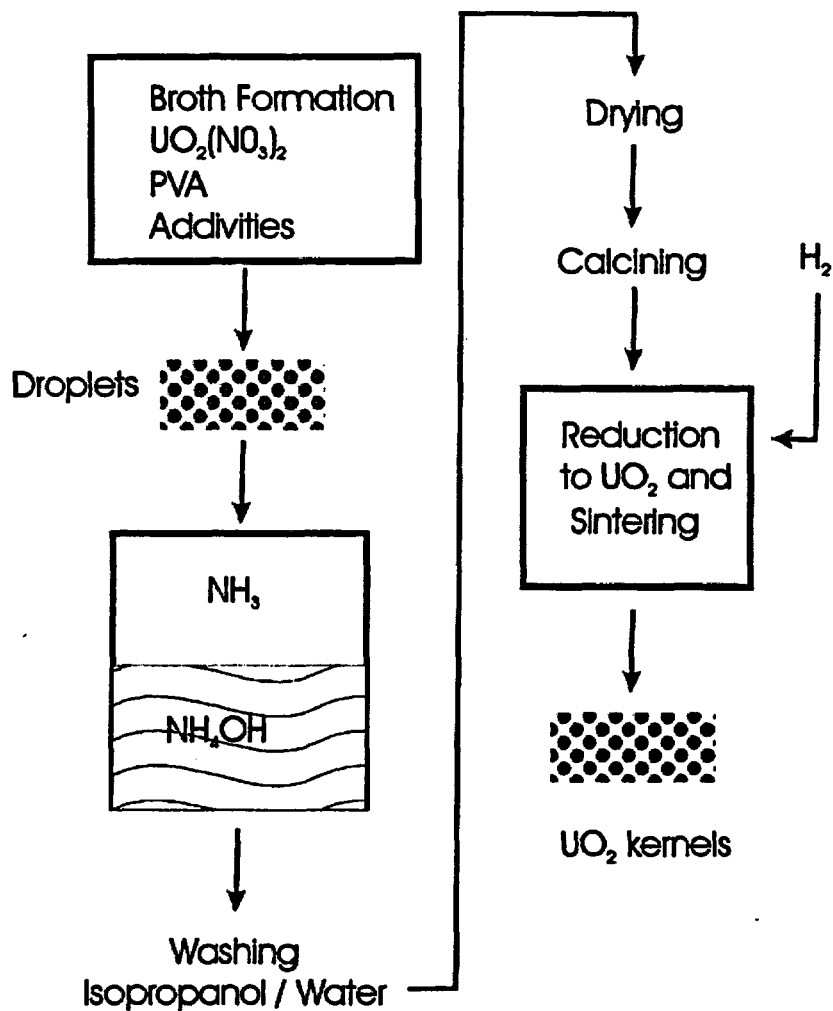


Figure 2-16 Flow diagram of external gelation kernel fabrication process

Table 2-17 Kernel Properties and QC Methods

Kernel Attribute	QC Method
Density	Pycnometry, density column
Diameter	Particle size analyzer, imaging (sphericity)
C/U and O/U	Combustion and wet chemistry, metallography/image analysis (phases)
Impurities	Spectrographic (mass) methods and wet chemistry

2.3.2.1 Kernel Manufacturing Phenomenon Identified By The PIRT Panel

Table 2-18 lists the kernel manufacturing factors identified by the PIRT panel.

Table 2-18 Kernel Manufacturing Factors Identified By The PIRT Panel

Kernel Manufacturing Factor	Rationale
Density	The density of the kernel determines the fissile material present and thus power. It may also affect the HCl reactivity during coating.
Microstructure – UO ₂	Microstructure is known to affect performance in other types of reactor fuel.

2.3.3 Coated Particles

The coating layers are deposited on the kernel in a fluidized bed by the thermal cracking of the appropriate gas in a fluidizing gas such as argon [2-8, 2-18, 2-25 to 2-27, 2-37 to 2-38]. Hydrocarbon gases such as acetylene and propylene are used for the carbon layers. MTS is used for the SiC layer and it is reduced by hydrogen. Temperatures are in the range of 1200 to 1500°C and the flow rates of the gases are adjusted to achieve the desired deposition rate.

Layer properties are controlled by temperature, coating rate, coating gas composition, bed loading, and particle size. In general, each layer has its own optimal combination of parameters that are determined experimentally for a particular coater. A flow diagram of the process is shown in Fig. 2-17. Note that the process may be continuous or interrupted. In the continuous process, the particles remain in the coater and the composition of the gases and furnace temperature are changed so the coatings can be put on one after another. In the interrupted process, the coater is unloaded after each coating and the particles can be checked and sorted for gross defects such as out-of-roundness. Sampling can be used for destructive investigation. The bad particles (or a bad batch) are discarded before the next layer is applied.

At the present time, the continuous coating method has been demonstrated to give acceptable results, but this conclusion is still tentative. The current trend is toward continuous coating and the highest quality fuel (reference material) has been produced by this method.

An item of interest for the PIRT review is that the specification of layer product properties is not sufficient to ensure satisfactory irradiation performance. At the present state of the art, modest changes in the operation of the coater (such as design issues, coater size, and exactly where the bed temperature is measured) can lead to coating property changes that can result in substandard irradiation performance. These changes either cannot be observed by the present QC methods or the changes in material properties are not currently measured.

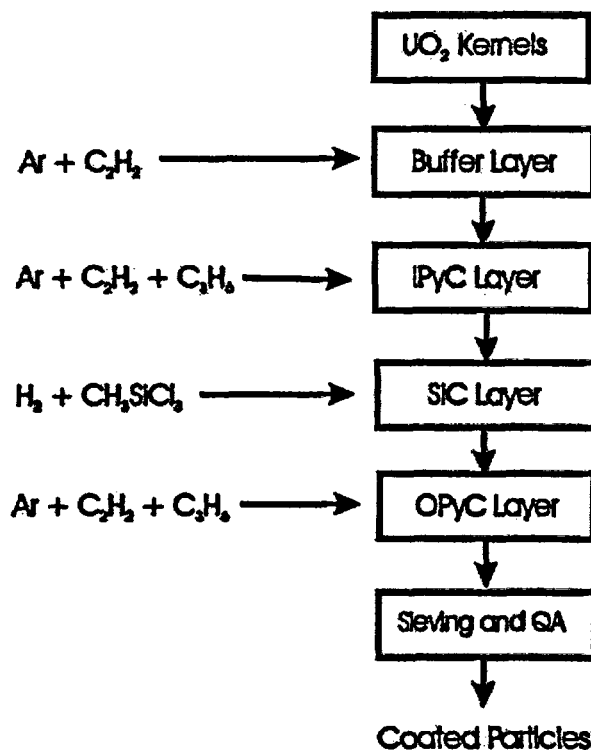


Figure 2-17. Flow diagram of the continuous coating process

This is addressed by having both layer fabrication process and layer product specification. Thus, both process knowledge and product measurements are required to determine if the fuel has been properly fabricated. This issue appears to be particularly important for pyrocarbon layers as was discussed in the design section. The BAF measurement technique is also important. The SiC layer is very important for the control of fission product transport and it is sensitive to the details of coater operation.

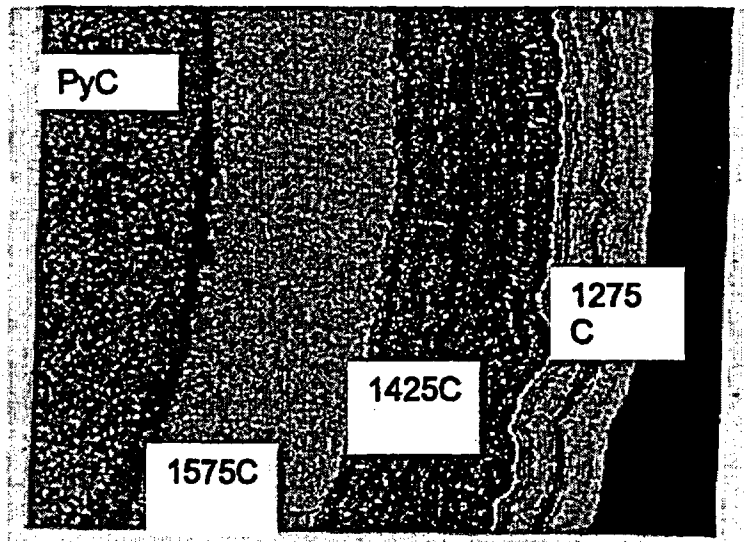
Figure 2-18 shows how the nature of deposited SiC can change with temperature. The fabricator would like to control free silicon, grain size and grain orientation. SiC has shown good irradiation properties, but like pyrocarbon, a clear one to one correlation between measured properties and irradiation behavior is not available at present.

Table 2-19 shows the coating layer product properties measured during fabrication and the measurement methods that are typically employed. The reader is cautioned that measurements alone do not provide a complete picture of the fabrication parameters and must be used in conjunction with process knowledge [2-27, 2-32, 2-33, 2-37, 2-39].

2.3.3.1 Coated Particles Manufacturing Factors Identified By The PIRT Panel

Table 2-20 lists the manufacturing factors identified by the PIRT panel.

Finally Fig. 2-19 shows that particles don't have to be perfect; some out of "roundness" can be tolerated. Severely malformed particles, however, are to be removed from the lot.



Etched SiC
ORNL/TM-5152

Figure 2-18 SiC structure as a function of coater temperature



Malformed Particle



R71610 (C9900814-23) 200x

**Particles with facets
have performed well
(FTE-13 Pu,Th)**

Figure 2-19 Performance of non-spherical particles

Table 2-19 Coating Layer Product Factors and Typical QC Methods

Layer Attribute	QC Method
Buffer Layer	
Thickness	Radiography, metallography
Density	Mercury pycnometry and carbon content analysis (LECO)
Missing or thin layer (a failure mechanism)	Radiography
IPyC Layer	
Thickness	Radiography, metallography
Density	Liquid gradient column
Anisotropy	BAF (other methods under study)
Microstructure	Coating rate and process conditions (temperature, coating gases, time) [Process Knowledge]
Permeability (The heavy metal dispersion will signal a missing layer)	Heavy metal dispersion into layers (Radiography, chemical analysis)
SiC Layer	
Thickness	Radiography, metallography
Density	Liquid gradient column
Microstructure	Coating rate and process conditions (temperature, coating gases, time) [Process Knowledge], metallography
Spatial defects or missing layer	Burn/leach
Strength	Crush tests, brittle ring tests
OPyC Layer	
Thickness	Radiography, metallography
Density	Coating weight and pycnometry
Anisotropy	BAF
Microstructure	Coating rate and process conditions (temperature, coating gases, time) [Process Knowledge]
Missing or defective layer	Optical microscopy
Surface connected porosity	Mercury porosimetry

Table 2-20 Manufacturing Layer Product Factors Identified by the PIRT Panel

Coating Layer Manufacturing Factor	Rationale
Buffer Layer	
Thin (less than specified)	A thin buffer layer can lead to particle failure due to overpressure.
Density and open porosity	The buffer layer is the void volume to accumulate the released fission gases and any generated CO. It determines the internal pressure.
IPyC Layer	
Porosity	High porosity can allow HCl liberated during SiC deposition to attack the kernel and spread fissile material to the other layers.
Bonding strength to SiC	The bonding strength determines how forces are transmitted from one layer to another. May be most important for IPyC.
Anisotropy	The anisotropy is important as it determines the dimensional stability of the layer under irradiation.
SiC Layer	
Defects	Defects in the SiC can allow fission products to diffusion out of the particle.
Heavy metal dispersion	Heavy metal in the SiC layer will fission and damage it.
Stoichiometry	High quality SiC is important. Free silicon may be detrimental.
Bonding strength to OPyC	The bonding strength determines how forces are transmitted from one layer to another.
Density	Density can indirectly determine retention properties and strength.
Fracture strength	The strength of the layer determines the integrity of a particle. The tails of the distribution determine the particles with marginal strength
Grain size and microstructure	The microstructure determines the layer diffusion properties.
OPyC Layer	
Porosity	The porosity of the OPyC can determine the strength of the OPyC to matrix bond.
Anisotropy	The anisotropy is important as it determines the dimensional stability of the layer under irradiation.

2.3.4 Fuel Element Manufacture

Once the particles have been coated and inspected, the next step is to form the fuel element. Over the years, several fuel element forms have been considered, but two are now of contemporary interest to US HTGR licensing. They are: fuel compacts in prismatic graphite blocks (US) and fuel pebbles (Germany, reference case). The fuel form and particle loading depends on the power required from the element, the required fissile loading, and the temperature and temperature gradients. In addition, the tolerable particle breakage depends on the fuel element loading as higher particle loading generally increases the risk of particle damage [2-9].

An important goal of fuel element fabrication is to minimize the amount of uranium outside the particles by limiting the number of defective particles from the manufacturing process, minimizing the damage done to particles during the element forming process, and minimizing the uranium impurities in the fuel element feedstock materials. With particle defects at the 10^{-5} level, limited particle damage during handling, and high purity materials, the exposed uranium in a fuel element is expected to be equivalent to no more than a particle defect fraction of $\sim 10^{-5}$.

The fuel element (compact or pebble) is formed from the fuel particles, which may or may not be overcoated with a matrix material, and the fuel element matrix material. The matrix material is a mixture of binder (resin or pitch), graphite flour, additives, and graphite shim (if required). The binder may be a thermosetting type (resin) that becomes rigid with exposure to elevated temperatures or a thermoplastic type (often a pitch) that always softens and flows with exposure to elevated temperatures.

Fuel element fabrication may be cast into two broad categories [2-1 to 2-4, 2-9]. The first is the so called "Admix" process where the particles, matrix, and any shim material are first mixed together and then molded to shape at temperature (used for reference fuel). With this process, the particles are often first overcoated with matrix material. The matrix material used is a highly viscous mixture of binder and graphite powder that does not flow. This process is generally limited to lower particle packing fractions of no more than roughly 30-40%. Somewhat higher packing fractions are possible, but the probability of particle breakage increases with higher packing fractions. Figure 2-20 illustrates the general process.

The particles are usually first overcoated with matrix material. The overcoated particles are then mixed with additional matrix material (as necessary) to create a uniformly random distribution of particles and matrix material of a specific volume, which is then placed into a mold. If the particles are not overcoated first, the matrix material may be introduced as a powder or flakes and melted during processing; it need not be "wet" to start with. Pressure and heat are applied to form the fuel element to shape. To add the unfueled layer of a pebble, the fueled center is fabricated as described above, then surrounded by more unfueled matrix material, placed in a larger spherical mold, and formed as before. The result is a "green" fuel element ready for carbonizing.

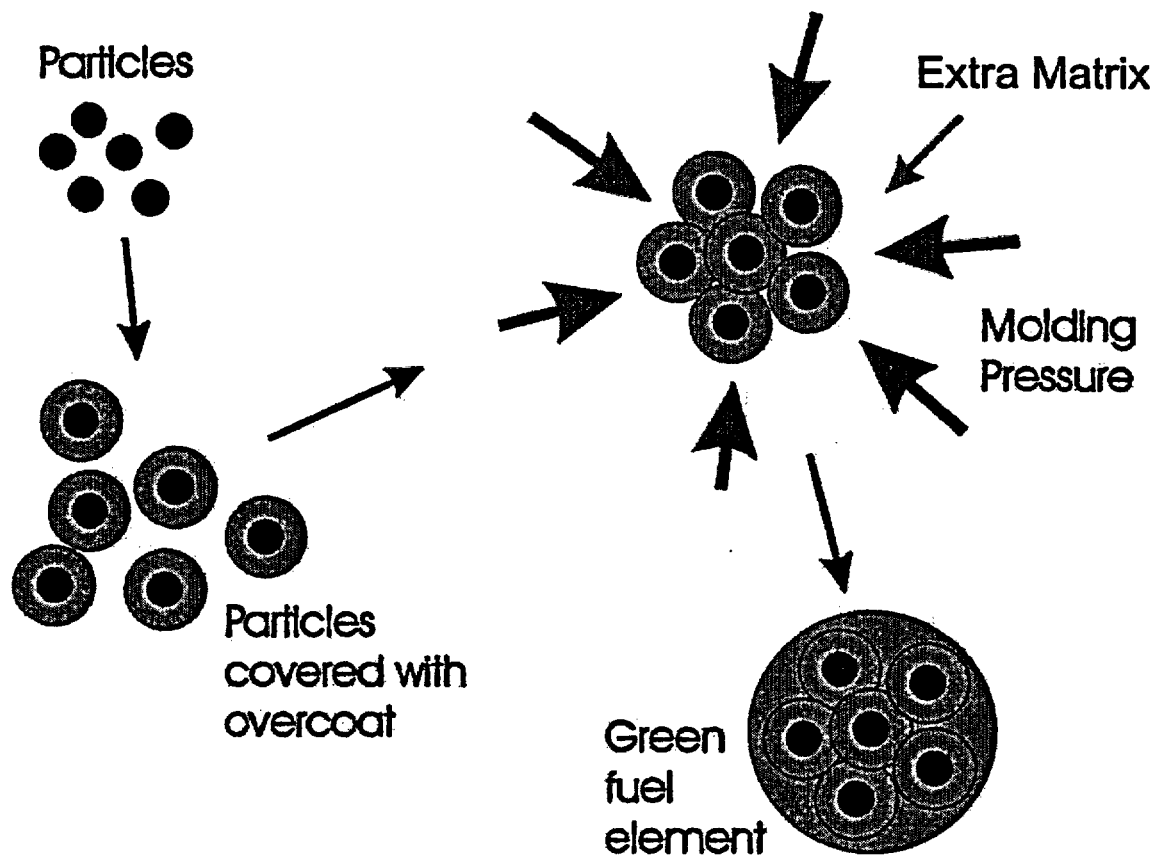


Figure 2-20 Illustration of the Admix fuel element forming process

Either thermosetting or thermoplastic binder may be used, but thermosetting resin is often chosen, as the "green" element will not slump upon further heating.

The second process is the injection method. With this process, the particles and any shim are first put into a mold and compressed by a piston. Next a flowable mixture of binder (usually pitch) and graphite flour is injected into the mold and allowed to harden by cooling the mold for thermoplastic binder or elevating the temperature to the set point for thermosetting binder. After the element has hardened, it is ejected from the mold. See Fig. 2-21. This method has often used thermoplastic pitch to get the desired matrix and fabrication properties.

Because this method needs a flowable mixture, less filler material can be used in the matrix, making it weaker. However, much higher particle packing fractions can be accommodated ~50-60%.

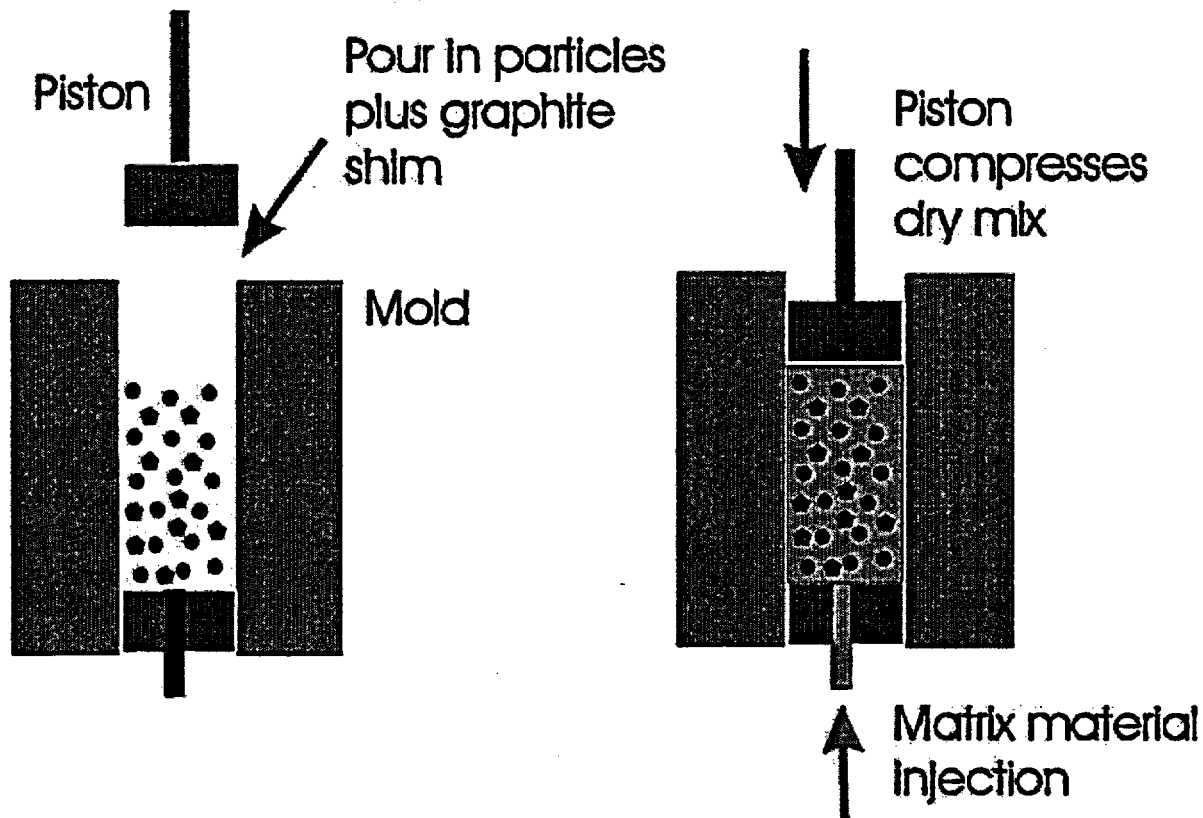


Figure 2-21 Illustration of the injection method

Both methods can damage particles by crushing and care needs to be taken to control forces and packing fraction. The current trend is toward the Admix process with thermosetting resin and the best performing fuel has used this method. It is likely that all future HTGR fuel element fabrication will be based on the Admix rather than the Injection process unless high particle packing fractions are required.

A common QC method to check for broken particles in a fuel element is the burn-leach method. A fuel element is slowly oxidized in air in a furnace at approximately 800°C to remove the matrix material and particle outer pyrocarbon layer. Flaws in the SiC larger than roughly 1 micron that expose the inner pyrocarbon will also allow the IPyC layer and the buffer layer to be oxidized during the burn [2-33, 2-38, 2-39]. The resulting burned back particles are then leached in hot nitric acid to dissolve any exposed uranium. The leachant is then analyzed for uranium and an estimate for the damaged particle fraction determined.

Another variable is the matrix mix. The resin is the glue (binder) that holds the mixture together, the graphite flour or flakes is the filler material that forms the foundation of the element, and the additives make the mixture free flowing (if necessary) and limit the adhesion of the resin to the OPyC.

Another factor of the element fabrication process is the adhesion between the matrix material and the OPyC. This was discussed previously (see Fig. 2-14). If the adhesion is too strong, the OPyC will be damaged as the matrix material shrinks during irradiation. This is less important with the Admix process because of the low percentage of binder and high filler content, but is more important for the injection process because of its high binder content and lower viscosity, which gives it better penetration ability. To limit the binder penetration into the OPyC, additives are added to the matrix material. These additives vaporize during the carbonizing process.

To summarize, the Admix process:

- 1) Uses a low percentage of binder and a high percentage of filler
- 2) Doesn't flow – can't be used for injection molding
- 3) Produces a relatively strong dense matrix
- 4) Few problems with OPyC penetration
- 5) Limits particle packing fractions to 30-40% (perhaps even up to 50% in some cases)

The Injection process:

- 1) Has a high binder content and a low filler content
- 2) Flows well – designed for injection molding
- 3) Produces a less dense, weaker matrix
- 4) Additives must be used to limit penetration into the OPyC
- 5) Supports higher packing fractions of 50-60%

The required strength of the fuel element depends on its application. A pebble, which is repeatedly dropped several meters, requires greater strength than a fuel compact that is surrounded by a fixed graphite block. Thus, element strength is a parameter that can be part of a design trade off – say, for higher packing fraction.

The next step after the green element has been made is carbonizing. The green fuel elements are baked in an inert atmosphere furnace at approximately 800°C to carbonize the binder material and vaporize and remove any process additives. Fuel elements made with thermosetting resin are carbonized free standing, as the resin will not resoften. Elements made with thermoplastic resin (pitch) are packed in beds of aluminum oxide to support them as they will “slump” (i.e. deform) as the resin softens with the temperature increase.

During the carbonizing process, care must be taken not to introduce impurities either from the furnace atmosphere or bakeout bed. Metals like iron and chrome can diffuse through the carbon layers and attack the SiC layer. To limit problems with impurities, the fuel elements can be purged with HCl after carbonizing. The HCl converts many impurities to volatile chlorides that leave the fuel element at processing temperatures. The HCl process was used by the US in a few cases. Other countries did not use this step.

Finally, the fuel elements are baked at 1650 to 1950°C to their final form. The purpose of this high temperature firing is to further the carbonization, improve the crystallinity of the

matrix binder, and to remove any residual volatile impurities. Short times, ~1 hour, at these temperatures do not appear to effect the SiC (slight grain growth). Impurity control during high firing is important because at these high temperatures impurities can quickly diffuse through the matrix and pyrocarbons to the SiC and damage it. Impurities can come from the initial matrix mix, the carbonizing bed, the firing furnace, and from handling equipment. Figure 2-22 illustrates the fuel element baking steps.

The final fuel element parameters of interest are:

- 1) Thermal conductivity and its changes with irradiation
- 2) Strength for general handling, and for pebbles, dropping toughness during normal operating conditions
- 3) Dimensional stability under irradiation and both cracking and microcracking
- 4) Corrosion behavior under air and water ingress conditions
- 5) Ability to sorb fission product metals

Some typical QC methods used for fuel element examination are detailed in Table 2-21 [2-38].

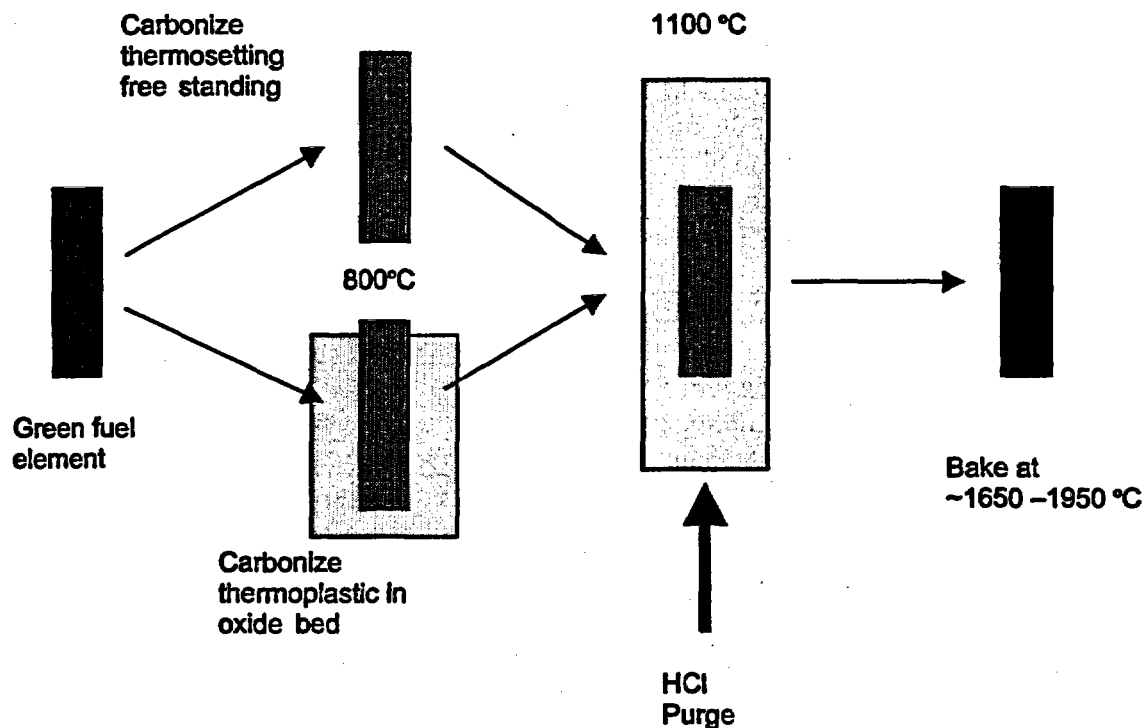


Figure 2-22 Green fuel element bakeout process

Table 2-21 Typical Fuel Element QC Methods

Fuel Element Attribute	QC Method
General integrity	Visual inspection
Dimensions	Gauging, contact and non-contact
U Content (total)	Wet chemistry
Particle distribution (homogeneity)	Gamma spectroscopy, radiography, metallography
Defective SiC	Burn leach
U contamination	HCl leaching
Impurities	Spectrographic methods and wet chemistry
Strength and toughness	Crush, drop
Thermal	General thermal analysis methods

2.3.4.1 Fuel Element Manufacturing Factors Identified By The PIRT Panel

The fuel element manufacturing factors identified by the PIRT panel are listed in Table 2-22.

Table 2-22 Fuel Element Manufacturing Factors Identified by the PIRT Panel

Fuel Element Manufacturing Factor	Rationale
Particle overcoating	The overcoating layer helps protect the particle during fuel element fabrication by slightly deforming, providing a spacing function, and integrates the particle into the matrix.
Matrix and Binder	The “glue” that holds the matrix together. May be thermosetting or thermoplastic.
Bonding strength between the OPyC and the matrix	If the bonding strength of the matrix to the fuel particle is too high, the OPyC may be torn away as the matrix undergoes irradiation-induced shrinkage.
Compacting (molding and pressing)	This process can result in broken or damaged particles.
Carbonization	This is the process of driving off the volatiles and converting the resin to carbon.
Heat treatment	The high temperature process that completes carbonization, improves the crystallinity of the matrix, and degasses the element.
Impurity control	Impurities can come from many sources and the metals can damage the SiC at high temperatures.
Tramp uranium	This is uranium contained in the raw materials used in the manufacturing process.
Strength	The fuel element must be strong enough for its application.
Initial particle defect fraction due to manufacture	Exposed kernels at the completion of fuel element fabrication increases fission product releases.

2.4 Normal Operation

2.4.1 General

During normal operation the fuel failure rate is required to be very low. The cause of fuel failures during operation is a function of its design, manufacture and operating environment. For example, in service failures of some past fuels were believed to come from the very small fraction of particles with thin or missing buffer layers [2-7, 2-20 to 2-24, 2-34]. Less than optimal pyrocarbon layers that crack or debond under irradiation can also contribute to failure [2-27, 2-30]. Failures due to misshaped particles are expected to be small with current QC methods. Adverse stress conditions due to statistical variations in fuel particle layer characteristics can also result in particle failures. Another potential source of failures are fuel particles that are in the "hot spots" of the core. Extended operation at temperatures near and above 1300°C can result in weakening or failure of particles due to fission product corrosion [2-35, 2-36]. Proper core design should eliminate these "hot spots".

Fission product releases during normal operation come from at least four sources:

- 1) Fabrication-induced particle defects and tramp uranium. Release from defective (e.g. flawed SiC) particles, particles broken during fuel element fabrication, and uranium impurities in the fuel element fabrication materials will be present from the start of operation. All three of these sources have uranium outside of the SiC coating, the pyrocarbon, or both.
- 2) Releases from particles that fail during normal operation. For a properly designed core, one source of release may be from particles that fail due to missing or thin buffer layers (or perhaps, poor quality pyrocarbon that cracks). These particles will result in excessive internal pressure and break sometime during the core life. If the particles are fabricated correctly and operated within limits, failures due to statistical variations or coating faults such as pyrocarbon, overpressure, or SiC problems should be very small.
- 3) If there are hot spots in the core, the probability of failure from other sources such as amoeba (UO₂) or fission product corrosion of the SiC could be significant for a limited number of particles.
- 4) Silver releases from particles at temperatures above 1100°C. SiC does not retain silver well above approximately 1100°C and silver is likely to be released. Silver-110m is considered to be an occupational dose issue rather than a public health and safety issue for present designs.

Released fission gases will quickly migrate to the coolant and can be removed by the coolant gas cleanup system. Metals, however, will remain on the reactor internal components and perhaps on dust. There appears to be no practical way to remove metallic releases from an operating reactor.

To meet the proposed HTGR licensing-basis offsite dose criteria, safety analysis assumptions, the initial releases would have to be equivalent to a particle failure fraction of about $1-5 \times 10^{-5}$. Failures during normal operation would also have to increase by no more than a factor of about 2 to 5. An illustration of selected operational failure mechanisms attributed to US fuel manufactured in the past is shown in Fig. 2-23. The

detailed analysis of acceptable fuel failure fractions and mechanisms was outside the scope of this PIRT. Other fission product transport means such as dust were deferred to future PIRT exercises.

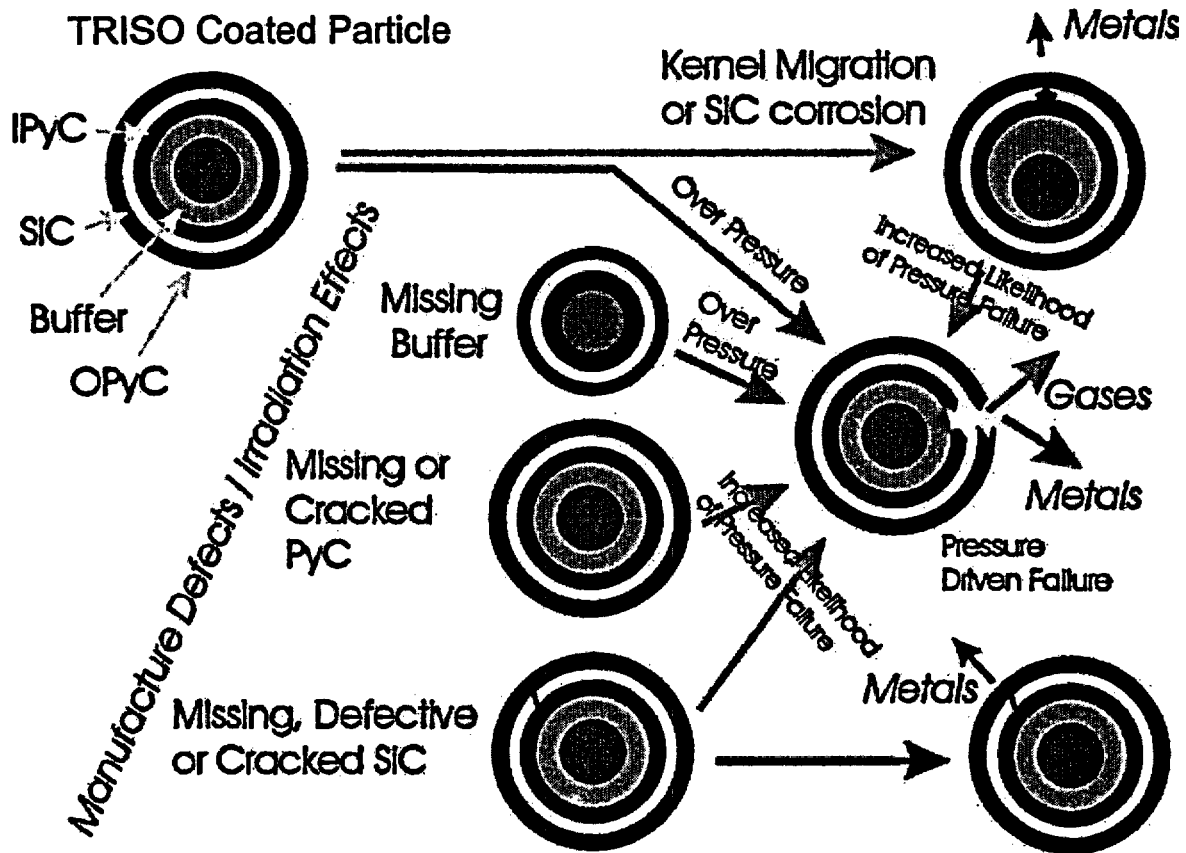


Figure 2-23 Illustration of selected particle failure mechanisms during normal operations

Figure 2-24 illustrates fractional releases (fission products outside fuel sphere divided by the total integrated fission products produced by fission) that have been calculated for pebble fuel during its life in the core of a small (170MW thermal) pebble bed reactor. Note the temperature cycling as it traverses the core. Also, note that the cesium release fraction is largely determined by the defective particles. These model calculations were done using the FRESKO-II code (German) [2-6].

Many of the particle failure mechanisms and phenomena associated with normal operation were covered in the design section. This section will not repeat these mechanisms and phenomena, but will focus on the general goals of operation.

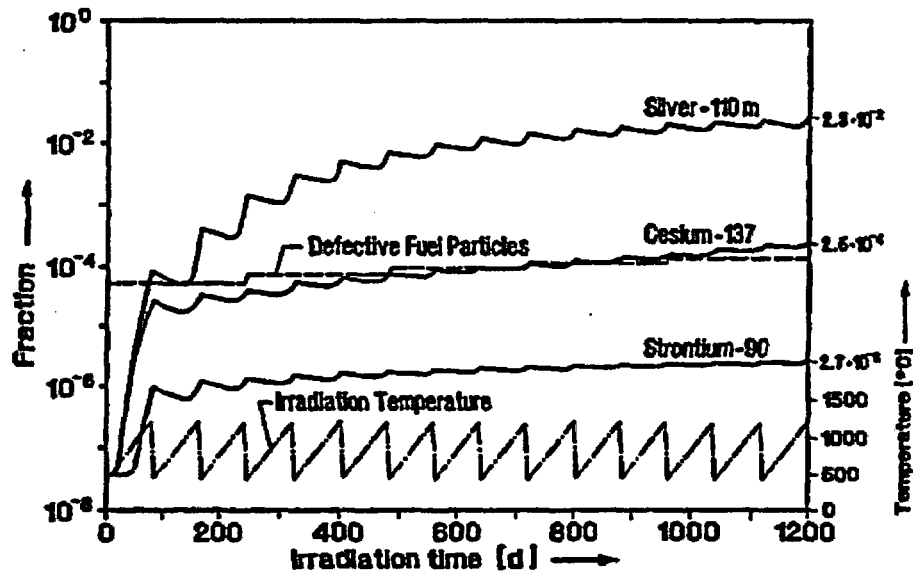


Figure 2-24 Model calculation-pebble fractional release over its lifetime (IAEA TECDOC-978)

2.4.2 Kernel

During normal operation, the kernel is expected to perform the functions outlined in the Section 2.2.2. Two design functional objectives are to control the oxygen potential to limit kernel migration and particle CO pressure and to retain the rare earths. Figure 2-25 shows two extremes of this situation. In the first case (left) a UO_2 kernel has moved in the direction of increasing temperature (amoeba effect). The time averaged temperature was 1180°C , the temperature gradient was $990^\circ\text{C}/\text{cm}$, and the burnup was 80% FIMA. In the second case (right), rare earths from a UC_2 kernel have migrated in the direction of decreasing temperature to the SiC layer. For this case, the time averaged temperature was 1130°C , the thermal gradient was $990^\circ\text{C}/\text{cm}$, and the burnup was also 80% FIMA. Both situations can cause SiC failure. In both cases the test conditions exceeded the design conditions that would be present in a power reactor environment.

While the kernel will also contain gases to some extent, the change in microstructure due to burnup may prevent high gas retention in the kernel, especially for accident temperatures. High burnup fuel contains many voids and the change in lattice structure with burnup increases the diffusion of fission products. Lower burnup fuel, <10% FIMA, will have less kernel microstructure damage and may better retain fission gases. This is different than the LWR case where high levels of fission gas retention (>95%) are common. Thus, the kernel is not expected to be retentive of all fission products, but rather to focus on particular ones and assume a new role of controlling oxygen potential.

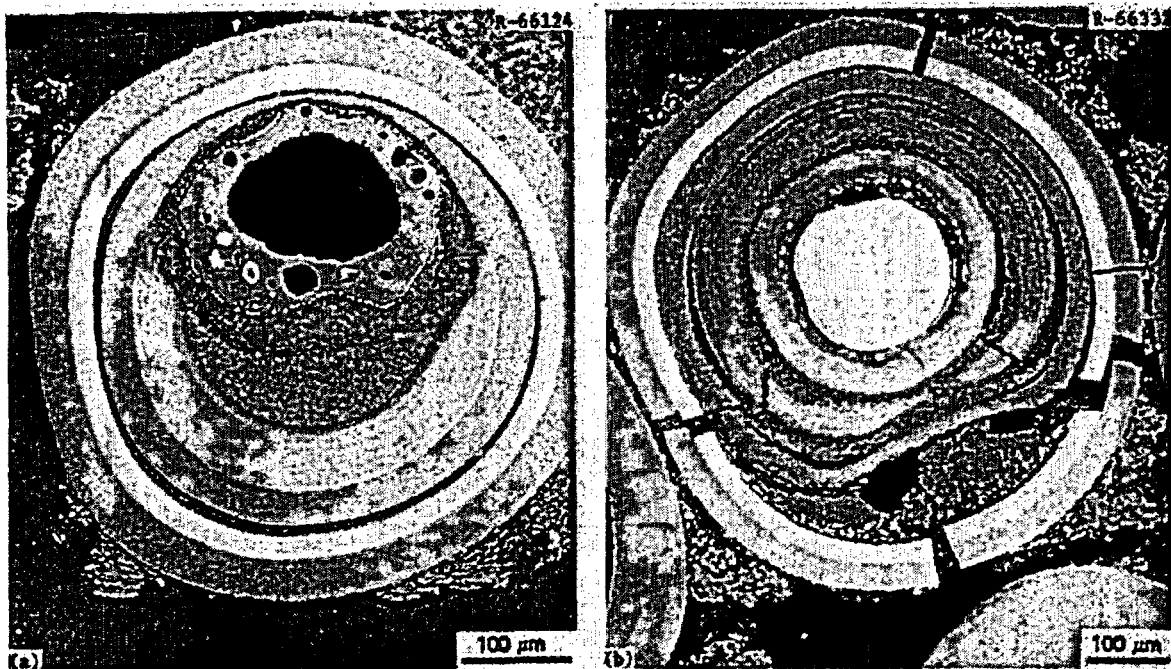


Figure 2-25 Kernel performance issues. The kernel on the left is a UO_2 kernel that is moving up the temperature gradient (amoeba effect). The particle on the right is a UC_2 kernel showing the accumulation of rare earth fission products on the cold side of the particle. The hot side is at the top of the photo

2.4.2.1 Kernel Operating Factors Identified By The PIRT Panel

Table 2-23 lists the kernel operating factors identified by the PIRT panel. This table also includes some general items that apply.

2.4.3 Buffer

The main design functional objective of the buffer is to provide a free space for the released fission gases and any generated CO. Service failures of fuel particles can be caused by missing buffers. Lacking sufficient volume to accommodate the volume of generated gas, the particle can fail by overpressure. Figure 2-26 shows a failure (in this case a BISO particle with no SiC layer) due to a missing buffer layer. The design section details other factors associated with the buffer.

An excessively thick (out of specification) buffer could increase thermal impedance. However, the temperature gradient across the particle due to its own heat generation is small ($<100^\circ\text{C}$) and this extra impedance does not appear to adversely affect particle performance, at least with the current level of understanding.

However, some recent calculations indicate that large thermal gradients can drive fission product diffusion; this is an area of current study.

Table 2-23 Kernel Operating Factors Identified By The PIRT Panel

Kernel Operations Factor	Rationale
CO production	CO production influences particle pressure and kernel migration.
Burnup	The burnup state determines the chemical environment in the kernel and its ability to retain fission products.
Swelling	The buffer is designed to accommodate the kernel distortions.
Microstructure changes	The crystal structure of the kernel can influence the hold up of fission products
Fission product chemical form	The chemical form of the fission products determines their mobility within the kernel and affects the CO pressure.
Buffer interaction	The periphery of the kernel may react with the buffer layer carbon.
Kernel migration (fuel dependent)	Temperature gradients can drive carbon transfer and result in the movement of the kernel toward the coatings.
Fission product generation	Different fissile isotopes will give different mixes of fission products. Since the noble metals attack the SiC, isotopes that generate more noble metals may degrade performance.
Temperature gradient	The macro temperature gradient across the kernel drives the amoeba effect and rare earth migration.
Isotope half life	Determines which fission products will survive the diffusion to and through the coatings.

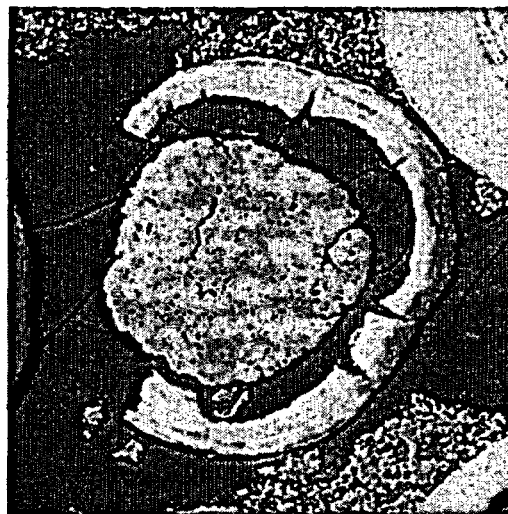


Figure 2-26 Failure in a BISO particle due to a missing Buffer layer

2.4.3.1 Buffer Operating Factors Identified By The PIRT Panel

The operating factors identified by the PIRT panel for the buffer layer are listed in Table 2-24. This table also carried forward the items discussed in previous sections that are relevant.

Table 2-24 Buffer Operating Factors Identified By The PIRT Panel

Buffer Operations Factor	Rationale
Pressure	The buffer function is to provide void volume to control particle pressure.
Shrinkage	Controlling buffer shrinkage is desirable to control cracks, and minimize kernel extrusion.
Cracking	See Shrinkage. May also allow recoil path to IPyC.
Carbonyl vapor species	No past examination of this; new issue identified by panel.
Temperature gradient	An excessive gradient can lead to higher kernel temperatures.
Condensed phase diffusion	The buffer layer is the medium connecting the kernel to the IPyC layer and first sees the fission products released from the kernel.
Gas phase diffusion	
Recoil effects	The buffer layer protects the IPyC layer by attenuating the fission product recoils.

2.4.4 IPyC Layer

The design functional objective of the IPyC is to remain dimensionally stable and intact during the fuel lifetime. Cracks (or debonding) in the IPyC can place high local tensile stresses on the SiC that can crack it if the bonding between layers is strong enough. Cracks can also expose the SiC to CO, which can corrode the SiC at high temperatures. The same issues that were covered in the design section are important during normal operation. In particular, the shrinkage of the IPyC is controlled and accommodated to some extent by IPyC creep to keep the stresses in IPyC the layer within acceptable limits.

The IPyC also limits transport of fission products to the SiC; it is highly impermeable to fission gases, but will allow the diffusion of metallic fission products.

2.4.4.1 IPyC Operating Factors Identified By The PIRT Panel

Table 2-25 lists the operating factors identified by the PIRT panel for the IPyC layer. It also includes the relevant factors identified in the previous sections.

2.4.5 SiC Layer

The SiC layer is the principle barrier to the release of fission products from the fuel particle. During normal operation, the SiC diffusion coefficients and temperatures are low enough that releases to the coolant are expected to be dominated by the initial defective fuel fraction

Table 2-25 IPyC Operating Factors Identified By The PIRT Panel

IPyC Operations Factor	Rationale
Radiation induced creep	IPyC creep relieves some of the stress in the IPyC caused by irradiation-induced shrinkage and pressure.
Fast fluence	The fluence dose has an impact on the shrinkage, creep, and layer stresses.
Dimensional change	The stresses caused by irradiation can result distortion and debonding of the IPyC from the SiC.
Anisotropy	The anisotropy is considered to be any important predictor of the IPyC dimensional stability.
Cracking	Cracking can result from the shrinkage and debonding from the SiC.
Debonding	Shrinkage and dimensional instability can result in the IPyC pulling away from the SiC and increasing peak local tensile stresses on the SiC layer.
Condensed phase diffusion	The IPyC layer is the first reasonably retentive layer.
Gas phase diffusion	The IPyC layer is the first reasonably retentive layer. The layer retains fission gases well.

and failures caused by other phenomena. The exception is silver. Extended fuel operation above about 1100°C will allow diffusion of silver through the SiC and into the coolant. The implications of this diffusion depend on the reactor design.

Extended high temperature operation of the fuel, above approximately 1300°C, can lead to corrosion of the SiC by noble metals and CO, especially if the IPyC is cracked. The noble metal of greatest concern is palladium as it easily migrates (diffuses) to the SiC and attacks it.

Figure 2-27 shows migration of Pd to the SiC layer for a plutonium kernel. The kernel type can be important as different fissile materials can have much higher yields of noble metals.

If the kernel does not retain the rare earth elements as oxides, they too can attack the SiC as was noted in the section dealing with the kernel.

If heavy metal contamination of the SiC layer occurs during fabrication, fissioning of this material will damage the SiC and lead to its early failure. If the PyC layers are intact, A SiC layer failure will not be detected by an increase in the circulating fission gas inventory. Fission product metals will be released, however. The same behavior will occur if the SiC is cracked, perhaps by handling (again, good PyC).

In general, an intact PyC layer or SiC layer will retain the fission gases making individual layer failure difficult to detect during normal operation. During normal operation, migration of the metals is limited and collecting and analyzing them is difficult in the absence of a special collection device.

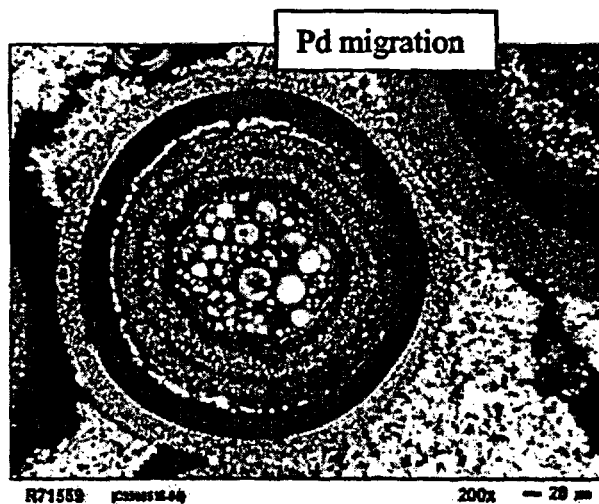


Figure 2-27 Pd migration: 70% burnup Pu kernel. FTE-13, $\text{PuO}_{1.68}$, 1150°C, polarized light

2.4.5.1 SiC Operating Factors Identified By The PIRT Panel

Table 2-26 lists the SiC layer operating factors identified by the PIRT panel.

Table 2-26 SiC Operating Factors Identified By The PIRT Panel

SiC Operations Factor	Rationale
Kernel interaction with SiC layer	See the previous comments on kernel migration.
Fission product corrosion	Noble metals present a corrosion hazard at the higher temperatures. CO can attack the SiC with a cracked IPyC at high temperatures.
Heavy metal attack	If fissile material is present in the SiC from fabrication, fissions in the SiC will damage it.
Cracking	Cracking during normal operation will cause the particle to release metallics, but not gases if one of the PyCs remains intact.
Condensed phase diffusion Gas phase diffusion	SiC is the primary diffusion barrier and it retains both metallic and gaseous fission products well, with the exception of silver.

2.4.6 OPyC Layer

The design functional objective of the OPyC is to remain dimensionally stable and intact over the fuel lifetime. It is the interface between the SiC and the fuel element matrix. Failure of the OPyC could increase the failure probability of the SiC. The same phenomena that were covered in the design section are important during normal operation. In particular, the shrinkage of the OPyC is controlled and accommodated to some extent by OPyC creep to keep the stresses in the layer within acceptable limits.

The OPyC limits the transport of fission gases, but will allow the migration of metals. One also wants to control the OPyC-matrix interactions so that the OPyC is not damaged by matrix shrinkage or micro cracks that occur in the matrix material.

2.4.6.1 OPyC Operating Factors Identified By The PIRT Panel

Table 2-27 lists the OPyC layer operating factors identified by the PIRT panel.

Table 2-27 OPyC Operating Factors Identified by The PIRT Panel

OPyC Operations Factor	Rationale
Radiation induced creep	This creep relieves some of the stress caused by shrinkage and pressure.
Dimensional change	The stresses caused by irradiation can result distortion and perhaps breakage of the OPyC layer.
Anisotropy	The anisotropy is considered to be an important predictor of the OPyC dimensional stability.
Condensed phase diffusion	The OPyC is not strongly retentive of metallics.
Gas phase diffusion	The OPyC layer functions as a barrier in the event of SiC failure.
Cracking	The OPyC layer functions as a barrier in the event of SiC failure.

2.4.7 Fuel Element

The major design functional objective of the fuel element during normal operation is to

- 1) Maintain dimensional stability
- 2) Not transmit undue stresses to the fuel particles
- 3) Withstand being dropped for pebble fuel
- 4) Maintain good thermal properties
- 5) Act as a sink for any released metallic fission products

Stability is a function of the fabrication of the fuel element; elements made with a high filler content tend to be more stable than those with low filler content. Shrinkage of the matrix material may result in microcracks and voids in the fuel element. As long as particles are not damaged and the thermal properties are within design limits, minor cracking is tolerable.

The tolerance for large cracks depends on the application. For fuel compacts inserted into a prismatic graphite block, a through crack may not be desirable, but it may not seriously affect the performance of the compact. However, the situation is different for a pebble that must be capable of being dropped from a height of several meters and traversing the reactor core without breakage. A through crack would increase the probability of pebble breakage and the fragments would have to be removed.

Corrosion by coolant impurities can affect fuel elements and result in small regions (<0.2mm deep) of "peeling" or "spalling" on the surface of pebbles. Corrosion resistance

to coolant impurities can be greatly increased by high temperature baking of the pebbles at 1950°C during manufacture [2-9].

It should be noted that the fuel element matrix is not solid graphite and the irradiation performance is not the same as graphite and will vary with the actual composition of the matrix. Different sources and mixes of binder, graphite, shim materials, and processing conditions can lead to different results, both in initial properties and during irradiation.

As the matrix material accumulates irradiation damage, its mechanical and thermophysical properties are affected [2-9]. For the reference fuel pebbles, matrix irradiation performance was very good for the operating temperatures and fast fluences of interest (<1400°C and <9 x 10²⁵ n/m²). Under irradiation the pebbles shrank less than 2% in diameter. Shrinkage was about the same in the radial and tangential directions up to a fast fluence of 5 x 10²⁵ n/m² and then deviated by about 30% as the fast fluence increased. Strength increased about 10% at moderate fast fluences and the elastic modulus increased with irradiation, up to 70% (700°C), and then only slightly decreased at the higher fast fluences (the increase was much less and the decrease greater at higher temperatures). Crush strength almost doubled.

Thermal conductivity decreased about 60% and the coefficient of thermal expansion increased by about 40% with irradiation. Both of these properties decreased initially and then remained fairly constant with increasing fluence. Irradiation temperature and accumulated fast fluence strongly influences property changes, but the pebbles maintained integrity under the irradiation conditions of interest.

The extent to which of the fuel element matrix retains metallic fission products depends on many factors, but in practice the matrix material appears to either sorb metallic fission products or delay their migration into the coolant at normal operating temperatures. Gases readily migrate through the matrix material.

2.4.7.1 Fuel Element Operating Factors Identified By The PIRT Panel

Table 2-28 lists the Fuel Element Operating Factors Identified by The PIRT Panel.

Table 2-28 Fuel Element Operating Factors Identified By The PIRT Panel

Fuel Element Operations Factor	Rationale
Temperature	Matrix behavior and stability is a function of temperature/fast fluence.
Fast fluence	Matrix behavior is related to the fast fluence. In particular shrinkage and cracks.
Power density	Power affects the operating temperature and gradients.
Temperature difference	The fuel particle behavior can be influenced by the macro temperature gradient.
Temperature time histories	Important for determining corrosion and diffusion.
Condensed phase diffusion	The matrix material can sorb/trap significant amounts of the less volatile fission products.
Gas phase diffusion	The element doesn't provide significant retention of gases.
Corrosion by coolant impurities	PPM levels of coolant impurities can corrode or damage the fuel element matrix material

2.5 Accident Conditions

For the purposes of identifying phenomena that are considered important to the performance of coated particle fuel, four classes of accident conditions were considered by the PIRT panel:

- 1) *Core heatup*: Loss of helium pressure and flow, core heatup and subsequent cooldown, with or without a SCRAM. This accident results in the reactor achieving a peak fuel temperature of roughly 1600°C; however, 1800°C was examined to envelope phenomena of interest. The core temperature rises from normal operating temperatures to a maximum over a period of 20 to 30 hours and slowly cools down over a period of several hundred hours in an assumed helium environment. Loss of coolant pressure is more challenging than simply a loss of flow, because natural convection can reduce the peak fuel temperature to some extent in the normal pressure case.
- 2) *Water ingress*: Failure of a heat exchanger tube with reactor depressurization. Since the reactor designs currently under study do not have steam generators and the water coolant in the heat exchangers is lower than core pressure, significant water entry into the core is not expected; however, 1% water vapor was assumed to be present in the core during the postulated accident (balance helium). The failure of the pressure boundary and depressuring the core with a heat exchanger failure would allow water entry under low driving pressure.
- 3) *Air ingress*: Complete severing of the horizontal vessel between the reactor vessel and the power conversion system vessel followed by depressurization and air diffusion into the core. Both high temperatures and chemical attack are considered. The PIRT panel considered oxidation of the core structure, but not structural collapse or major relocation of fissile material.
- 4) *Reactivity insertion*: A sudden reactivity addition could result in locally high fuel temperatures and/or fuel damage. Pulse lengths are on the order of seconds and a fraction of the fuel is assumed to fail by cracking of the PyC and SiC, but the kernel and buffer remain intact. A postulated rod ejection accident was considered to be the basis for the accident conditions. The on-line refueling of the pebble bed reactor results in small excess reactivity and the use of burnable poisons in the prismatic reactor also limits excess reactivity.

The PIRT panel considered the aforementioned postulated events as a basis for establishing an "envelope of accident conditions" as fuel environmental conditions from which to identify important fuel phenomena. The conditions were intended to be a "realistically conservative" upper bound for each postulated class of accidents that might be included in the licensing basis.

Unlike an LWR, an HTGR does not have core internals that would melt and rapidly lose core configuration under accident conditions, although an earthquake could cause some damage. In addition, the chemical reactions that result in the degradation of core internals proceed at a much slower rate. Thus, the dynamics of these types of accidents are much slower than LWR accidents. Reactivity insertion accidents are expected to be less severe in an HTGR, both in intensity and because the large thermal inertia of the

graphite provides a heat sink. However, this accident needs more study for the particular design of interest.

2.5.1 Heatup Accident

The most significant condition associated with this accident is the elevated temperature over time. The environment remains essentially inert (helium). Thermal power is at a low level, either from afterheat or from the low nuclear power level achieved by the negative reactivity with the failure to SCRAM. Heat is transferred from the core through the reactor vessel to the cavity cooling equipment and structures.

Figure 2-28 shows the calculated temperature versus time curve for a depressurized heatup accident, the temperatures used for experimental fuel testing (horizontal lines), and a conservative heatup accident curve for a small modular type reactor.

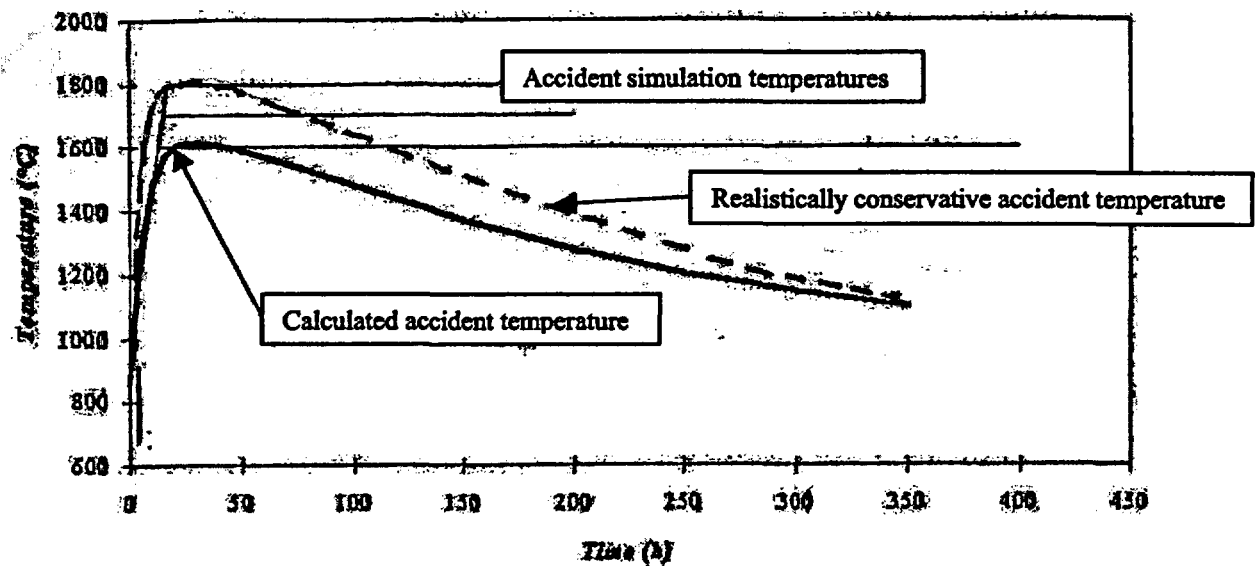


Figure 2-28 Time versus temperature heatup accident curve considered by the PIRT

In general, fuel element releases tend to increase with time at temperature, burnup, and temperatures above $\sim 1600^{\circ}\text{C}$ [2-6, 2-7, 2-20 to 2-24]. Figure 2-29 shows ^{85}Kr releases for German program test compacts illustrating the burnup and temperature observation for about a 300-hour heating time [2-6].

2.5.1.1 Kernel

High temperatures during a Heatup accident will increase the diffusion of fission products from the kernel. The SiC is the primary barrier to release, but diffusion through the kernel can have a minor effect. Of special interest is the more rapid diffusion of fission products (mostly noble

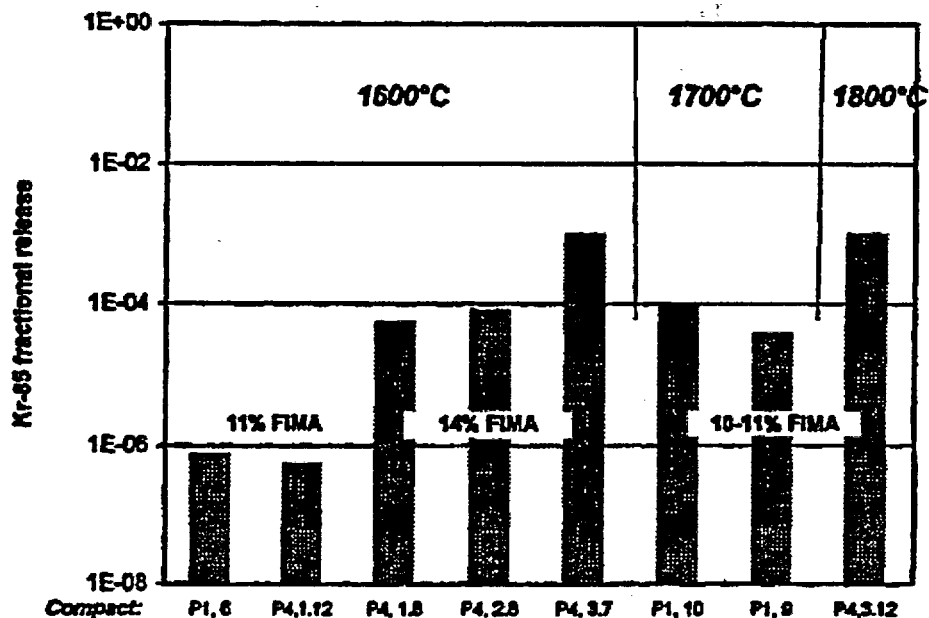


Figure 2-29 ^{85}Kr releases as a function of burnup and test temperature. (IAEA TECDOC-978)

metals) that are known to attack the SiC layer. If the SiC is already weak due to corrosion during normal operation, the additional attack due to newly diffusing material, higher gas pressures, and the higher temperature may fail the SiC layer if the time at temperature is long enough. Cracks in the IPyC may allow CO to attack the SiC as well as increasing the stress loading of the layers. These effects are considered a function of burnup.

The temperatures in the fuel are expected to be below the melting point of the kernel material. The vapor pressure of the volatile species could increase however. As the temperature increases, the oxygen potential of the kernel may change and this could shift the equilibrium somewhat, but the fuel design should anticipate this situation [2-8, 2-43].

Temperature gradients in the fuel are expected to decrease under accident conditions compared to normal operation.

2.5.1.1.1 Kernel Heatup Accident Factors Identified By The PIRT Panel

Table 2-29 lists the phenomena identified by the PIRT panel for the kernel under heatup accident conditions.

Table 2-29 Kernel Heatup Accident Factors Identified By The PIRT Panel

Kernel Heatup Accident Factor	Rationale
Maximum fuel temperature	Temperature affects the rate at which material diffuses out of the kernel.
Temperature vs time transient conditions	The time-dependent variation of the fuel with time will determine diffusive release.
Energy Transport: conduction within kernel	The gradient within a kernel is due to the transport of decay heat
Thermodynamic state of fission products	The chemical state of the fission products determines how they migrate and vapor pressures. A goal is to tie the rare earths and limit CO production (same as normal operation).
Condensed phase diffusion	Higher temperature increases the diffusion rate.
Gas phase diffusion	Higher temperature increases the diffusion rate.
Oxygen flux	Diffusion would increase, but not known in detail.
Grain growth	Grain growth may increase fission product transport, but it has not been explored.
Buffer carbon-kernel interaction	Some interaction between the kernel and the buffer carbon may be possible.

2.5.1.2 Buffer Layer

The design performance objective of the buffer layer during a heatup accident is to control the gas pressure by providing a void volume as it is for normal conditions. It provides little retention of fission products. Some distortion of the buffer is expected during irradiation and is not expected to affect accident performance.

2.5.1.2.1 Buffer Layer Heatup Accident Factors Identified By The PIRT Panel

Table 2-30 lists the buffer layer heatup accident factors identified by the PIRT panel under heatup accident conditions. Many of these issues are the same as noted for normal operation.

2.5.1.3 IPyC Layer

Depending on the bonding between the IPyC and the SiC, the IPyC can help keep the SiC in compression; breaking or cracking of the IPyC can result in higher localized stresses in the SiC layer. A crack can also expose the SiC to CO that can cause corrosion at the higher accident temperatures. Complete debonding of the IPyC may cause a shift in the pressure loading; a structural model is necessary to determine the effect. This is an area of active research.

Table 2-30 Buffer Layer Heatup Accident Factors Identified By The PIRT Panel

Buffer Heatup Accident Factor	Rationale
Gas phase diffusion	The fission product transport through the buffer layer is expected to be high at accident temperatures.
Condensed phase diffusion	
Response to kernel swelling	The buffer layer is designed to be weak enough that it will deform to accommodate the kernel.
Maximum fuel gaseous fission product uptake	The buffer layer is designed to have sufficient free volume to accommodate the fission products at an acceptable pressure.
Layer oxidation	Any oxygen released from the kernel will oxidize a small portion of the buffer. This may be of little consequence for the buffer, but may increase the particle pressure.
Thermal gradient	During heatup conditions, the gradient across the buffer is much less than normal operation due to the much lower heat generation rate.
Irradiation and thermal shrinkage	The buffer is designed to isolate the kernel from the IPyC, but small cracks could locally concentrate fission products on the IPyC.

Decomposition or chemical reactions of the IPyC layer are not an important phenomena for a heatup accident; dimensional stability is the important concern as it is during normal operation. Metallic fission products will diffuse through the layer at a greater rate, but the gaseous diffusion should still be small for an intact layer.

2.5.1.3.1 IPyC Layer Heatup Accident Factors Identified By The PIRT Panel

Table 2-31 lists the IPyC layer heatup accident factors identified by the PIRT panel. The relevant general issues identified before are also included.

2.5.1.4 SiC Layer

An intact SiC layer is the primary barrier to the release of metallic fission products at accident temperatures. It also effectively contains gaseous fission products. The primary challenges to layer integrity are pressure, corrosion, and decomposition. The pressure can be controlled by the design of the particle, corrosion by the tie up of most fission products and limiting the operating temperature to control Pd attack (and CO attack if the IPyC cracks), and decomposition by limiting the maximum accident temperature.

Decomposition results in the disassociation of the SiC into silicon and carbon at temperatures above about 1600-1800°C [2-6, 2-20 to 2-24, 2-34]:

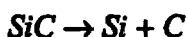


Table 2-31 IPyC Layer Heatup Accident Factors Identified By The PIRT Panel

IPyC Heatup Accident Factor	Rationale
Gas phase diffusion	Gaseous fission products are generally retained well by the IPyC layer even at higher temperatures.
Condensed phase diffusion	Metallic fission products are not retained well.
Pressure loading (fission products)	The IPyC can help keep the SiC in tension and prevent it from failing if the bonding between layers is strong (same as normal operation).
Pressure loading (CO)	The same CO issues apply here. High CO production will result in high pressures (same as normal operation).
Layer oxidation	In some cases internal oxidation of the layer could be significant. IPyC cracks can allow CO to the SiC and corrosion may result.
Stress state (compression/tension)	If this layer breaks or debonds, the changes in stress distribution of the particle could cause it to fail.
Cracking	Cracks could change the stress distribution; same as normal operation.
Intercalation Trapping	The IPyC can accumulate fission products during normal operation that could be released during a heatup accident.

At about 2000°C, thermal decomposition of SiC is a dominate failure mechanism. However, above about 1600°C decomposition affects in the SiC such as the development of porosity are noted, implying that thermal decomposition mechanisms are active. Above the assumed particle temperature limit, ~1600°C, diffusion of fission products begins to increase (over normal operating values) and limits the time at temperature [2-6, 2-21 to 2-24].

Figure 2-30 shows the relative effective SiC thinning rates due to corrosion and decomposition predicted for past US fuel at 16% FIMA, a fast flux of 4.0×10^{15} n/m²/s, and an irradiation temperature of 1000°C. Decomposition is considered a significant factor above 1600°C. Corrosion can take place during normal operation and weaken the SiC layer, which then might fail under the greater pressure at accident temperatures.

SiC is stable to oxidation over the temperature region of interest. Figure 2-31 shows an oxidation diagram for converting selected carbides to oxides.

SIC "Thinning"

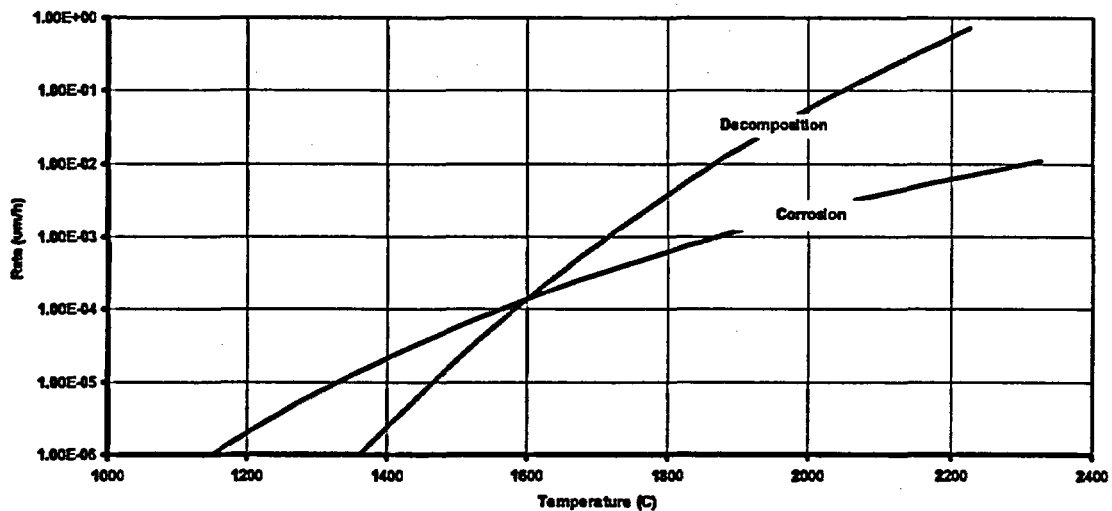


Figure 2-30 Effective SiC thinning due to corrosion and decomposition. Comparison of frequency factors for failure (data from Goodin, 1989)

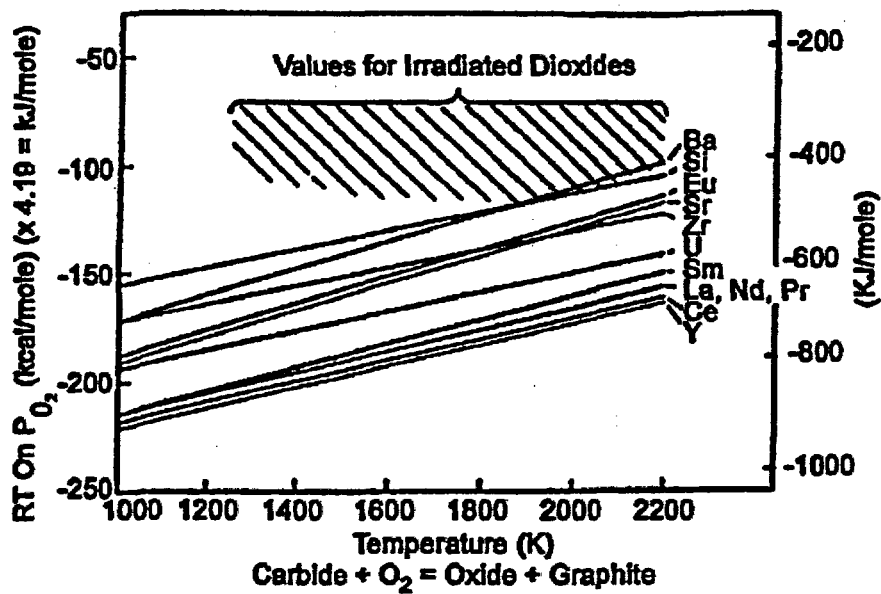


Figure 2-31 Oxidation diagram for carbides of interest

As the temperatures increase and the time at temperature becomes significant, diffusion of silver and radiological important fission products through the SiC can occur. Figure 2-32 shows the fractional releases from a German pebble at 1600°C. Note that silver is not effectively retained by the SiC layer and a significant portion of the relatively small amounts of the other released fission products are sorbed on the matrix graphite. In particular, ⁹⁰Sr levels approaching 1% (after 500h at 1600°C) are seen in the matrix, but the fractional release from the sphere is only $\sim 10^{-7}$ [2-6].

Accident releases tend to increase with peak accident temperature. Figure 2-33 shows the fractional ⁸⁵Kr releases as a function of temperature. The general rule is that larger releases are seen above 1600°C.

2.5.1.4.1 SiC Layer Heatup Accident Factors Identified By The PIRT Panel

Table 2-32 lists the SiC layer heatup accident factors identified by the PIRT panel. Included are the relevant general items discussed in previous sections.

Table 2-32 SiC Layer Heatup Accident Factors Identified By The PIRT Panel

SiC Heatup Accident Factor	Rationale
Gas phase diffusion	Except for silver, fission product diffusion is low through the SiC even at accident temperatures.
Condensed phase diffusion	
Thermal deterioration or decomposition	Above about 1600-1800°C the SiC begins to decompose and its ability to retain fission products is greatly reduced.
Fission product corrosion	Some fission products may migrate to the SiC and corrode it. This corrosion process is a function of temperature and can begin during normal operation. Pd is believed to be the main concern, but others are possible as well.
Heavy metal diffusion	The diffusion of heavy metal through SiC could relocate fissile material (not noted to date).
Layer oxidation	Local attack of the SiC layer by CO due to a cracked IPyC at high temperatures may be possible.
Fission gas release through undetected defects	In order to release gases, both PyCs must be cracked in addition to a failed SiC. The SiC can be attacked by fission products and fabrication impurities (see manufacturing).
Fission product release through failures (e.g. cracking)	
Thermodynamics of the SiC fission product system	At the higher temperatures of interest, SiC is just stable to oxidation in its intact particle environment. See corrosion issues.
Sintering	Accident temperatures could change the crystal or grain structure of the SiC layer (not noted to date).

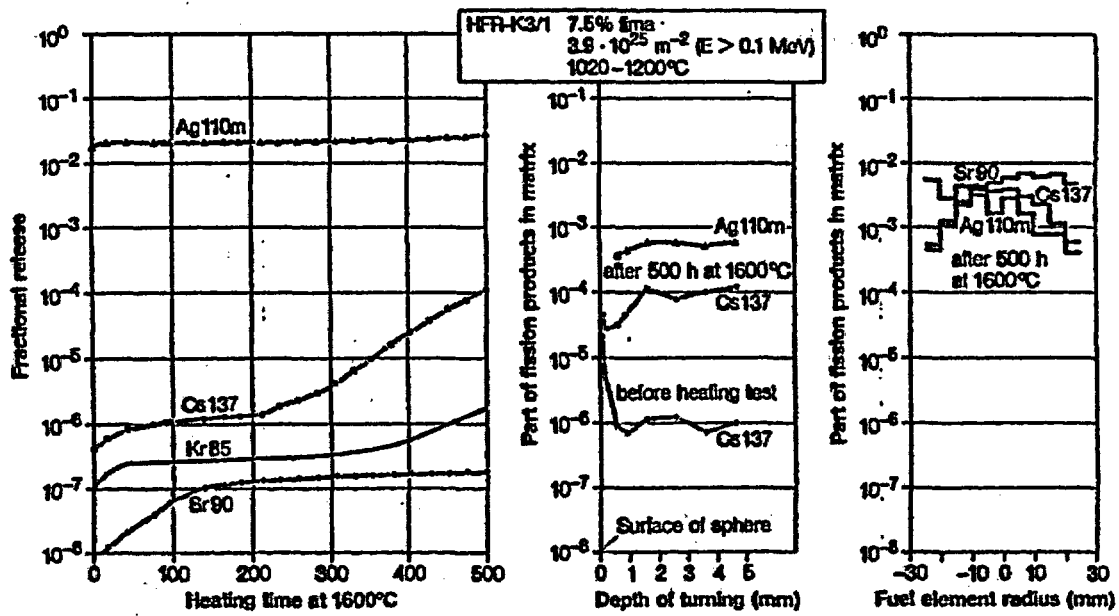


Figure 2-32 Fission product release from a fuel sphere at 1600°C. (IAEA TECDOC-978)

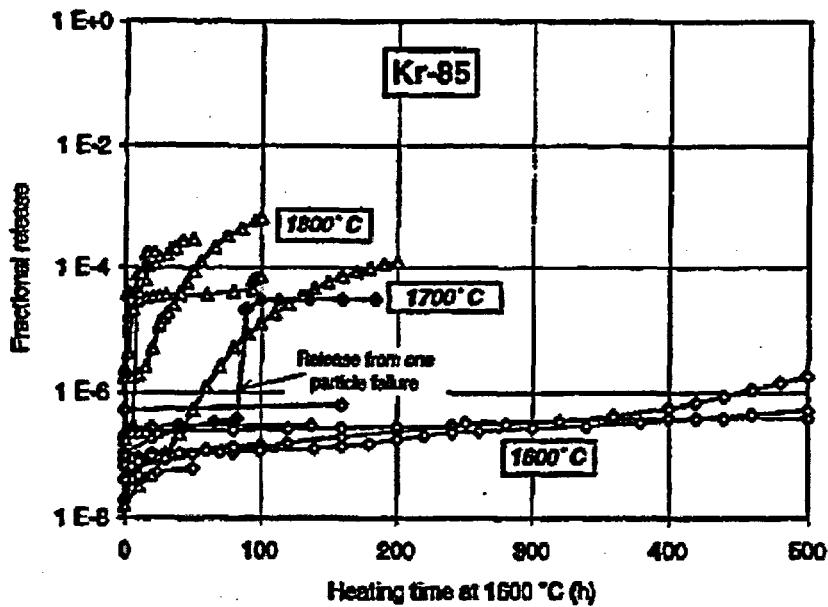


Figure 2-33 ^{85}Kr release as a function of heating temperature. (IAEA TECDOC-978)

2.5.1.5 OPyC Layer

The OPyC can help keep the SiC layer in compression; breaking or cracking of the OPyC can result in higher local stresses in the SiC and increase its likelihood of failure. It also protects (delays) the SiC layer from chemical attack

Decomposition or chemical reactions of the OPyC layer are not an issue for a heatup accident; dimensional stability is still the important concern. Metallics will diffuse through the layer at a greater rate, but the gaseous diffusion should still be small for an intact layer. It is possible that fission products trapped within the layer (intercalation) could be released at the higher temperatures. No new issues with matrix interactions are expected.

2.5.1.5.1 OPyC Heatup Accident Factors Identified By The PIRT Panel

Table 2-33 lists the OPyC heatup accident factors identified by the PIRT panel.

Table 2-33 Identified OPyC Heatup Accident Factors Identified By The PIRT Panel

OPyC Heatup Accident Factor	Rationale
Gas phase diffusion	Gaseous diffusion is low, while metallic diffusion is high.
Condensed phase diffusion	
Layer oxidation	Cracked layers may allow CO to the OPyC or coolant impurities may attack it.
Stress state (compression/tension)	See general discussion on the stress of the particle. OPyC loss is generally not as bad as IPyC loss.
Intercalation	Because the fission product inventory is low in this layer, these two items may be important.
Trapping	
Cracking	Cracks can lead to a higher probability of SiC failure. Gases will be released if the other layers have failed.

2.5.1.6 Fuel Element

During a heatup accident, the fuel element performs three main functions that are essentially the same required during normal operation. The first is dimensional stability; by remaining stable and intact no undue mechanical stresses will be placed on the fuel particles. Modest element cracking can often be tolerated as long as the particles are not affected. The second function is heat transfer. Adequate thermal conductivity is necessary to couple the particles to the core and coolant. Finally, the third function is to sorb released metallic fission products. The matrix material of some fuel element types may be capable of retaining a significant portion of the released metallic fission products. Gases generally are not retained. Figure 2-32 shows that some of the less volatile fission products are retained in the element matrix material even if they are released from the

particles [2-6]. Some of these fission products migrate from the fuel element to the coolant and other reactor components [2-7, 2-20 to 2-24]

2.5.1.6.1 Fuel Element Heatup Accident Factors Identified By The PIRT Panel

Table 2-34 lists the Fuel Element heatup accident factors identified by the PIRT panel.

Table 2-34 Fuel Element Heatup Accident Factors Identified By The PIRT Panel

Fuel Element Heatup Accident Factor	Rationale
Irradiation history	Matrix behavior (shrinkage) is related to time temperature history, particularly temperatures and fast fluence.
Condensed phase diffusion Gas phase diffusion	In the matrix gas diffusion is high, while metallic diffusion is variable. The less volatile metals can be sorbed in the matrix material to a high degree.
Transport of metallic FPs through fuel element – chemical form	The chemical form of the fission product determines its transport behavior. The chemical environment outside the fuel kernel may be different than inside. Generally, significant sorbing of the metallics is seen.

2.5.2 Air and/or Water Intrusion Accident

Unlike the heatup accident detailed in the previous section, an accident with subsequent air and/or water intrusion can result in the additional effect of chemical attack of the fuel elements [2-6, 2-20 2-24, 2-42 to 2-44]. The temperature of the fuel depends on whether or not the reactor remains pressurized, if the control and shutdown rods insert, if significant heat is added by chemical reactions, or if heat transfer conditions change significantly during the accident.

A major difference between chemical intrusion accidents and a heatup accident is that the fuel element matrix material and the particle coating layers can be subject to a chemical reaction and transport of fission products can be by a means other than diffusion. Also, unlike the simple heatup case, the structural integrity of the fuel element may be degraded and particle coatings may even be damaged or fail. Some core designs involve changes in core geometry if the chemical reactions were sufficiently extensive. However, for purposes of the PIRT assessment, core support structural damage was assumed to be limited and slow.

The generally low chemical reactivity of the nuclear grade graphite fuel blocks in a prismatic core reactor can protect the fuel compacts and coated fuel particles to some extent. In a pebble bed reactor core, the fuel zone is surrounded by a relatively thin layer of matrix material that is directly exposed to the coolant. The matrix material is more

reactive than nuclear grade graphite so fuel element oxidation in air or water attack could be more rapid.

Current reactor designs are based on a direct cycle gas turbine design that does not have a source of high pressure, high volume water such as a steam generator, so extensive water ingress due to equipment failure is not possible as it was with the past designs. However, design specifics will need to be examined.

Exposed kernels are most affected by water ingress. Intact particles are much less affected even for extended periods of exposure to water [2-6, 2-43].

For air ingress, controlling or limiting the oxidation rate and exposure duration is a primary objective. This can be achieved by delaying the entry of air into the core until the core temperatures have been reduced and by limiting the air flow rate through the core. The loss of protective matrix material can expose fuel particles and release sorbed fission products into the coolant. Chemical attack of the fuel particles could follow. As long as the fuel temperatures and flow rate of reactants are limited, fuel particle damage can be avoided. The establishment of an air flow path that would allow rapid core matrix material loss to occur at temperatures above 1600°C could result in significant particle damage rates.

This flow path can principally be established in two ways. The first is the development of a "chimney" by having the reactor pressure boundary fail in both the top and bottom of the vessel. Natural convection via buoyancy forces then drives a flow. The second way involves a breach in a single location. In this case, gaseous diffusion allows the entry of air from outside the break into the core volume and the establishment of convective flow on a longer time scale [2-45].

Contemporary designs limit the water available by using heat exchanger water side pressures below core pressure and limit the natural convection with high core flow impedance. However, these are design specific issues and need to be assessed on a case-by-case basis. Figure 2-34 illustrates how chemical attack of the fuel might occur. Air attack of the carbon materials is the most aggressive [2-6].

Figure 2-35 shows the results of a fuel sphere exposed to water vapor at a temperature of 800°C. The water vapor reacts with exposed kernels (fabrication defects) and releases fission products [2-6, 2-43].

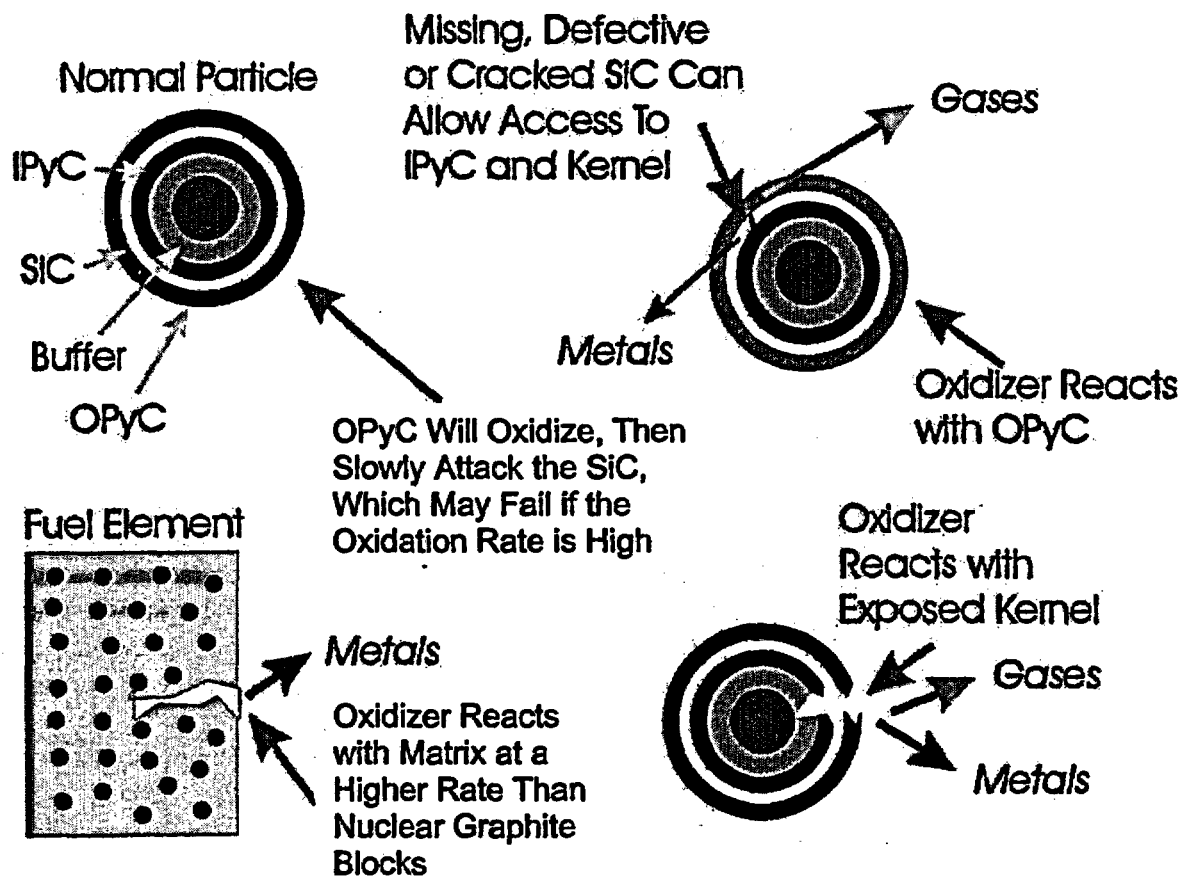


Figure 2-34 An illustration of the chemical attack of a fuel element and fuel particles

Air ingress is a complex thermochemical phenomena, as the reaction can be non-self sustaining or, in extreme situations, self sustaining. The balance between heat production, heat removal, and gas flows all influence the reaction. In addition, the fuel particles are usually shielded from the reactor coolant by several millimeters of highly graphitized material such as the webs of a prismatic fuel block or the outer few millimeters of relatively ungraphitized carbon matrix material of the outer shell of a pebble fuel element. The oxidizer must first penetrate this material before the fuel particles are exposed. Thus, there is a varying amount of "sacrificial" material to limit the damage that might be caused by a modest amount of air.

Sustained air ingress with high carbon reaction rates is possible only if a self-sustaining flow of air is established while the fuel is still at a relatively high temperature. If this should happen, the behavior of SiO_2 becomes important. In such a case, SiO_2 would be produced as SiC is oxidized and it forms a layer on the particle that impedes further reaction. However, in an oxygen-limited atmosphere above about 1300°C , SiO_2 may be

converted to SiO, which is volatile and will allow the SiC to SiO reaction to continue unabated.

Figure 2-36 shows the particle failure fraction from irradiated fuel spheres (about 9% burnup) at 1300°C and 1400°C as well as a set of 10 particles at 1500°C while heating in air [2-6]. In an unlimited air supply, failure rates can be high, much greater than in a heatup without air ingress. This event is more aggressive than water ingress, which is primarily a factor with exposed kernels.

2.5.3 Water Ingress Accident Phenomena

The following sections detail the PIRT panel selected coated particle fuel factors, characteristics, and phenomena for water ingress.

2.5.3.1 Kernel

If the fuel particle is intact during a water ingress accident, the kernel behavior is much the same as during a heatup event (described previously). If the kernel is exposed, it can be oxidized by water [2-6, 2-22, 2-24, 2-43]. During the process of oxidation, the structure of the kernel changes and it releases much of its stored fission product inventory relatively quickly. This effect appears to be burnup dependent. After the kernel completes the process, the kernel release rates return to approximately the pre-oxidation level.

Figure 2-37 shows this effect after exposure to water vapor.

Exposed kernels are most susceptible to water vapor because they react rapidly and intact particles are little affected. Thus, under water ingress conditions, fuel releases are dominated by exposed kernel releases (at least at modest temperatures). This behavior is dependent on the water partial pressure and Figure 2-38 shows the relationship between released stored fission gas and water partial pressure. Finally, it is not known if a catalysis could increase reaction rates under certain conditions.

2.5.3.1.1 Kernel Water Ingress Accident Factors Identified By The PIRT Panel

Table 2-35 lists the kernel water ingress accident factors identified by the PIRT panel along with the relevant general issues identified previously.

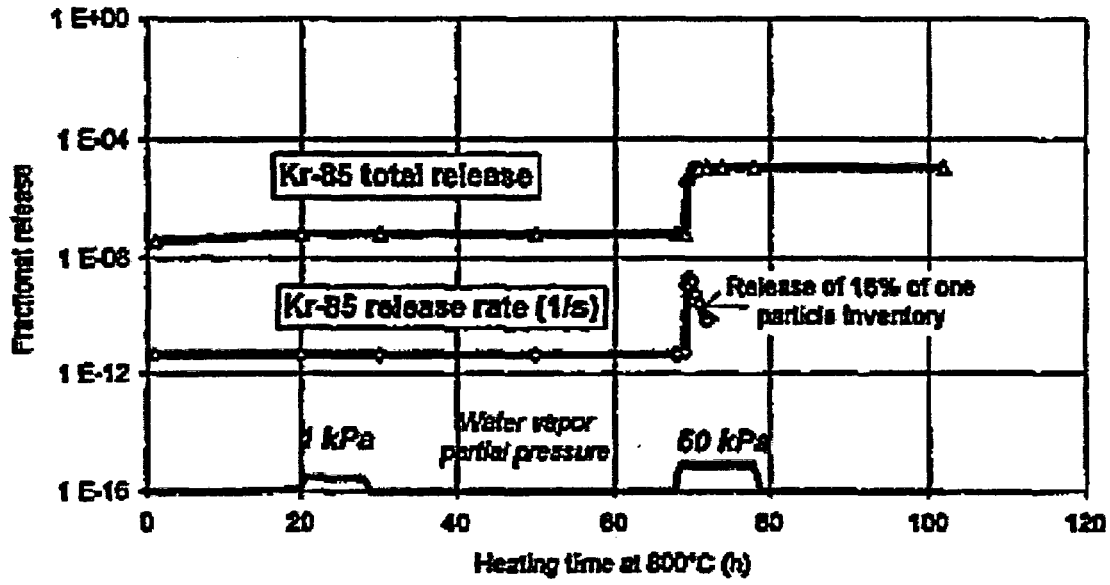


Figure 2-35 ^{85}Kr release from a fuel sphere exposed to water vapor (AVR 92/7, type GLE-3, 9.2% FIMA) at 800C (IAEA TECDOC-978)

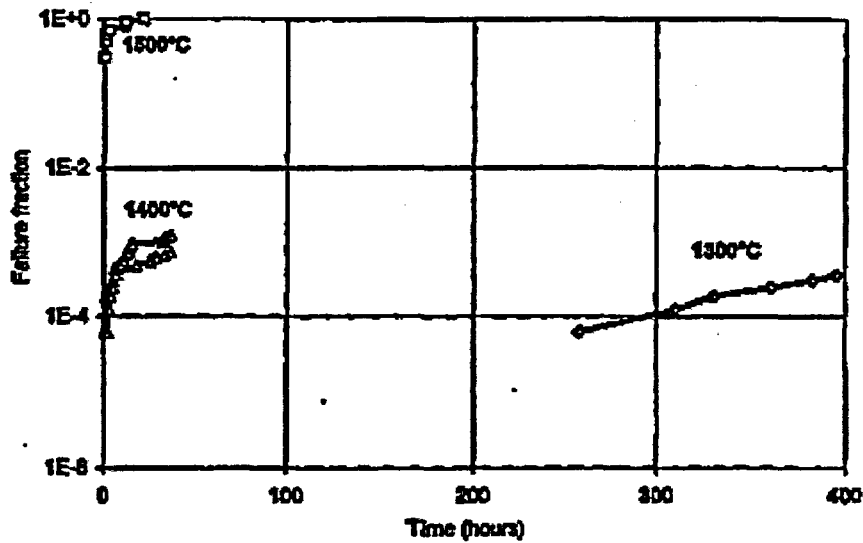


Figure 2-36 Sphere particle failure fractions and 10 unbonded particles (1500°C line) heated in air (IAEA TECDOC-978)

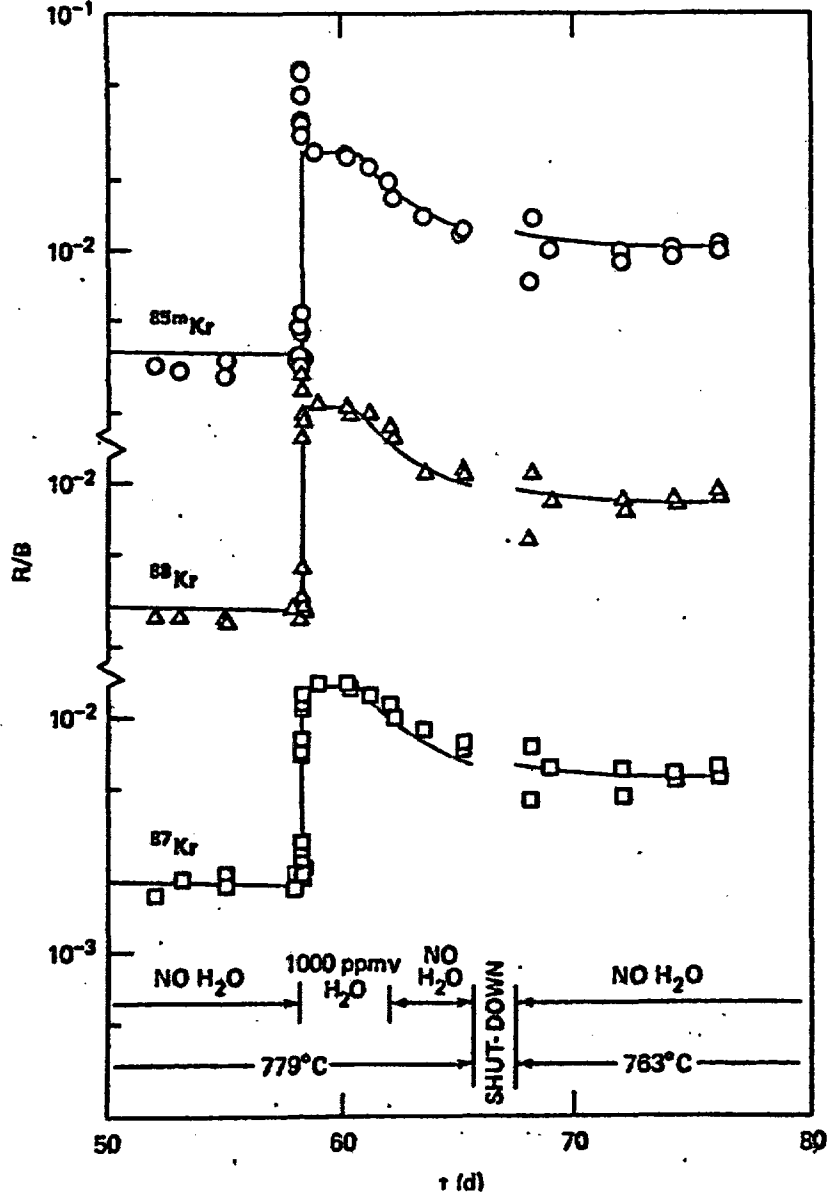


Figure 2-37 Expose to water vapor causes the kernel to restructure and release much of its stored inventory (From Meyers, DOE-HTGR-88486)

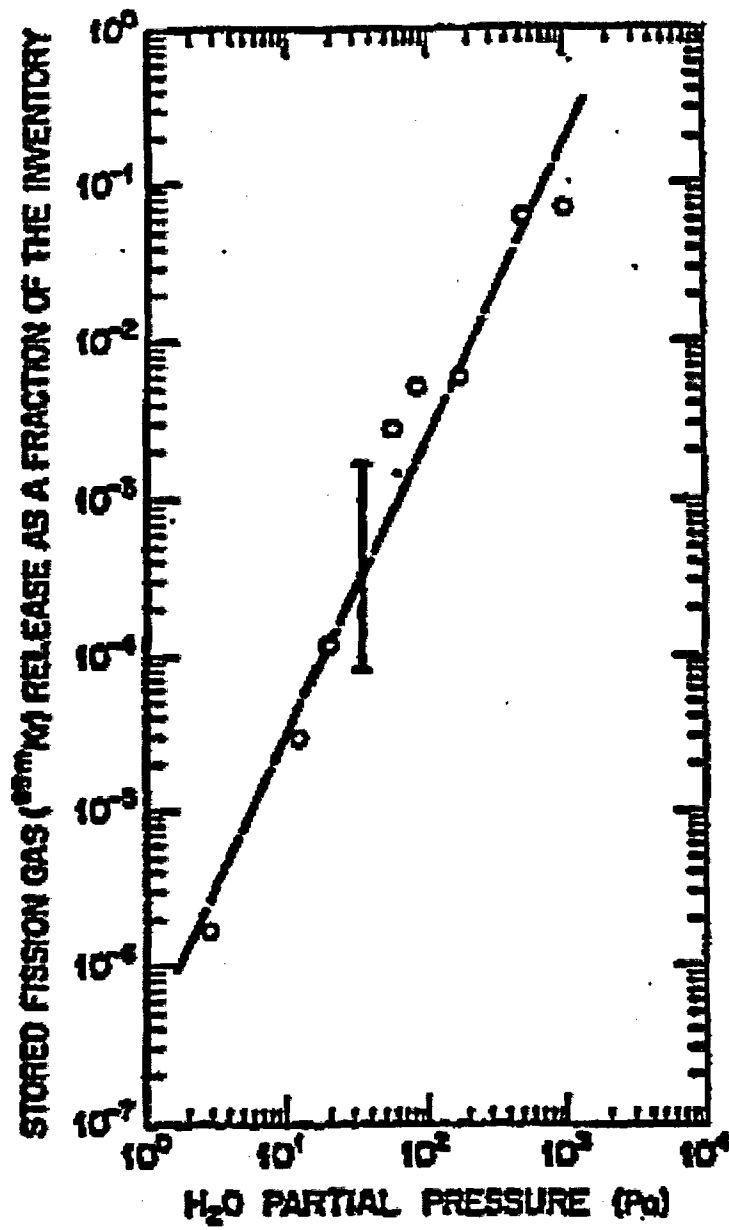


Figure 2-38 Stored fission gas release versus water partial pressure for exposed kernels at 770°C for experiments HFR-B1 and HRB-17 (IAEA TECDOC-978)

Table 2-35 Kernel Water Ingress Accident Factors Identified By The PIRT Panel

Kernel Water Ingress Factor	Rationale
Maximum fuel temperature	Chemical reactions and fission product diffusion are strongly influenced by temperature.
Temperature vs. time transient conditions	Time at temperature strongly influences the amount of material reacted or fission products released.
Energy Transport: Conduction within kernel	Determines kernel temperature and fission product diffusion from the kernel.
Thermodynamic state of fission products	The diffusivity of fission products is strongly influenced by their chemical form.
Oxygen flux	A significant redistribution of oxygen has the potential to change the oxygen potential and thus the fission product chemical species within the kernel.
Grain growth	Grain growth could release fission products from the grain to the grain boundary region, thus enhancing transport.
Buffer carbon-kernel interaction	The kernel periphery may react with the Buffer carbon.
Chemical attack by water - Kinetics	The reaction rates will determine the rate of fission product release.
Chemical attack by water - Catalysis	Some impurities or fission products may increase the reaction rate.
Chemical attack by water - Changes in chemical form of fission products	The changes in chemical form of the fission products may change transport properties.
Chemical attack by water - Changes in kernel properties	Structural and chemical changes to the kernel may release stored fission products.

2.5.3.2 Buffer Layer

The buffer layer plays a role similar to that played during a heatup accident for an intact particle. Once exposed, it offers little resistance to fission product transport and may be slowly oxidized by exposure to water. It will also quickly transport water vapor to the kernel.

2.5.3.2.1 Buffer Layer Water Ingress Accident Factors Identified By The PIRT Panel

Table 2-36 lists the buffer layer water ingress accident factors identified by the PIRT panel. Many of the factors are the same as discussed in previous sections with similar behavior.

Table 2-36 Buffer Layer Water Ingress Accident Factors Identified By The PIRT Panel

Buffer Water Accident Ingress Factor	Rationale
Gas phase diffusion	This layer offers little impedance to the transport of fission products.
Condensed phase diffusion	
Response to kernel swelling	The buffer will have to accommodate any kernel distortion to protect the other layers.
Maximum fuel gaseous fission product uptake	The buffer layer must have sufficient free volume to withstand the pressure.
Layer oxidation	The buffer will be oxidized from the outside if the particle is cracked or broken.
Thermal gradient	The gradient may influence the transport of fission products to the other layers.
Irradiation and thermal shrinkage	The buffer is expected to isolate the kernel from the other layers. Damage to it may compromise this ability.
Chemical attack by water - Kinetics	The reaction rates will determine the rate of fission product release.
Chemical attack by water - Changes in chemical form of fission products	The changes in chemical form of the fission products may change their transport properties.
Chemical attack by water - Changes in graphite properties	Changes in the graphite (or PyC) properties may affect the transport of fission products or the release of trapped fission products.
Chemical attack by water - Holdup reversals	Stored fission products in the buffer may be released quickly if its structure is seriously attacked.
Chemical attack by water - Temperature distributions	The temperature of the buffer and surrounding materials determines reaction rates and transport.

2.5.3.3 IPyC Layer

The factors for the IPyC during air or water ingress are similar to those for heatup with the additional aspect of chemical attack. If the OPyC and SiC remain intact, the IPyC will not be exposed to a new environment. However, if the other layers become damaged or cracked, this layer would be exposed to water and be subject to a chemical reaction. Since this layer would be the final barrier for gases (metals will have begun diffusing through the layer), its failure would allow the release any stored gases and expose the kernel to the oxidizing environment with the subsequent kernel reaction.

2.5.3.3.1 IPyC Layer Water Ingress Accident Factors Identified By The PIRT Panel

Table 2-37 lists the IPyC layer water ingress accident factors identified by the PIRT panel.

Table 2-37 IPyC Layer Water Ingress Accident Factors Identified By The PIRT Panel

IPyC Water Ingress Accident Factor	Rationale
Gas phase diffusion	Gas diffusion is low, while metallic diffusion is high; chemical attack could increase both rates.
Condensed phase diffusion	
Pressure loading (fission products)	High pressures can challenge this layer. The IPyC can help keep the SiC in compression if the bonding between layers is strong.
Pressure loading (CO)	The same CO issues apply here. High CO production will result in high pressures.
Layer oxidation	If the IPyC cracks or otherwise allows internal CO to the SiC, corrosion may result (inside out). Cracks in the OPyC and SiC will allow oxidation of the IPyC (outside in).
Stress state (compression/tension)	See general discussions on coating stress distributions.
Cracking	Same situation as layer oxidation and stresses. If other layers are broken, cracking will allow the oxidizer to the kernel.
Intercalation	Chemical attack of the IPyC may allow release of trapped fission products.
Chemical attack by water - Kinetics	The reaction rates will determine the rate of fission product release.
Chemical attack by water - Catalysis	Some impurities or fission products may increase the reaction rate.
Chemical attack by water - Changes in chemical form of fission products	The changes in chemical form of the fission products may change their transport properties.
Chemical attack by water - Changes in graphite properties	Changes in the graphite (or PyC) properties may affect the transport of fission products or the release of trapped fission products.
Chemical attack by water - Holdup reversal	Serious damage to the IPyC will allow access to the Buffer and its relatively large inventory of fission products.
Chemical attack by water - Temperature distributions	The temperature of the IPyC and surrounding materials determines reaction rates and transport.

2.5.3.4 SiC Layer

Under water ingress conditions, the SiC layer performs in a manner similar to that of a heatup accident until the OPyC begins to be subject to chemical attack. As the OPyC becomes weakened and fails, the stress state of the SiC would change. This may lead to failure if the SiC has been weakened by other causes. The SiC would then be exposed to water and perhaps some generated CO [2-6, 2-31].

Thinning of this layer can cause the particle to fail by pressure vessel failure and penetration of the layer will cause the release of metallic fission products and expose the IPyC to oxidation.

2.5.3.4.1 SiC Layer Water Ingress Accident Factors Identified By The PIRT Panel

Table 2-38 lists the SiC layer water ingress accident factors identified by the PIRT panel.

2.5.3.5 OPyC Layer

Under ingress conditions, the OPyC first functions in the same way as in the heatup case; it then suffers erosion. Its loss due to chemical attack has a similar effect except that the SiC is now exposed to attack (covered previously).

2.5.3.5.1 OPyC Layer Water Ingress Accident Factors Identified By The PIRT Panel

Table 2-39 lists the OPyC layer water ingress accident factors identified by the PIRT panel.

2.5.3.6 Fuel Element

Under ingress conditions, the fuel element responds first and would be in a manner similar to that for a heatup condition. However, the matrix material of an element is more reactive than either the fuel particle pyrocarbon or core graphite blocks and is the first material to be damaged due to chemical attack (if exposed, in some cases a thick reflector region may first see the ingress and consume the water). For low levels of water this could be an advantage as there are large amounts of matrix material and some protection could be provided to the fuel particles. Some fuel forms have a thick outer layer that must be consumed before the fuelled region can be reached and other forms are imbedded into graphite blocks so specifics of the situation must be considered.

Loss of significant amounts of matrix material is not desirable, however. Increased porosity and cracks can expose the fuel particles to the water and consumption of the matrix material might structurally weaken the fuel element. Fission products sorbed in the matrix during normal operation would be released into the remaining coolant as the matrix material reacts with the water.

For the water-carbon reaction, the reaction is endothermic and is driven by the nuclear decay heat, so high temperatures and high material consumption rates driven by aggressive chemical reactions are not expected.

Table 2-38 SiC Layer Water Ingress Accident Factors Identified By The PIRT Panel

SiC Water Ingress Accident Factor	Rationale
Gas phase diffusion	The SiC layer is the major barrier to the transport of fission products. Significant changes in the transport properties can greatly increase release of fission products.
Condensed phase diffusion	
Thermal deterioration or decomposition	Above about 1600-1800°C the SiC begins to decompose and its ability to retain fission products is greatly reduced.
Fission product corrosion	Some fission products may migrate to the SiC and damage it. This process is a function of temperature and can begin during normal operation. Pd is the main concern
Heavy metal diffusion	If fissile material were to be transported across the SiC layer, a possible core configuration issue may arise (considered unlikely).
Layer oxidation	Attack of the SiC layer by CO could occur due to a failed OPyC at high temperatures (outside in). The SiC can also be damaged by CO exposure due to IPyC failure (inside out).
Fission product release through undetected defects	Undetected SiC defects could have poor fission product retention behavior not apparent during normal operations.
Fission product release through failures, e.g. cracking	Failure of the SiC will allow the release of metallic fission products even with intact PyCs.
Thermodynamics of the SiC fission product system	SiC is known to be attacked by some noble metals. At higher burnups and temperatures, other chemical concerns may arise.
Sintering	High temperatures could results in microstructural changes to the SiC that change transport behavior.
Chemical attack by water - Kinetics	The reaction rates will determine the rate of fission product release.
Chemical attack by water - Catalysis	Some impurities or fission products may increase the oxidation rate.
Chemical attack by water - Changes in chemical form of fission products	The changes in chemical form of the fission products may change their transport properties.
Chemical attack by water - Changes in SiC properties	Changes in the SiC properties may affect the transport of fission products or the release of trapped fission products.
Chemical attack by water - Holdup reversal	Extensive damage to the SiC would allow access to the IPyC and its relatively poor retention of metallic fission products.
Chemical attack by water - Temperature distributions	The temperature of the SiC and surrounding materials determines reaction rates and transport.

Table 2-39 OPyC Layer Water Ingress Accident Factors Identified By The PIRT Panel

OPyC Water Ingress PIRT Factor	Rationale
Gas phase diffusion	Gas diffusion is low, while metallic diffusion is high; chemical attack could increase both rates.
Condensed phase diffusion	
Layer oxidation	The OPyC is the most exposed layer. It would be the first layer subjected to oxidation (sound particle).
Stress state	See general discussions on coating stress distributions. Its failure will increase the likelihood of SiC failure.
Intercalation	Chemical attack of the OPyC may allow release of trapped fission products.
Trapping	Chemical attack of the OPyC may allow release of trapped fission products.
Cracking	Failure of the OPyC will change the stress state of the particle; if the other layers are breached, the gases will be released.
Chemical attack by water - Kinetics	The reaction rates will determine the rate of fission product release.
Chemical attack by water - Catalysis	Some impurities or fission products may increase the reaction rate.
Chemical attack by water - Changes in chemical form of fission products	The changes in chemical form of the fission products may change their transport properties.
Chemical attack by water - Changes in graphite properties	Changes in the graphite (or PyC) properties may affect the transport of fission products or the release of trapped fission products.
Chemical attack by water - Holdup reversal	Attack of the OPyC may result in the release of any stored fission products.
Chemical attack by water - Temperature distributions	The temperature of the OPyC and surrounding materials determines reaction rates and transport.

2.5.3.6.1 Fuel Element Water Ingress Accident Factors Identified By The PIRT Panel

Table 2-40 lists fuel element water ingress accident factors identified by the PIRT panel. Many of these factors are the same as were seen for the heatup conditions.

Table 2-40 Fuel Element Water Ingress Accident Factors Identified By The PIRT Panel

Fuel Element Water Ingress Accident Factor	Rationale
Irradiation history	Matrix behavior is strongly affected by fast fluence and temperature exposure, which may cause shrinkage of the matrix and change its chemical reactivity.
Condensed phase diffusion Gas phase diffusion	Gas diffusion is high, while metallic diffusion is variable. The less volatile metals can be sorbed in the matrix material. Chemical attack could increase the transport.
Gaseous transport - holdup	Gas transport through the matrix is generally high.
Transport of metallic FPs through fuel element - Chemical form	Changes in the chemical form of the fission products could increase their transport rate through the matrix.
Chemical attack by water - Kinetics	The reaction rates will determine the rate of fission product release.
Chemical attack by water - Catalysis	Some impurities or fission products may increase the reaction rate.
Chemical attack by water - Changes in chemical form of fission products	The changes in chemical form of the fission products may change their transport properties.
Chemical attack by water - Changes in graphite properties	Changes in the graphite (matrix) properties may affect the transport of fission products or the release of trapped fission products.
Chemical attack by water - Holdup reversal	Serious damage to the matrix may allow release of sorbed fission products.
Chemical attack by water - Temperature distributions	The temperature of the matrix and surrounding materials determines reaction rates and transport.

2.5.4 Air Ingress Accident Phenomena

The following sections detail the PIRT panel selected coated particle fuel factors, characteristics, and phenomena for air ingress. As part of the PIRT process, the 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 was available at the INEEL to address the important phenomena related to air ingress events in a pebble bed reactor. Appendix G contains the results of the MELCOR calculations performed for the air-intrusion accident scenario.

2.5.4.1 Kernel

If the fuel particle is intact during an ingress accident, the kernel behavior is much the same as during a heatup event (described previously). If the kernel is exposed, it can be oxidized by oxygen or CO (the oxygen is converted to CO by the large amount of carbon in the reactor system) [2-6, 2-22, 2-24]. During the oxidation process, the structure of the kernel changes and it releases much of its stored fission product inventory relatively quickly. After the kernel completes the process, the kernel releases return to approximately the pre-oxidation level.

Finally, it is not known if a catalysis could increase reaction rates under certain conditions.

2.5.4.1.1 Kernel Air Ingress Accident Factors Identified By The PIRT Panel

Table 2-41 lists the kernel air ingress accident factors identified by the PIRT panel along with the relevant general rationales identified previously.

Table 2-41 Kernel Air Ingress Accident Factors Identified By The PIRT Panel

Kernel Air Ingress Accident Factor	Rationale
Maximum fuel temperature	Chemical reactions and fission product diffusion are strongly influenced by temperature.
Temperature vs. time transient conditions	Time at temperature strongly influences the amount of material reacted or fission products released.
Energy Transport: conduction within kernel	Determines kernel temperature and fission product diffusion from the kernel.
Thermodynamic state of fission products	The diffusivity of fission products is strongly influenced by their chemical form.
Oxygen flux	A significant redistribution of oxygen has the potential to change the oxygen potential and thus the fission product chemical species within the kernel.
Grain growth	Grain growth could release fission products from the grain to the grain boundary region, thus enhancing transport.
Buffer carbon-kernel interaction	The kernel periphery may react with the buffer carbon.
Chemical attack by air - Kinetics	The reaction rates will determine the rate of fission product release.
Chemical attack by air - Catalysis	Some impurities or fission products may increase the reaction rate.

**Table 2-41 Kernel Air Ingress Accident Factors Identified By The PIRT Panel
(continued)**

Chemical attack by air - Changes in chemical form of fission products	The oxygen potential of the kernel may increase due to the available oxygen. The changes in chemical form of the fission products may change transport properties.
Chemical attack by air – Changes in graphite properties	Changes in the graphite (or PyC) properties may affect the transport of fission products or the release of trapped fission products.
Chemical attack by air - Holdup reversal	Structural and chemical changes to the kernel may release stored fission products.
Chemical attack by air – Temperature distributions	The temperature of the kernel and surrounding material will affect reaction rates and the transport of fission products.

2.5.4.2 Buffer Layer

The buffer layer plays a role similar to that played during a heatup accident for an intact particle. Once exposed, it offers little resistance to fission product transport and will be oxidized by exposure to air. It will also quickly transport oxidizer to the kernel. Air attack is much more aggressive than water. It is possible a catalysis could increase reaction rates under certain conditions if present.

2.5.4.2.1 Buffer Layer Air Ingress Accident Factors Identified By The PIRT Panel

Table 2-42 lists the buffer layer air ingress accident factors identified by the PIRT panel. Many of the factors are the same as discussed in previous sections with similar rationales.

2.5.4.3 IPyC

The factors for the IPyC during air ingress are similar to those for heatup with the additional aspect of chemical attack. If the OPyC and SiC remain intact, the IPyC will not be exposed to a new environment. However, if the other layers become damaged or cracked, this layer will be exposed to air and CO and be subject to a chemical reaction. Since this layer is now the final barrier for gases (metals will have begun diffusing through the layer), its failure will release any stored gases and expose the kernel to the oxidizing environment with the subsequent kernel reaction.

2.5.4.3.1 IPyC Layer Air Ingress Accident Factors Identified By The PIRT Panel

Table 2-43 lists the IPyC layer air ingress accident factors identified by the PIRT panel.

Table 2-42 Buffer Layer Air Ingress Accident Factors Identified By The PIRT Panel

Buffer Air Ingress Accident Factor	Rationale
Gas phase diffusion	This layer offers little impedance to the transport of fission products.
Condensed phase diffusion	
Response to kernel swelling	The buffer will have to accommodate any kernel distortion to protect the other layers.
Maximum fuel gaseous fission product uptake	The buffer layer must have sufficient free volume to accommodate the fission products at an acceptable pressure.
Layer oxidation	The buffer layer may react with oxide materials in the kernel (prior to air exposure).
Thermal gradient	The gradient may influence the transport of fission products to the other layers.
Irradiation and thermal shrinkage	The buffer is expected to isolate the kernel from the other layers. Damage to it may compromise this ability.
Chemical attack by air - Kinetics	The reaction rates will determine the rate of fission product release.
Chemical attack by air - Catalysis	Some impurities or fission products may increase the reaction rate.
Chemical attack by air - Changes in chemical form of fission products	The changes in chemical form of the fission products may change their transport properties.
Chemical attack by air - Changes in graphite properties	Changes in the graphite (or PyC) properties may affect the transport of fission products or the release of trapped fission products.
Chemical attack by air - Holdup reversal	Stored fission products in the buffer may be released quickly if its structure is seriously attacked.
Chemical attack by air - Temperature distributions	The temperature of the buffer and surrounding materials determines reaction rates and transport.

2.5.4.4 SiC Layer

Under air ingress conditions, the SiC layer performs in a manner similar to that of a heatup accident until the OPyC begins to be subject to chemical attack. If the OPyC becomes weakened and fails, the stress state of the SiC would change. This may lead to failure if the SiC has been weakened by other causes. After OPyC loss, the SiC would then be exposed to air and CO. Depending on the conditions, either SiO₂ or SiO (low oxygen) can be formed. SiO is volatile while SiO₂ is not. SiO₂ will impede the reaction rate as the reactant has to diffuse through it. Since SiO is gaseous, it does not offer this protection. Thus, the specific details of the reacting environment determine the damage and the rate of damage to the SiC layer [2-6, 2-31].

Thinning of this layer can cause the particle to fail by pressure vessel failure and penetration of the layer will cause the release of metallic fission products and expose the IPyC to oxidation.

Table 2-43 IPyC Layer Air Ingress Accident Factors Identified By The PIRT Panel

IPyC Air Ingress Accident Factor	Rationale
Gas phase diffusion	Gas diffusion is low, while metallic diffusion is high; chemical attack could increase both rates.
Condensed phase diffusion	
Pressure loading (fission products)	High pressures can challenge this layer. The IPyC can help keep the SiC in compression if the bonding between layers is strong.
Pressure loading (CO)	The same CO issues apply here. High CO production will result in high pressures.
Layer oxidation	If the IPyC cracks or otherwise allows internal CO to the SiC, corrosion may result (inside out). Cracks in the OPyC and SiC will allow oxidation of the IPyC (outside in).
Stress state (compression/tension)	See general discussions on coating stress distributions.
Cracking	Same situation as layer oxidation and stresses. If other layers are broken, cracking will allow the oxidizer to the kernel.
Intercalation	Chemical attack of the IPyC may allow release of trapped fission products.
Chemical attack by air - Kinetics	The reaction rates will determine the rate of fission product release
Chemical attack by air - Catalysis	Some impurities or fission products may increase the reaction rate.
Chemical attack by air - Changes in chemical form of fission products	The changes in chemical form of the fission products may change their transport properties.
Chemical attack by air - Changes in graphite properties	Changes in the graphite (or PyC) properties may affect the transport of fission products or the release of trapped fission products.
Chemical attack by air - Holdup reversal	Serious damage to the IPyC will allow access to the buffer and its relatively large inventory of fission products.
Chemical attack by air - Temperature distributions	The temperature of the IPyC and surrounding materials determines reaction rates and transport.

2.5.4.4.1 SiC Layer Air Ingress Accident Factors Identified By The PIRT Panel

Table 2-43 lists the SiC layer air ingress accident factors identified by the PIRT panel.

Table 2-44 SiC Layer Air Ingress Accident Factors Identified By The PIRT Panel

SiC Air Ingress Accident Factor	Rationale
Gas phase diffusion	The SiC layer is the major barrier to the transport of fission products. Significant changes in the transport properties can greatly increase release of fission products.
Condensed phase diffusion	
Thermal deterioration or decomposition	Above about 1600-1800°C the SiC begins to decompose and its ability to retain fission products is greatly reduced.
Fission product corrosion	Some fission products may migrate to the SiC and damage it. This process is a function of temperature and can begin during normal operation. Pd is the main concern
Heavy metal diffusion	If fissile material were to be transported across the SiC layer, a core configuration issue may arise.
Layer oxidation	Attack of the SiC layer by CO due to a failed OPyC at high temperatures problematic. The SiC can also be damaged by CO exposure due to IPyC failure (inside out). The formation of either SiO or SiO ₂ can determine the rate at which the SiC is eroded.
Fission product release through undetected defects	Undetected defective SiC could have poor accident behavior not apparent during normal operations.
Fission product release through failures, e.g. cracking	Failure of the SiC will allow the release of metallic fission products even with intact PyCs.
Thermodynamics of the SiC fission product system	SiC is known to be attacked by some noble metals. At higher burnups and temperatures, other chemical concerns may arise.
Sintering	High temperatures could results in microstructural changes to the SiC that change transport behavior.
Chemical attack by air - Kinetics	The reaction rates will determine the rate of fission product release.
Chemical attack by air - Catalysis	Some impurities or fission products may increase the oxidation rate.
Chemical attack by air - Changes in chemical form of fission products	The changes in chemical form of the fission products may change their transport properties.
Chemical attack by air - Changes in SiC properties	SiC property changes may affect the transport of fission products or release of trapped fission gases.
Chemical attack by air - Holdup reversal	Serious damage to the SiC will allow access to the IPyC and its relatively poor retention of metallic fission products.
Chemical attack by air - Temperature distribution	The temperature of the SiC and surrounding materials determines reaction rates and transport.

2.5.4.5 OPyC

Under air ingress conditions, the OPyC first functions in the same way as in the heatup case; it then suffers erosion. Its loss due to chemical attack has a similar effect except that the SiC is now exposed to attack (covered previously).

2.5.4.5.1 OPyC Layer Air Ingress Accident Factors Identified By The PIRT Panel

Table 2-44 lists the OPyC layer air ingress accident factors identified by the PIRT panel.

Table 2-45 OPyC Layer Air Ingress Accident Factors Identified By The PIRT Panel

OPyC Air Ingress Accident Factor	Rationale
Gas phase diffusion	Gas diffusion is low, while metallic diffusion is high; chemical attack could increase both rates.
Condensed phase diffusion	
Layer oxidation	The OPyC is the most exposed layer. It would be the first layer subjected to oxidation
Stress state	See general discussions on coating stress distributions. Failure will increase the likelihood of SiC failure.
Intercalation	Chemical attack of the OPyC may allow release of trapped fission products.
Trapping	Chemical attack of the OPyC may allow release of trapped fission products.
Cracking	OPyC failure will change the stress state of the particle; gases will be released if other layers breached.
Chemical attack by air - Kinetics	The reaction rates will determine the rate of fission product release
Chemical attack by air - Catalysis	Some impurities or fission products may increase the oxidation rate.
Chemical attack by air - Changes in chemical form of fission products	The changes in chemical form of the fission products may change their transport properties.
Chemical attack by air - Changes in graphite properties	Changes in the graphite (or PyC) properties may affect the transport of fission products or the release of trapped fission products.
Chemical attack by air - Holdup reversal	Attack of the OPyC may result in the release of any stored fission products.
Chemical attack by air - Temperature distribution	The temperature of the OPyC and surrounding materials determines reaction rates and transport.

2.5.4.6 Fuel Element

Under air ingress conditions, the fuel element responds first in a manner similar to that for a heatup. However, the matrix material of a fuel element is more reactive than either the fuel particle pyrocarbon or core graphite blocks and is the first material to suffer damage due to chemical attack (if exposed, in some cases a thick reflector region may first see the air ingress and buffer the damage). For small amounts of air this could be an advantage as there are large amounts of matrix material and some protection could be provided to the fuel particles. Some fuel forms have a thick outer layer that must be consumed before the fuelled region can be reached and other forms are imbedded into graphite blocks so specifics of the situation must be considered.

Loss of significant amounts of matrix material is not desirable, however and air ingress is more aggressive than water ingress. Increased porosity and cracks can expose the fuel particles to the air and consumption of the matrix material might structurally weaken the fuel element.

Fission products sorbed in the matrix would be released into the remaining coolant-air mix as the matrix material reacts with the oxidizer. The chemical forms of the released fission products may change (oxidize) if large amounts of air enter the core. A sudden release of this sorbed material might change the accident analysis if the chemical attack is extensive.

Generally, the heat generated by these reactions is considered to be small compared to the nuclear decay heat, but this must be examined on a case-by-case basis. Experiments in air have seen greater releases from fuel elements than from unbonded particles at similar apparatus temperatures, suggesting that the energy of combustion may have an important local effect.

Figure 2-39 shows the oxidation of two similar fuel spheres in air. Note that the matrix material was oxidized at 1100°C with no releases. Releases were seen from the remaining fuel particles when the temperature was raised to 1400°C. In an inert environment, no failures would be expected [2-6, 2-20 to 2-24].

2.5.4.6.1 Fuel Element Air Ingress Accident Factors Identified By The PIRT Panel

Table 2-46 lists the fuel element air ingress accident factors identified by the PIRT panel. Many of these issues are the same as were seen for the coated particle fuel ingress and heatup conditions.

Table 2-46 Fuel Element Air Ingress Accident Factors Identified By The PIRT Panel

Fuel Element Air Ingress Accident Factor	Rationale
Irradiation history	Matrix behavior is strongly affected by fast fluence and temperature exposure, which may cause shrinkage of the matrix and change its chemical reactivity.
Condensed phase diffusion	Gas diffusion is high, while metallic diffusion is variable. The less volatile metals can be sorbed in the matrix material. Chemical attack could increase the transport.
Gas phase diffusion	
Transport of metallic FPs through fuel element - Chemical form	Changes in the chemical form of the fission products could increase their transport rate through the matrix.
Chemical attack by air - Kinetics	The reaction rates will determine the rate of fission product release
Chemical attack by air - Catalysis	Some impurities or fission products may increase the oxidation rate.
Chemical attack by air - Changes in chemical form of fission products	The changes in chemical form of the fission products may change their transport properties.
Chemical attack by air - Changes in graphite properties	Changes in the graphite (or PyC) properties may affect the transport of fission products or the release of trapped fission products.
Chemical attack by air - Holdup reversal	Significant damage to the matrix material could allow the release of the sorbed fission products.
Chemical attack by air - Temperature distribution	The temperature of the matrix and surrounding materials determines reaction rates and transport.

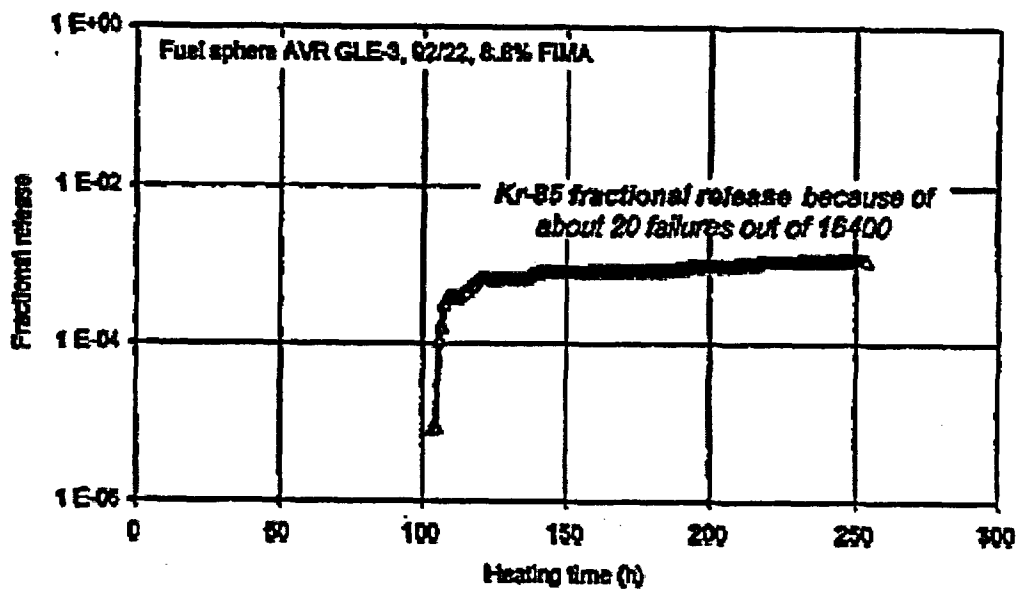
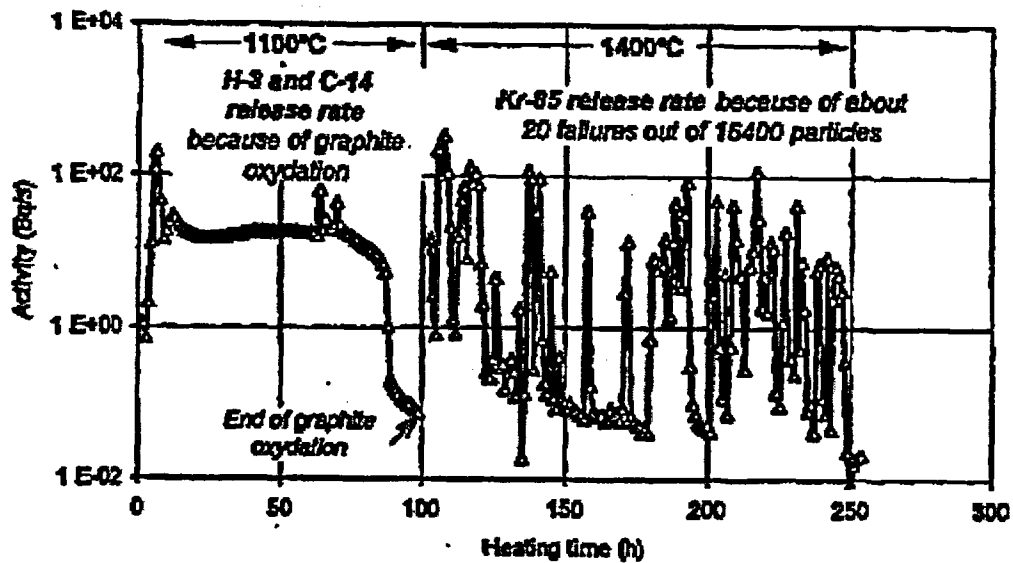


Fig. 2-39 Oxidation of two similar fuel spheres in air. Top is from AVR 92/8, 9% FIMA, bottom is from AVR 92/22, 8.8% FIMA (IAEA TECDOC-978)

2.5.5 Reactivity Accident

An important class of potential accidents for reactors in general is the sudden increase in reactor local or core-wide power due to a reactivity increase. This might be caused by a control system malfunction, control rod ejection, or a sudden change in the core internal arrangement such as pebble compaction in a pebble bed reactor.

Because of the constant cycling of the fuel, a pebble bed reactor has low excess reactivity. The prismatic core design is more like an LWR in terms of excess reactivity (and burnable poisons) at the start of life, which is reduced as the core nears end of life. The designers of each type strive to minimize excess reactivity and to limit control rod worth and accident movement, so the actual accident pulse could be modest.

A sudden pulse of power might damage the fuel elements and the fuel particles, leading to a large release of fission products from the fuel. If the pressure boundary has also been damaged, such as for a rod ejection accident, a driving force would be available to transport fission products outside of the reactor boundary. For a reactor like the HTTR design, a certain regulatory event could lead to a pulse length of 8 seconds with an energy deposition of 1.26×10^4 J/g of UO_2 (no mitigation) [2-6, 2-44]. However, for other postulated HTGR events, pulses could be much shorter with much higher energy deposition. While limited reactivity insertion accident (RIA) testing has been done and much of it is at difference energies and pulse lengths, an understanding has evolved [2-6].

The large amount of graphite in the core along with its high temperature capability eliminates concerns of core melting, but the kernel can still see high temperatures and the resulting pressures can fail coatings.

The examination of Japanese fuel compacts after pulse testing (10-30 ms) showed internal UO_2 kernel melting and central vaporization for coated particles with an energy deposition of 2300 J/g UO_2 . Microprobe analysis revealed that uranium vapor penetrated the cracks in the coating layers. Particles that saw lower energies appeared almost unchanged, but layer cracking was still present [2-6].

Russian pulse tests used both short pulses and long pulses. In a first set of tests done at the Impulse Graphite Reactor (IGR) reactor, a pulse of duration (half width peak) 0.7 seconds and energy of 2.6×10^4 J/g UO_2 was deposited into spherical fuel elements, which remained intact. A second set of tests with a pulse duration of 30 seconds and an energy of 9×10^4 J/g UO_2 resulted in the failure of the coated particles and fragmentation of the fuel element sphere [2-6].

A set of short pulses (1-2 ms) was also conducted by the Russians in the HYDRA reactor with energies of 100 to 1700 J/g UO_2 . They observed coating cracking at < 1050 J/g UO_2 and kernel restructuring at > 1300 J/g UO_2 . Figure 2-40 outlines this behavior. Three particle types are shown. A normal density 490 micron diameter kernel (10.8 g/cm^3), a lower density 532 micron diameter kernel (7.9 g/cm^3), and a particle with a layer composed of both SiC and PyC on both sides of the SiC [2-6].

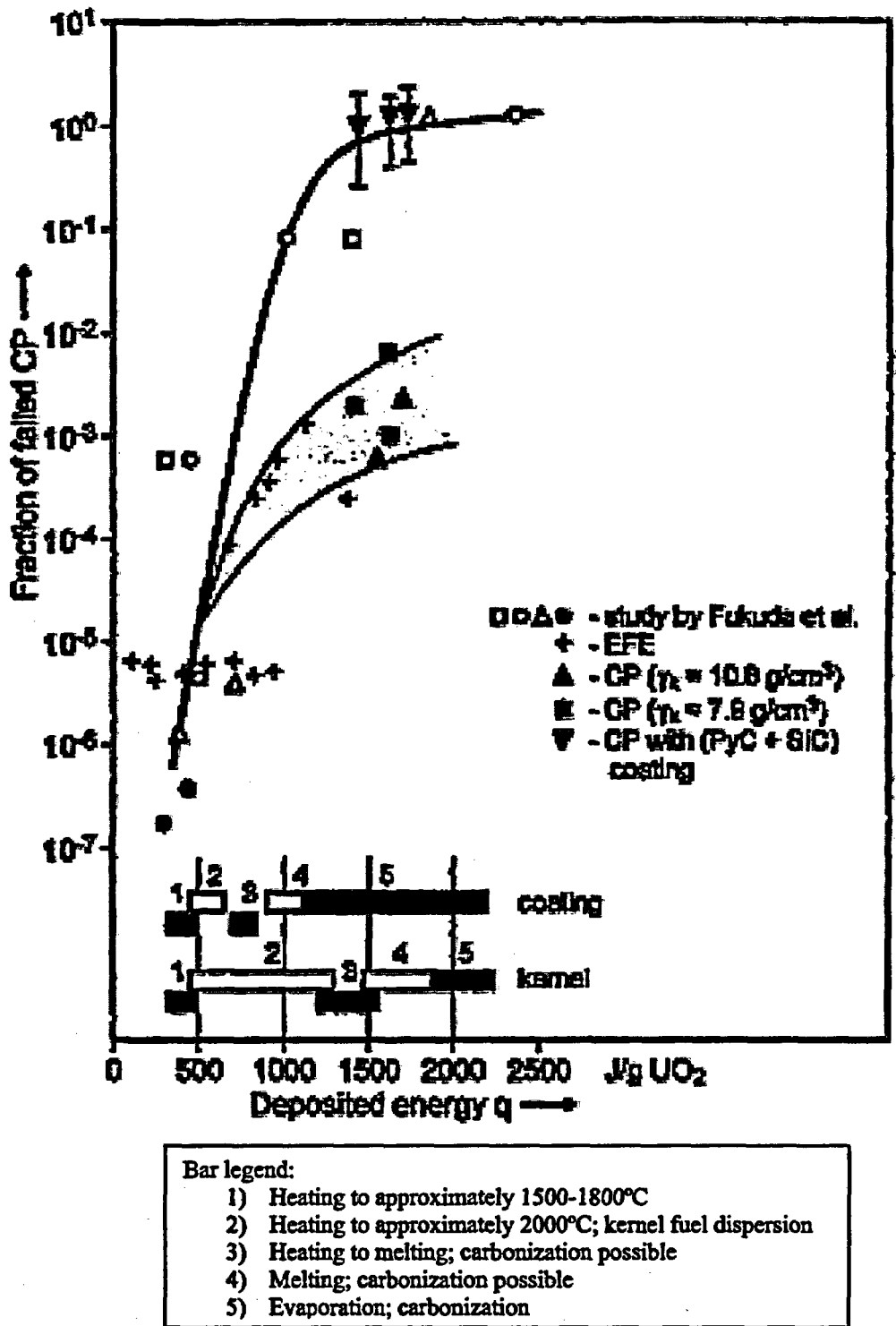


Fig. 2-40 Particle failure rate versus pulse energy deposition (IAEA TECDOC-978)

The Russian fuel is different than US or German fuel because different layer thickness are used, so the results may not be directly transferable.

2.5.5.1 Kernel

The energy is deposited in the kernel and a sudden deposition of energy will raise the temperature of the kernel causing the sudden release of fission products trapped in the grains and crystal structure and even kernel melting. A sudden pressure increase or pressure pulse may over pressurize and break the coating layers as well as increase the temperature of the coatings.

Past testing indicates that the energy deposition rate for fuel damage is in the range of 1000-2000 J/g [2-6].

2.5.5.1.1 Kernel Reactivity Accident Factors Identified By The PIRT Panel

Table 2-47 lists the kernel reactivity accident factors identified by the PIRT panel as well as the environmental conditions of interest.

Table 2-47 Kernel Reactivity Accident Factors Identified By The PIRT Panel

Kernel Reactivity Accident Factor	Rationale
Maximum fuel temperature	Chemical reactions and fission product diffusion are strongly influenced by temperature.
Temperature vs. time transient conditions	Time at temperature strongly influences the amount of material reacted or fission products released.
Energy deposition (total)	Determines the fuel and core temperature
Energy deposition rate	Determines the likelihood of impulsive fuel damage and system response time.
Energy Transport: Conduction within kernel	Determines kernel temperature and fission product diffusion from the kernel.
Thermodynamic state of fission products	The diffusivity of fission products is strongly influenced by their chemical form.
Gas phase diffusion	The details of the event, such as melting of the kernel, can modify the diffusion of fission products.
Condensed phase diffusion	
Oxygen flux	A significant redistribution of oxygen has the potential to change the oxygen potential and thus the fission product chemical species within the kernel.
Grain growth	Grain growth could release fission products from the grain to the grain boundary region, thus enhancing transport.
Buffer carbon-kernel interaction	The kernel periphery may react with the buffer carbon.

2.5.5.2 Buffer Layer

The buffer layer affects the response of the coated fuel particle to a reactivity event because it provides the expansion space for the particle gases. Any gases suddenly released from the kernel during the accident would have to diffuse into the buffer layer. This process could result in a brief pressure pulse that could damage the coatings. Otherwise the buffer plays the same role as described previously.

2.5.5.2.1 Buffer Layer Reactivity Accident Factors Identified By The PIRT Panel

Table 2-48 lists the buffer layer reactivity accident factors identified by the PIRT panel plus the relevant general issues.

Table 2-48 Buffer Reactivity Accident Factors Identified By The PIRT Panel

Buffer Reactivity Accident Factor	Rationale
Gas phase diffusion	The fission product transport through the buffer layer is expected to be high at accident temperatures.
Condensed phase diffusion	
Response to kernel swelling	The buffer layer must be weak enough that it will deform to accommodate the kernel.
Maximum fuel gaseous fission product uptake	The buffer layer must have sufficient free volume to accommodate the fission products at an acceptable pressure.
Layer oxidation	Any oxygen released from the kernel will oxidize a small portion of the buffer. This is of no consequence for the buffer, but may increase the particle pressure.
Thermal gradient	Gradients could be high for a high energy pulse.
Irradiation and thermal shrinkage	The buffer is designed to isolate the kernel from the IPyC, but small cracks could act to concentrate fission products.

2.5.5.3 IPyC Layer

During the pulse, the particle pressure may stress the IPyC. The main goal is to maintain particle integrity by accommodating the particle pressure. This is similar to normal operation, expect that the pulse may impose increased stresses in the layer.

2.5.5.3.1 IPyC Layer Reactivity Accident Factors Identified By The PIRT Panel

Table 2-49 lists the IPyC layer reactivity accident factors identified by the PIRT panel.

Table 2-49 IPyC Layer Reactivity Accident Factors Identified By The PIRT Panel

IPyC Reactivity Accident Factor	Rationale
Gas phase diffusion	Gaseous fission products are generally retained by the IPyC, but metallics transport is high. High local accident temperatures could increase the diffusion rate.
Condensed phase diffusion	
Pressure loading (fission products)	High pressure could challenge this layer. The IPyC can help keep the SiC in tension if the bonding between layers is strong (same as normal operation).
Pressure loading (CO)	The same CO issues apply here. High CO production will result in high pressure (same as normal operation).
Layer oxidation	In some cases internal oxidation of the layer could be significant. IPyC cracks can allow CO to the SiC and corrosion may result.
Stress state	See general discussion on particle layers. An impulse load may be more demanding. If this layer cracks or debonds, the stress distribution of the particle could change.
Intercalation	Material trapped in the layer could be released.

2.5.5.4 SiC Layer

The main goal is for the SiC layer is to stay intact under the induced stresses in the layer. If the accident causes a significant internal pressure pulse, fracture toughness of the SiC could be important. One factor is the temperature of the layer during and after the event. High-pressure stresses and layer temperatures near or above 1600°C could result in failure.

The details of the accident need to be modeled to get a reasonable estimate of the evolution of the event so that proper analysis and testing can be done.

2.5.5.4.1 SiC Layer Reactivity Accident Factors Identified By The PIRT Panel

Table 2-50 lists the SiC layer reactivity accident factors identified by the PIRT panel. Generally, many of the factors are the same as those that were discussed before.

Table 2-50 SiC Layer Reactivity Accident Factors Identified By The PIRT Panel

SiC Reactivity Accident Factor	Rationale
Gas phase diffusion	Except for silver, fission product diffusion is low through the SiC even at accident temperatures.
Condensed phase diffusion	
Thermal deterioration or decomposition	Above about 1600-1800°C the SiC begins to decompose into Si and C and its ability to retain fission products is greatly reduced.
Fission product corrosion	Some fission products may migrate to the SiC and damage it. This process is a function of temperature and can begin during normal operation. Pd is believed to be the main source of chemical attack, but others are also possible.
Heavy metal diffusion	The diffusion of fissile material could change the core configuration. A concern is major particle cracking and the expulsion of the kernel material during the pulse.
Layer oxidation	Attack by CO due to a cracked IPyC at high temperatures may be possible.
Fission product release through undetected defects, e.g. cracking	In order to release gases, both PyCs must be cracked in addition to a failed SiC. The SiC can be attacked by fission products and fabrication impurities (see manufacturing). Also, the impulse loads of this event may be important.
Fission product release through failures, e.g. cracking	
Thermodynamics of the SiC fission product system	At the temperature of interest, SiC is just stable to oxidation in its intact particle environment. (See corrosion issues.)
Sintering	High temperatures could result in changes to the microstructure and changes in fission product transport.

2.5.5.5 OPyC Layer

The main goal of the OPyC is to support the SiC during the event to keep it from exceeding its ultimate stress. Many of the factors that have been discussed previously apply.

2.5.5.5.1 OPyC Layer Reactivity Accident Factors Identified By The PIRT Panel

Table 2-51 lists the OPyC layer reactivity accident factors identified by the PIRT panel. Note that, like the other layers, they overlap with other events discussed previously.

Table 2-51 OPyC Layer Reactivity Accident Factors Identified By The PIRT Panel

OPyC Reactivity Accident Factor	Rationale
Gas phase diffusion	Gaseous diffusion is low, while metallic diffusion is high.
Condensed phase diffusion	
Layer oxidation	Coolant impurities could be a factor.
Stress state	See general discussion on the stress of the particle. OPyC loss is generally not as significant as IPyC loss.
Intercalation	Because the fission product inventory is low in this layer, these two items may be important in determining transport.
Trapping	
Cracking	Cracks can lead to a higher probability of SiC failure. Gases will be released if the other layers have failed.

2.5.5.6 Fuel Element

The purpose of the fuel element form during a reactivity accident event is to prevent relocation of the fuel during the accident should the particles fail and to sorb a portion of the released fission products. Cracks in the fuel element may occur, but fragmentation of the element is not expected.

2.5.5.6.1 Fuel Element Reactivity Accident Factors Identified By The PIRT Panel

Table 2-52 lists the fuel element reactivity accident factors identified by the PIRT panel. These concerns are similar to those previously identified.

Table 2-52 Fuel Element Reactivity Insertion Factors Identified by the PIRT Panel

Fuel Element Reactivity Accident Factor	Rationale
Irradiation history	Matrix behavior (shrinkage) is related to time temperature history, particularly temperatures and fast fluence.
Condensed phase diffusion	In the matrix gas diffusion is high, while metallic diffusion is variable. The less volatile metals can be sorbed in the matrix material to a high degree.
Gas phase diffusion	
Transport of metallic FPs through fuel element - Chemical form	The chemical form of the fission product determines its transport behavior. The chemical environment outside the fuel kernel may be significantly different than inside. Generally, significant sorbing of the metallics is observed.

2.6 Summary of Fuel Failure Mechanisms

The previous sections detailed the fuel behavior on a layer-by-layer basis so the PIRT process could be applied to each aspect of the fuel constitution. This section will briefly review the fuel particle damage/failure mechanisms on a broader scale so that the reader might better catalog the general overall picture.

A review of the irradiation and safety testing of coated particle fuel reveals a number of potential failure mechanisms. These failure mechanisms are functions of temperature, burnup, fluence, and macroscopic temperature gradient across the particle. Mechanisms that may result in particle failure, which ultimately leads to fission product release, are:

- 1) Pressure vessel failure caused by internal gas pressure
- 2) Pyrocarbon layer cracking and/or debonding due to irradiation induced shrinkage that ultimately leads to the failure of the SiC layer
- 3) Fuel kernel migration (amoeba effect), which leads to interactions with the coating layers
- 4) Fission product/coating layer chemical interactions
- 5) Matrix/OPyC interaction
- 6) As-manufactured defects produced during fabrication of fuel particles or during pressing of fuel compacts/spheres
- 7) Thermal decomposition of the SiC layer at very high temperatures
- 8) Enhanced SiC permeability and/or SiC degradation (high burnup considerations)
- 9) Chemical attack (ingress accidents)
- 10) Reactivity insertion (accident)

In this section, these mechanisms and the variables that control them are briefly described; for more detail refer to the previous section(s).

2.6.1 Pressure Vessel Failure

Under irradiation, coated particle fuel is subjected to a number of forces that put stress on the TRISO coating. One of the earliest recognized mechanisms is overpressure due to gas generation under irradiation. During irradiation, fission gases are released from the kernel to the porous buffer layer. The pressure that is generated exerts tensile forces on the layers of the particle. In addition to fission gas, in coated particle fuel with UO₂ kernels, there is excess oxygen released during fission. This excess oxygen will react with the buffer to form CO gas. Both the fission gas and CO production are functions primarily of burnup and temperature. In UCO fuels, CO is not produced provided sufficient uranium carbide is added to the kernel to buffer the oxygen over the burnup life of the fuel. The key variables that affect this mechanism are burnup and temperature. Fluence does not significantly affect these processes. Particles are generally sized with a large enough buffer to ensure that nominal particles do not fail by overpressure. Particle failure is postulated to occur in the event that during the coating process, particles are coated with an insufficient or missing buffer layer (i.e., insufficient void volume to accommodate the gases). Thus, fabrication specifications limit the number of particles produced with thin

or missing buffer layers and impose limits on the statistical variation in kernel diameter and buffer thickness. This is a much analyzed but seldom seen failure mechanism. No indications of pressure vessel failure were observed in the past German pebble fuel irradiations.

2.6.2 Irradiation-induced IPyC Cracking and Debonding

Under irradiation, PyC shrinks in both the radial and tangential direction. At modest fluences ($\sim 2 \times 10^{25}$ n/m²) depending on the density, temperature and anisotropy of the material, it begins to swell in the radial direction and continues to shrink in the tangential direction. This behavior puts the PyC layers into tension in the tangential direction. At longer irradiation times, irradiation induced creep works to relieve the tensile stress in the PyC layer. If the IPyC is strongly bonded to the SiC layer, the IPyC shrinkage provides a strong compressive stress in the SiC layer that offsets the tensile stresses generated by gas production. In fact, the particles are designed such that in intact particles, the SiC layer remains in compression throughout the irradiation.

The shrinkage, swelling and creep behavior of the pyrocarbons is complex and depends strongly on the fabrication details. If the shrinkage is much larger than anticipated the tangential stresses in the PyC can be high enough to cause cracking in the layer. These cracks can lead to stress concentrations in the SiC layer high enough to cause failure of that layer. This failure mechanism has been attributed to high anisotropy in the PyC layer.

Post irradiation examination of German pebble fuel did not reveal any shrinkage cracks in the IPyC layer as has been observed in many U.S. irradiations. Thus, the experimental evidence to date suggests that this mechanism is most likely not important for very isotropic IPyC, but may play a role in less isotropic IPyC. The issue is complicated because the PyC isotropic measurement is somewhat controversial and US fuels often saw much more aggressive irradiation conditions. Control of the fabrication process appears to be the most reliable current way to assure sound PyC properties.

In addition to irradiation-induced shrinkage, debonding at the IPyC/SiC interface has been observed in many U.S. irradiations. This debonding is believed to be related to the nature of the IPyC/SiC interface. Weakly bonded coating layers can partially detach because of the tensile stresses generated by the PyC shrinkage under irradiation. A particle for which partial debonding of the IPyC from the SiC has occurred can develop relatively large tensile stresses in the SiC (although significantly smaller than in the case of a cracked IPyC). Tensile stresses occur at the point of IPyC/SiC contact as the IPyC shrinks under irradiation. Irradiation induced creep relieves the stress at longer times. When these stresses are used in concert with Weibull statistics to calculate the SiC failure probability, it is found that the SiC fails at a low, but not insignificant, rate.

2.6.3 Kernel Migration

Kernel migration is defined simply as movement of the kernel in the coated particle toward the TRISO coating. If the migration is excessive, the kernel will penetrate the TRISO coating leading to failure of the particle. Kernel migration is associated with carbon transport in the particle in the presence of a temperature gradient. In the fuel kernel equilibrium is established among C, UO₂ and CO. When there is a thermal

gradient across the particle, the equilibrium is different on each side of the particle. The different equilibrium conditions lead to mass transport of carbon down the temperature gradient. This movement of carbon appears in photomicrographs of fuel as a movement of the kernel up the temperature gradient and hence the name kernel migration. This phenomenon is strongly dependent on the temperature and the macroscopic temperature gradient in the fuel with secondary dependence on burnup. It can also occur as solid-state carbon transport through carbide kernels.

In prismatic cores with UO_2 fuel, where power densities in the particles are greater, the potential for kernel migration is greater. In pebble bed cores, the power densities and hence the thermal gradients are much smaller. For prismatic cores, this phenomenon prompted the U.S. to change their kernel design from UO_2 to UCO, an oxycarbide kernel, in which no CO is produced and thus the equilibrium and carbon transport phenomena mentioned above are not expected to occur.

2.6.4 Fission Product/Coating Layer Chemical Interactions

Past irradiation experiments indicate that fission products can be transported from the kernel to the inner surface of the SiC where they interact and can damage and potentially fail the SiC layer. In older uranium carbide kernels rare earth fission product migration was of concern. In UO_2 kernels, palladium is very important, as are some other noble metal fission products. In UCO kernels, the oxycarbide form of the kernel generally ties up all fission products with the exception of a few metals (e.g., Ag, Cs, Pd) as either carbides or oxides, which tend to limit their mobility in the UCO system. However, Pd transport has still been observed in UCO coated particle fuel. In addition, although not a failure mechanism, the migration of silver in both UO_2 and UCO has been observed. The silver can migrate through apparently intact particles and be released into the reactor coolant system where it will deposit on cold surfaces. For direct cycle gas reactors, this may be in the turbine, which has important maintenance (worker dose) implications. Studies have been conducted to understand the mechanism for the Ag migration through SiC and Pd attack of the SiC. The migration of the fission products is thought to be a function of temperature and burnup as well as temperature gradient. Although a complete understanding of the phenomena is not available, the role of temperature and temperature gradient are recognized as being critical. The degree of fission product attack is generally correlated with the temperature and temperature gradient in the fuel. Thus, these fission product attack mechanisms are expected to play a more important role in prismatic reactors where power densities in the particle are larger than corresponding particles in a pebble bed reactor (reference design for this PIRT).

Also of note here is the fact that the enrichment of the fuel is important in defining the magnitude of the Ag and Pd problem. The yields of Ag and Pd are 25 to 50 times greater for Pu than for U. Thus, in LEU fuels where at the end of life significant fission comes from Pu, the concentration of Ag and Pd can be much greater than in HEU fuel of similar burnups.

2.6.5 Matrix/OPyC Interaction

In early U.S. irradiations, high levels of OPyC failure due to cracking or debonding from the SiC layer were observed. These failures were attributed to intrusion of the low viscosity carbonaceous matrix material in the OPyC during compact fabrication followed

by shrinkage under irradiation. Specifications on this matrix material and its injection were developed based on the irradiation experiments to limit this failure mechanism. No similar behavior was observed in German pebble fuel because of the use of a high viscosity matrix/binder mix that does not tend to penetrate the OPyC and because of the higher isotropy of German OPyC.

2.6.6 As-Manufactured Defects

In the absence of any of the above failure mechanisms, fission gas and metal release during irradiation is attributed to heavy metal contamination outside of the SiC layer and to initially defective particles. Initially defective particles can be the result of undetected defective particles that have not been removed during fabrication, attack of the particles during fabrication or irradiation by impurity metals (e.g., Fe), or particles that have failed as a result of damage from fuel element fabrication. In pebble bed fuel, a soft overcoating is put on the particle after the OPyC layer to limit stresses induced by particle-to-particle contact during pebble manufacture. In prismatic fuel using the injection process, recent process development work has been carried out to reduce particle stresses and limit introduction of impurities during compact formation.

During the three decades of German particle fuel production, the fraction of as-manufactured defects has continuously dropped to very low levels ($< 1 \times 10^{-6}$). This is evident by the low beginning of life Kr-85m R/B values (reaching a minimum value of 2×10^{-10} in the FRJ2-K15 experiment) from each of the German experiments. Even at these low defect levels, as-manufactured defects were the most common source of particle abnormalities reported. In all, one fuel kernel was reported to be without coating in the FRJ2-P27 experiment and two kernels were reported to be without coating in the R2-K12 experiment.

2.6.7 SiC Thermal Decomposition

At very high temperatures (above 1600-1800°C), thermodynamics and data from German high temperature heating tests show that the SiC layer undergoes thermal decomposition at a significant rate. This phenomenon is primarily a function of temperature and time and has not played a major role in fuel failure at lower accident temperatures (1600°C) where safety testing has been routinely performed. Fuel releases generally increase at temperatures above 1600°C, with releases at 1800°C being much greater, although SiC behavior in the 1600-1800°C range may be a combination of corrosion and decomposition.

2.6.8 Enhanced SiC Permeability and/or SiC Degradation

Although not formally a failure mechanism, there is some limited evidence that fast neutron fluence and/or burnup plays a role in the permeability or degradation of the SiC layer with respect to fission products during high temperature heating. Pebbles exposed to higher fluence (4.6×10^{23} n/m²) and higher burnup (14 % FIMA) have exhibited a greater release of fission products (e.g., cesium) in heating tests than similar pebbles exposed to less severe conditions. This phenomenon could become more important as coated particle fuel is pushed to high burnup. The reference German pebble has not been tested at more aggressive irradiation conditions (temperature and burnup).

2.6.9 Chemical Attack (Ingress Accidents)

Under accident conditions, fuel may be exposed to air and/or water. Both will react with the carbon materials and the fuel kernels. Water ingress primarily affects exposed kernels, causing them to release a large fraction of their stored inventory. Reactions with the carbon materials are relatively modest at the temperatures of interest and the resulting fuel damage is not aggressive.

Air is much more aggressive than water and reacts not only with the exposed kernels, but also reacts with the carbon materials at a greater rate than water. The possibility of the establishment of a flow may result in significant fuel damage if allowed to continue unabated. In both cases, reactions with the carbon materials will release sorbed fission products.

2.6.10 Reactivity Insertion (Accident)

The sudden generation of high energies within the coated particle fuel can cause it to overheat, overpressure, and break, thus releasing its fission products. This accident is not well defined, but results to date indicate that coated particle fuel will fail with energy depositions in the range of 1000-2000 J/gm. Much higher energies may cause the fuel element to be damaged.

Past estimates for the reactivity insertion duration were in the seconds with energies much larger than that required to damage fuel particles.

2.7 References

Reference 6 is an excellent compilation of coated particle fuel information and is a good starting point for the interested reader. Reference 9 is a good starting point for understanding how coated particles are bonded into a fuel element.

- 2-1. Mehner, A. W., et.al., "Status of Qualification of High-Temperature Reactor Fuel Element Spheres, Nuclear Technology," 69 (1985), page 44.
- 2-2. "Spherical Fuel Elements for Advanced HTR Manufacture and Qualification by Irradiation Testing," Journal of Nuclear Materials, 171 (1990), pages 1-18.
- 2-3. Nickel, H., et. al., "Long Time Experience with the Development of HTR fuel Elements in Germany," Nuclear Engineering and Design, 217 (2002), pages 141-151.
- 2-4. Wolf, L., et. al., "Fuel Elements for the High Temperature Pebble Bed Reactor, Nuclear Engineering and Design," 34, (1975), pages 93-108.
- 2-5. Gontard, R., and H. Nabielek, "Performance Evaluation of Modern HTR TRISO Fuel," HTA-1B-05/90 (July 1990).
- 2-6. "Fuel Performance and Fission Product Behavior in Gas Cooled Reactors," IAEA-TECDOC-978 (1997).

- 2-7. Moormann, R., et. al., "Source Term Estimation for Small-Sized HTRs: Status and Further Needs, Extracted From German Safety Analysis," *Nuclear Technology*, 135, (2001), pages 183-193.
- 2-8. *Nuclear Technology*, Volume 35, Number 2, 1977 (entire issue is devoted to coated particle fuels).
- 2-9. "Fuel Compact Design Basis Report," DOE-GT-MHR-100212 (1994).
- 2-10. Proksch, E., et. al., "Production of Carbon Monoxide During Burn-up of UO₂ Kerneled HTR Fuel Particles," *Journal of Nuclear Materials*, 107 (1982) pages 280-285.
- 2-11. Horsley, G. W., et. al., "Influence of Irradiation Temperature, Burnup, and Fuel Composition on Gas Pressure (Xe, Kr, CO, CO₂) in Coated Particle Fuels," *Journal of the American Ceramic Society*, 59 (1976), Number 1-2, pages 1-4.
- 2-12. Stansfield, O. M., et. al., "Kernel Migration in Coated Carbide Fuel Particles," *Nuclear Technology*, 25 (1975), pages 517-530.
- 2-13. Martin, D. G., "Considerations Pertaining to the Achievement of High Burn-ups in HTR Fuel," *Nuclear Engineering and Design*, 213 (2002), pages 241-258.
- 2-14. Kaae, J. L., "A Mathematical Model for Calculating Stresses in a Pyrocarbon and Silicon Carbide Coated Fuel Particle," *Journal of Nuclear Materials*, 29 (1969), page 249.
- 2-15. Stevens, D. W., "An Explicit Solution for Stresses in Pyrocarbon-Coated Fuel Particles," *Nuclear Technology*, 10 (1971), page 301.
- 2-16. Kaae, J. L., "A Mathematical Model for Calculating Stresses in a Four-Layer Carbon-Silicon-Carbide-Coated Fuel Particle," *Journal of Nuclear Materials*, 32, (1969), page 322.
- 2-17. Gulden, T. D., et. al., "The Mechanical Design of TRISO-Coated Particle Fuels for the Large HTGR," *Nuclear Technology*, 16 (1972), pages 100-109.
- 2-18. TRISO Fuel Particle Coating Design Basis, DOE-GT-MHR-100225 (1994).
- 2-19. Miller, G. K., and D.C. Wadsworth, "Treating Asphericity in Fuel Particles Pressure Vessel Modeling," *Journal of Nuclear Materials*, 211 (1994), pages 57-69.

- 2-20. Verfondern, K., "Modeling of Fuel Performance and Metallic Fission Product Release During HTTR Normal Operating Conditions," Nuclear Engineering and Design, 210 (2001), pages 225-238.
- 2-21. Mitake, S., et. al., "An analytical Study of Volatile Metallic Fission Product Release From Very High Temperature Gas-Cooled Reactor Fuel and Core," Nuclear Technology, 81 (1988), pages 7-12.
- 2-22. Martin, R. C., "Compilation of Fuel Performance and Fission Product Transport Models and Database for MHTGR Design," ORNL/NPR-91/6 (1993).
- 2-23. Martin, R. C., "Revised MHTGR High-Temperature Fuel Performance Models," ORNL/NPR-92/16 (1993).
- 2-24. Verfondern, K., et. al., "Methods and Data for HTGR Fuel Performance and Radionuclide Release Modeling during Normal Operational and Accidents for Safety Analysis," Forschungszentrum Juelich GmbH, Juel-2721 (1992).
- 2-25. Godfrey, T. G., et. al., "Coated-Particle Fuels," ORNL-4324 (1968).
- 2-26. "TRISO Fuel Particle Coating Design Basis," DOE-GT-MHR-100225 (1994).
- 2-27. Petti, D. A., 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, also Nuclear Engineering and Design, 222 (2003) 281-297.
- 2-28. "Fission Recoil Damage to Pyrolytic Carbon," Carbon, 7 (1969), pages 703-706.
- 2-29. "MHTGR TRISO-P Fuel Failure Evaluation Report," DOE-HTGR-90390 (1993).
- 2-30. Miller, G., et. al., "Consideration of the Effects on Fuel Particle Behavior from Shrinkage Cracks in the Inner Pyrocarbon Layer," Journal of Nuclear Materials, 295 (2001), pages 205-212.
- 2-31. Minato, K., et. al., "Carbon Monoxide-Silicon Carbide Interaction in HTGR Fuel Particles," Journal of Materials Science, 26 (1991), pages 2379-2388.
- 2-32. Forthmann, R., et. al., "Influence of Material Properties on the Retention of Fission Products by Silicon Carbide Coatings," High Temperature - High Pressure 1982, Volume 14 (1982) pages 477-485.
- 2-33. "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).

- 2-34. Tokar, M., Evaluation of High Temperature Gas Cooled Reactor Fuel Particle Coating Failure Models and Data, NUREG-0111 (1976)
- 2-35. Tiegs, T. N., "Fission Product Pd-SiC Interaction in Irradiated Coated-Particle Fuels," Nuclear Technology, 57 (1982), pages 389-398.
- 2-36. Lauf, R., et. al., "Out-of-Reactor Studies of Fission Product-Silicon Carbide Interactions in HTGR Fuel Particles," Journal of Nuclear Materials, 120 (1984), pages 6-30.
- 2-37. Federer, J. I., "Fluidized Bed Deposition and Evaluation of Silicon Carbide Coating on Microspheres," ORNL/TM-5152 (1977).
- 2-38. "MHTGR Fuel Manufacturing Quality Assurance Plan," DOE-HTGR-88091 (1988).
- 2-39. "Data Support Document: Operating Procedures for SiC Defect Detection," DOE-HTGR-88359 (1991).
- 2-40. Bullock, R. E., "Fission-Product Release During Postirradiation Annealing of Several Types of Coated Fuel Particles," Journal of Nuclear Materials, 125 (1984), pages 304-319.
- 2-41. "Fission Product Plateout and Liftoff in the MHTGR Primary System: A Review," NUREG/CR-5647 (1991).
- 2-42. Myers, B., "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," DOE-HTGR-88486 (1991).
- 2-43. Moorman, R., "Chemical Behavior of Fission Products in Core Heatup Accidents in High-Temperature Gas-Cooled Reactors," Nuclear Technology, 94 (1991), pages 56-67.
- 2-44. "Design of High Temperature Engineering Test Reactor (HTTR)," Japan Atomic Energy Research Institute document JAERI 1332, Japan Atomic Energy Research Institute (September 1994).
- 2-45. Hishida, M., and T. Takeda, "Study on Air Ingress During an Early Stage of a Primary-Pipe Rupture Accident of a High-Temperature Gas-Cooled Reactor," Nuclear Engineering and Design, 126 (1991), pages 175-187.

3. FISSION PRODUCT TRANSPORT IN TRISO-COATED PARTICLE FUELS

3.1 Introduction

The purpose of this section is to discuss the potential phenomena (generalized to the term "factors" in this report) associated with the transport of fission products in TRISO-coated particle fuel. Fission product transport in the coated particle is a key component of the source term calculation for the high-temperature gas-cooled reactor and is very useful for evaluation of factors identified by the PIRT panel. TRISO-coated particle fuel is a complex fuel form from the perspective of fission product modeling. The multiple layers, the chemical state of the fission products, the different mechanisms responsible for gaseous and metallic fission product transport in each layer, and the projected high burnups and fast neutron fluences make the modeling of fission product transport challenging. Sections 3.2 through 3.5 discuss fission product transport in the TRISO-coated particle fuel layer by layer. Each section includes a review of the existing database for transport in the layer, discusses potential mechanisms responsible for the transport, and presents results of preliminary scoping calculations for the transport in the layer. In Section 3.6, a simplified integrated transport model is presented and some simple sensitivity results are discussed. These results are used to provide a better understanding of the individual sub-factors associated with the fission product transport factors identified by the PIRT panel. In Section 3.7, these factors are defined and the rationale for the selection of these factors to capture the overall complexity of fission product transport is discussed. Section 3.8, summarizes our findings.

3.2 The Fuel Kernel

Fission product transport in the kernel is complex. Important mechanisms (i.e., factors) include recoil, diffusion of fission products to grain boundaries, vaporization, and transport through the interconnected porosity of the kernel to the surface of the kernel and chemical reaction at the boundary of the kernel. These processes are functions of burnup and temperature and thus change over the life of the fuel.

3.2.1. Recoil

Recoil from the kernel can be estimated using the following equation:

$$(RF)_{\text{recoil}} = 0.25 [\tau_k^3 - (\tau_k - d)^3] / \tau_k^3$$

where RF is the release due to recoil, τ_k is the radius of the fuel kernel and d is the average fission fragment range. The average fission fragment ranges are calculated for a given fuel composition from experimental data [3-1]. Based on fission energies of 107 MeV for krypton and 72 MeV for xenon, the average krypton range is 5.8 microns and the average xenon range is 4.1 microns in UO_2 with a density of 10.5 g/cm^3 . Thus, for a 500-micron kernel, the recoil release fraction is about 1.5%. For a 350-micron kernel, the recoil release fraction is about 2%.

3.2.2. Chemical Reaction at the Fuel Kernel Boundary

Fuel kernels are chemically reactive with the surrounding graphite. This is especially true for UO_2 kernels. There will be some reaction of the graphite with the kernels to produce surface layers of uranium carbide or oxycarbide and carbon monoxide (CO). The structure of uranium carbide is different from the structure of uranium dioxide. The reaction is not topotactic¹ and restructuring of the surface material takes place. The restructuring causes the material to evolve toward a more nearly equilibrium state by expelling to its surfaces some fractions of the impurities including fission products. Because these fission products are moved during the recrystallization process to the exposed surfaces of the fuel kernel, they are usually considered to be released from the kernel. Because of the temperature dependence of the reaction of graphite with the kernel, reaction release of fission products can become progressively more important as temperatures increase.

During normal operations, kinetics of reaction limit the rate of fission product release from fuel kernels by reaction with the graphite. Out-of-pile studies of the reaction kinetics are of limited use because the effects of graphite irradiation is not accounted for. Irradiation of the graphite creates dislocations of the graphite structure that are energetic and more reactive than unirradiated graphite toward the fuel kernel.

3.2.3. Booth Diffusion

Far more important than either recoil or reaction as transport mechanisms of release (especially under accident conditions) is the conventional release process of fission product diffusion through grains to the grain boundaries and subsequent transport through the interconnected porosity. This mechanism has been studied extensively in the context of light water reactor fuel behavior. The Booth diffusion model has been used to estimate the release of fission gases via these mechanisms and has been used to describe fission product release from the kernel. The release fraction is given by [3-2]:

$$FR = 1 - \left(\frac{6}{D't}\right) \sum_{n=1}^{\infty} [1 - \exp(-n^2 \pi^2 D't)] / [n^4 \pi^4]$$

where D' is the reduced diffusivity, which is equal to D'/a^2 and t , is equal to time. The two key parameters in the model are a , the effective radius for diffusion, and D the diffusion coefficient. This equation has been used to establish reduced diffusivities (D'/a^2) from integral irradiation and high temperature experiments. This approach produces a reduced diffusion coefficient that is time-averaged and volume-weighted. The formulation for diffusion coefficients by Turnbull, which accounts for intrinsic, athermal and radiation-enhanced diffusion, is believed to be the most accurate for UO_2 . [3-3,3-4] The definition of the effective radius is usually taken to be the grain size of the UO_2 .

¹ topotactic transition: a transition in which the crystal lattice of the product phase shows one or more crystallographically equivalent, orientational relationships to the crystal lattice of the parent phase.

There are several limitations with the Booth model:

- a. The original Booth model was used to describe gas release from a fuel grain and not a fuel kernel or fuel pellet per se where the gas phase transport in the interconnected porosity is also important.

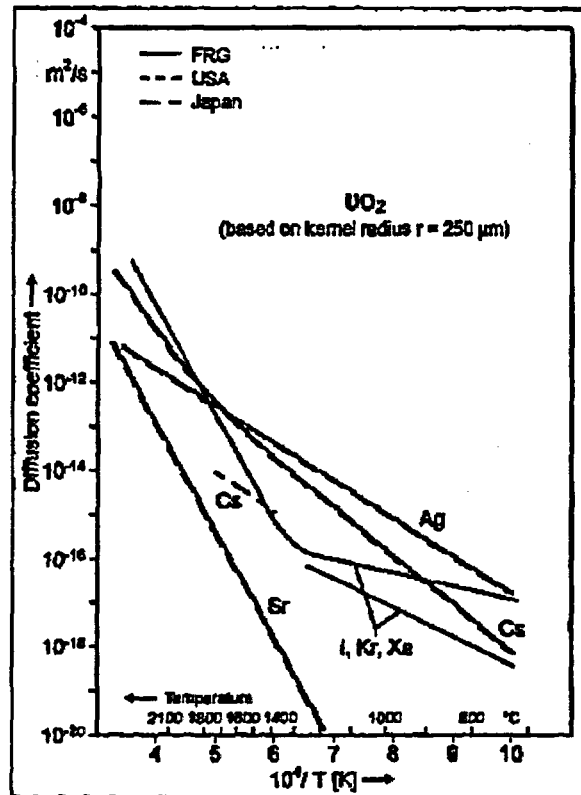


Figure 3-1 Comparison of measured diffusivities of fission gases and some fission metals in UO₂ kernels of coated particle fuel [3-5]

- b. The use of the Booth model makes it difficult to accurately capture the effect of burnup on the microstructural changes in the kernel and the subsequent impact on release.²

² The variability in the reduced diffusivity derived from the integral release measurements may be quite large when the morphology changes in the kernel with burnup are considered. Low releases are expected at low burnup. At moderate to high burnup, the restructuring of the kernel can be extensive resulting in large release. This is a key shortcoming in using such a simple model to account for very complex fuel microstructural evolution and attendant fission product release.

- c. The release of some of the metallic fission products, which tend to form nodules along grain boundaries in the fuel (e.g., Ru, Mo, Tc, Pd), is not governed by this classic diffusion mechanism.

Despite these shortcomings, many researchers have correlated or “force-fitted” release measurements to an “effective Booth model.” For coated particle fuels, reduced diffusivities exist for the fission gases and some fission metals like cesium, silver, and strontium. The effects of changes in the microstructure with burnup are not directly accounted for but are implicit in the values used for D . Figure 3-1 is a plot of the values of D measured on UO_2 coated particles by the Germans (assuming $a = 250$ microns) [3-5] and they form the baseline to be used for scoping analysis presented here. No diffusivity data exist for noble fission metals like Ru, Mo, Tc, and Pd. Similar data do not exist for UCO and thus UO_2 values are used in the interim.

This effective Booth model has been used with the measured diffusivities for UO_2 fuel to determine the impact of time (i.e., burnup) and temperature on the release of fission gas, cesium, silver and strontium from a 500-micron UO_2 kernel. Three specific calculations have been performed:

- A three-year 900°C irradiation, typical of the average exposure of a UO_2 coated particle in a prismatic reactor
- A three-year 1200°C irradiation, typical of the peak exposure of a UO_2 coated particle in a prismatic reactor
- A three-year 600 to 1200°C ten cycle exposure typical of peak exposure of a UO_2 coated particle in a pebble bed reactor.

The resultant fission product releases are shown in Figures 3-2, 3-3 and 3-4. The results indicate that time at temperature is important and can make a difference in the release fraction of the fission products from the kernel. Given the exponential nature of the diffusivities, as expected the release is dominated by the time at high temperature.

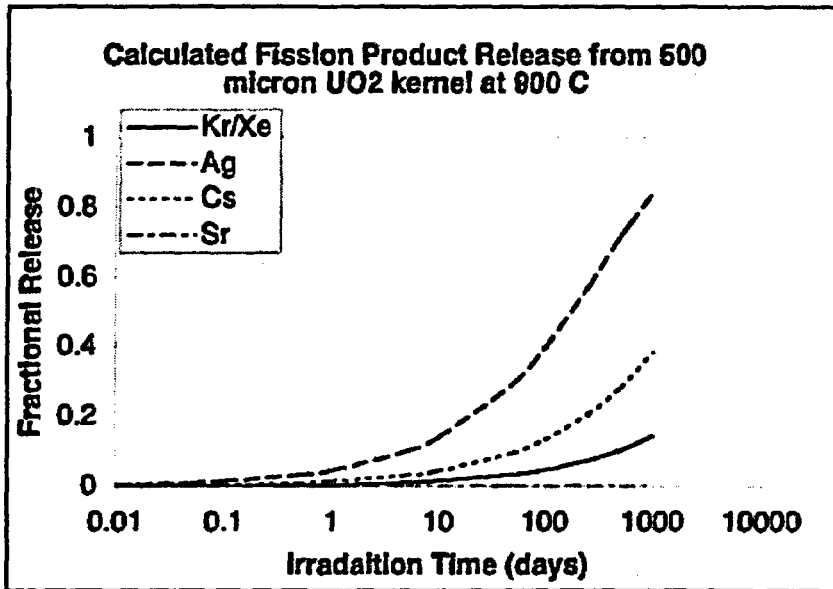


Figure 3-2 Calculated fission product release from 500 micron UO₂ kernel at 900°C

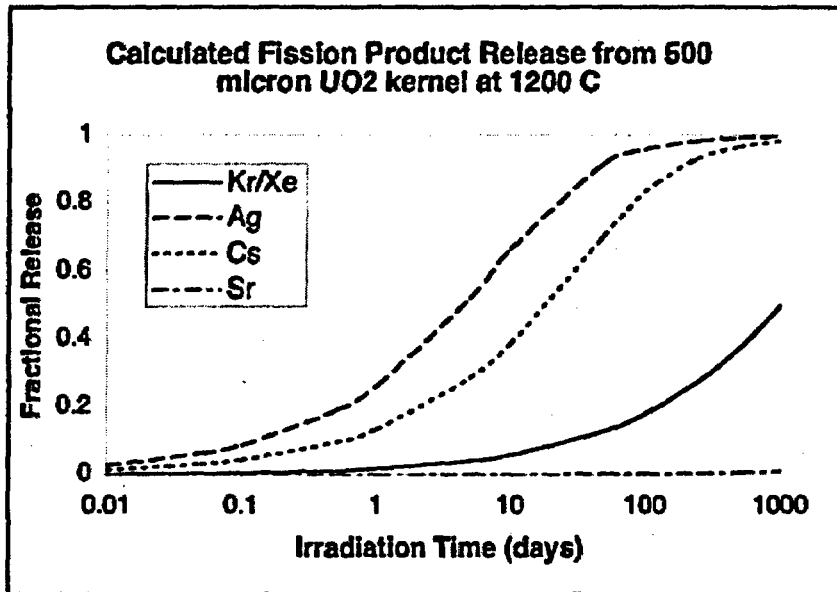


Figure 3-3 Calculated fission product release from 500 micron UO₂ kernel at 1200°C

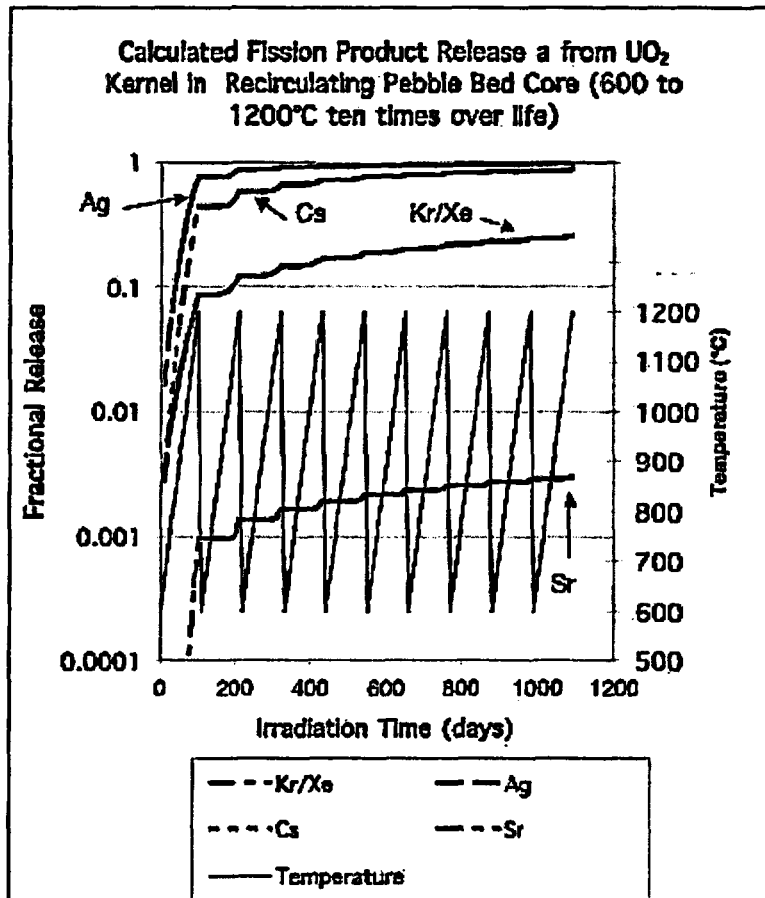


Figure 3-4 Influence of cyclic temperature in a pebble bed reactor on fission product release from a 500 micron UO₂ kernel

3.2.4. Vaporization: Fission Product Chemical Form

The estimation of fission product transport through the layers of coated particle fuel requires an understanding of the gas-phase speciation of fission products released from the fuel. The chemical environment of the fuel particle will be reducing and different than exists at any point in the release of fission products for light water reactor cores. The speciation will be sensitive to the reducing conditions. Furthermore, graphite and carbon monoxide produced by the reaction of graphite with oxygen liberated by the fission process can affect the speciation.

Speciation in terms of elemental vapor species and oxide vapor species can be determined with existing thermochemical data. There are, however, possibilities for vapor species that are not as well known forming in the environment of the coated particle fuels. These include impurities left from the manufacturing process such as HCl, which can affect speciation by the formation of chlorides of the fission products.

Chlorides are typically volatile. There are recognized databases on the thermochemical properties of condensed chlorides of most of the fission products. Data bases on vapor species, especially monochloride and dichloride vapor species or oxychloride vapor species, have not been as comprehensively compiled though data are available.

More exotic species in the sense that they are less familiar in the analysis of light water reactor accidents include vapor phase carbide species. There is also evidence for the formation of the vapor phases of BaC, SrC, ZrC and RuC. Again, the necessary review of the literature to produce a well-founded compilation of vapor-phase carbides has not been done.

Another class of species that is not well known in a thermochemical sense is the vapor phase carbonyls. Metal carbonyls $(CO)_n$ are well known chemically and used as precursors for the synthesis of organometallics. Notable species include $Ni(CO)_4$ and $Fe(CO)_5$ and carbonyls of many other transition elements. These, however, are not the species of primary interest in relation to the transport of fission products in coated particle fuels at the high temperatures arising in reactor accidents, because they are not radiologically important. In these conditions vapor species that are monocarbonyls (MCO) and dicarbonyls $(M(CO)_2)$ are likely to be of more interest [3-[6]. Thermochemical data for such species are not abundant simply because there has been little incentive to look for and characterize such species. This, however, does not mean that the species are unimportant in the particular situation of interest here. (The level of knowledge about vapor phase carbides and carbonyls is similar to that of vapor phase hydroxides 50 years ago. Their existence is not well established, but they proved important for the understanding of factors other than fission product transport such as flames, magmatic processes and even some corrosion processes. They were eventually found by experiment and characterized.)

Speciation of fission products can become more complicated during accidents involving air and water intrusion. Then, in addition to the vapor species already mentioned, vapor phase hydrides, hydroxides, nitrides and even cyanides may affect the potential for fission product release.

The thermochemical data used for the calculation of the vapor speciation are enthalpies of formation and free-energy functions. The free-energy functions are usually calculated for vapor species from spectroscopic data, some of which can be very complicated for high molecular weight fission product species. Enthalpies of formation are usually derived from mass spectroscopic estimates of the temperature dependencies of vapor pressures or inferred from transpiration experiments. The uncertainties in the enthalpies of formation of vapor species can be as high as ± 20 kcal/mole.

3.3 The Buffer Layer

The buffer layer plays a role in the coated particle from the perspective of fission product transport. Depending on the specific irradiation conditions, the nature of the shrinkage and densification of the buffer establishes the initial condition for fission product

transport during irradiation and under accident conditions. The buffer is a porous carbon layer (~50% dense initially) whose function is to serve as a void volume for fission gases and act a material to absorb fission recoils and swelling of the fuel kernel. Sometimes the buffer cracks because of tangential stresses developed under irradiation. Because of the high porosity of the layer, it has the lowest conductivity of any layer in the coated particle and thus the largest temperature drop. Depending on the power produced in the kernel, the temperature gradient in the buffer may cause thermal (or Soret) fission product diffusion in the layer.

3.3.1. Thermal Behavior of the Buffer

For a first approximation, to calculate the internal temperature distribution in a coated particle it can be assumed that heat transfer is predominantly by radial heat conduction and that the outer boundary temperature of the fuel particle is uniform. In a spherical fuel kernel with uniform heat generation rate, q_f''' (W/m^3), the steady state temperature rise from the center to the surface of the kernel is given by:

$$T_o - T_1 = - q_f''' r_1^2 / 6k_f$$

Where $T_o = T(0)$, $T_1 = T(r_1)$, $r_1 =$ fuel kernel radius, and $k_f =$ fuel kernel thermal conductivity. Ignoring heat generated in the buffer, the buffer temperature drop is given by:

$$T_1 - T_2 = q_f (r_2 - r_1) / 4\pi k_o r_1 r_2$$

Where $r_2 =$ buffer outer radius, $k_o =$ thermal conductivity of the buffer, and $q_f = (4/3)\pi r_1^3 q_f''' =$ thermal power generated in the fuel kernel. Assuming no gaps develop between layers, which can cause large temperature drops, similar equations apply to the temperature drops across other layers (IPyC, SiC, OPyC).

Table 3-1 presents the calculated temperature drop across each layer, and the layer's associated thermal properties for an average particle that generates ~ 62 mW of power, which is about the average power per particle in a pebble bed reactor core (PBR). Thus, for an average particle, the ~ 10 °K temperature drop across the buffer translates into ~ 100 °K/cm gradient across the layer.

Table 3-1 Calculated Temperature Drops Across Layers of a Coated Particle

	Outer Radius, μm	Conductivity k, W/m-K	Density ρ , kg/m^3	Heat Capacity C_p , J/kg-K	Temperature drop ΔT , $^\circ\text{K}$ Layer
UO ₂ kernel	$r_1 = 250$	2.5	10960	332	3.92
Buffer (50% dense graphite)	$r_2 = 345$	0.5	1100	1.5	10.88
IPyC	$r_3 = 385$	4.0	1700	1.5	0.37
SiC	$r_4 = 420$	13.9	3200	0.5	0.07
OPyC	$r_5 = 460$	4.0	1700	1.5	0.26
				Total $\Delta T =$	15.5

Figure 3-5 plots the thermal gradient and the temperature drop across the buffer as a function of the power per particle for a standard 500 micron UO₂ German coated particle. As the power increases, significant thermal gradients can develop. These thermal gradients lead to increasing thermal stresses in the layer. The stresses in the buffer due to thermal gradients and densification, if high enough, could cause cracking of the buffer. Furthermore, high thermal gradients across the buffer ($> \sim 1000 \text{ K/mm}$) can drive thermal diffusion (Soret effect) of fission products across the layer (see Section 3.3.3).

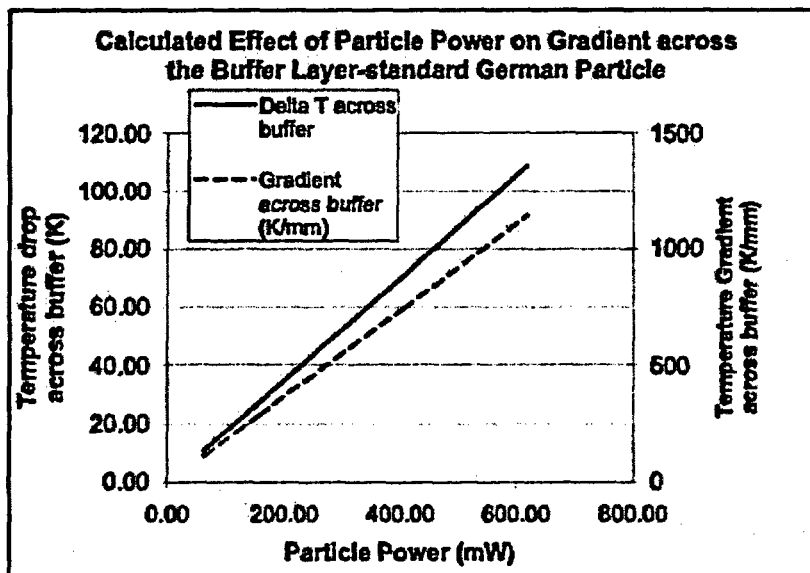


Figure 3-5 Calculated effect of particle power on temperature gradient and temperature drop across the buffer layer of a standard 500-micron UO₂ German particle

Figure 3-6 is a photomontage of different fuel particles irradiated under different power conditions. As shown in the figure, as the irradiation is accelerated the power in the particle is increased and the state of the buffer changes. The German LEU UO_2 particle from AVR shows very little change in the buffer after irradiation probably because of the low power being produced (the exact power history is not well know given the nature of pebble bed refueling). The LEU UCO particle from the HRB-14 irradiation shows a typical cracked buffer. These cracks can provide paths for more rapid fission product transport (see Section 3.3.2). The particle in HRB-15A is an example of more severe cracking of the buffer. The NPR-2 HEU UCO particle was irradiated at an accelerated factor of 10 compared to that expected in an HTGR. There is significant densification of the buffer on one side of the particle as the buffer shrank during the irradiation. (The cause of the excessive shrinkage in the NPR-2 photo is not known with certainty. It is the most accelerated irradiation ever conducted in the U.S. However, there may have been some chemical interactions between the kernel and the buffer that contributed to the final state shown in the micrograph).

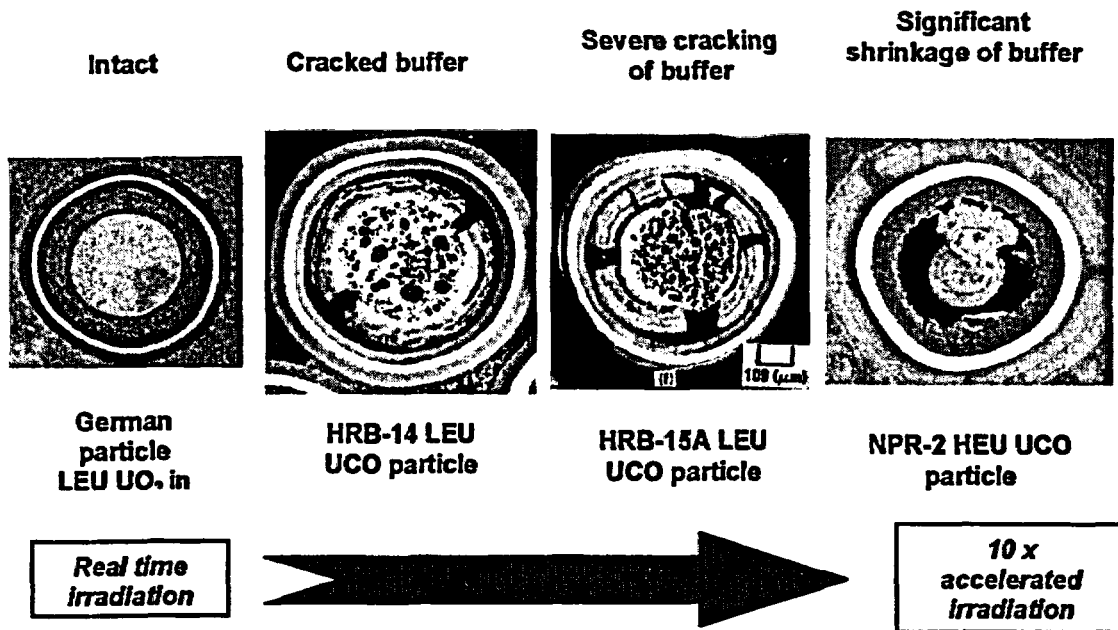







Figure 3-6 Different states of the buffer in coated particles following irradiation in the U.S.

Table 3-2 schematically presents this evolution of the buffer relative to particle power. The table describes possible locations where such powers might be found in a pebble bed reactor, in a prismatic reactor core or in an irradiation test reactor. In addition, the thermal gradient that develops across the buffer of a 500-micron UO_2 kernel has been estimated and some comments about the condition of the buffer are provided. (Note that the thermal gradients for a 350-micron kernel in a prismatic core would be about double that shown here for the same power level because of the smaller kernel size).

Table 3-2 Effects of Particle Power on the Buffer in Coated Particle Fuel

					
Description or location	PBMR low flux region; GT-MHR average	PBMR average	PBMR pebble and prismatic compact peak	Current prismatic irradiation limit	Very accelerated irradiations
Particle Power	25 to 40 mW	60 mW	100 mW	400 mW	500 to 5000 mW
Thermal gradient Across buffer (for 500 micron kernel)	< 50 K/mm	~ 100 K/mm	~ 250 K/mm	~ 750 K/mm	~ 900 to 9000 K/mm
Condition of buffer	Uniform shrinkage		Moderate tensile stress - some cracking	High tensile stress - many cracks	Excessive shrinkage; buffer and fuel side by side

3.3.2. Fission Product Transport in a Porous Medium

A complete description of fission gases and vapor in a porous media requires an understanding of multicomponent gas-phase mass transport. The multicomponent diffusion equation in the Chapman-Enskog [3-7] approximation is given by:

$$\left(\frac{P}{RT}\right)\vec{\nabla}x_i + \left(x_j - \frac{x_j m_j P / RT}{\rho}\right)\vec{\nabla} \ln P = \sum_{j=1}^N \left(\frac{x_i \vec{N}_j - x_j \vec{N}_i}{[D_{ij}]} \right) + \vec{\nabla} \ln T \sum_{j=1}^N \frac{1}{[D_{ij}]} \left(\frac{x_i D_j^{(T)}}{m_j} - \frac{x_j D_i^{(T)}}{m_i} \right)$$

where:

- X_i = mole fraction vapor species i
- $[D_{ij}]$ = first Chapman - Enskog approximation of the binary diffusion coefficient of species
- N_i = molar flux of species i (moles/cm²-g)
- P = total pressure
- R = gas constant
- T = temperature
- m_i = molecular weight of species i
- $D_i^{(T)}$ = thermal diffusion coefficient of species i

This formulation assumes that mass transfer occurs as a result of gradients in chemical composition (i.e., mole fractions), gradients in temperature³ (thermal diffusion or the Soret effect, see also Section 3.3.3) and gradients in pressure. (Note that as written above, the slip correction is not included in the pressure gradient coefficient. This slip correction, which accounts for relative velocity between the molecule and the surface when the characteristic size in the medium is on the order of the mean free path of the gas, has proven to be of some importance in the analysis of mass transport through graphite.) The dependence on pressure gradients can be important for mass transport across the SiC layer and is dominant in situations in which the porous medium has failed structurally and macroscopic cracks are present. The multicomponent diffusion equation, even in the absence of gradients in pressure and temperature, is difficult to solve. It also yields counter-intuitive results such as osmotic diffusion, barrier diffusion, and reverse diffusion [3-8]. These counter-intuitive results have generally been confirmed by experiment.

The solution of the binary form of the diffusion mass transport equation for transport of a vapor *i* in radial gradients in temperature and composition for a spherical shell with inner radius *A* and outer radius *A* + δ yields:

$$\frac{1}{A} \frac{dN_i}{dt} = \frac{PD_{12}(T_b) \Delta T}{RT_b^{1.5}} \frac{(A + \delta)}{2 A \delta} \ln \left(\frac{1 - x_b}{1 - x_s} \right) \frac{1}{[T_b^{1/2} - T_s^{1/2}]} + \frac{3\gamma D_{12}(T_b) P (\Delta T)^2 (A + \delta)}{4R \Delta x T_b^{1.5}} \frac{[x_b^2 - x_s^2]}{A \delta [T_b^{1.5} - T_s^{1.5}]}$$

where the subscript *b* denotes conditions at the outer radius and the subscript *s* denotes conditions at the inner radius. γ is related to the thermal diffusion coefficients of the stagnant and mobile gases by:

$$\gamma = \frac{(RT)^2 \rho D_1^{(T)}}{P^2 m_1 m_2 D_{*12}}$$

When γ is greater than zero, the mobile gas moves toward cooler regions. From the above expression, it is evident that temperature gradients have a more global effect on the mass transport kinetics than just thermal diffusion.

The above development has been in terms of the Chapman-Enskog model because it is usually more familiar. Most investigators [3-9, 3-10] of mass transport through porous media have chosen to use the development by Grad (the so-called '13-moment' method) because it allows the explicit consideration of the porous medium in the so-called 'dusty

³ There are temperature dependencies in this equation, most notably the gas phase binary diffusion coefficients, which typically have a $T^{1.5}$ scaling at the accident temperatures considered here.

gas' approximation developed extensively by Mason and Malinauskas. The isothermal, binary diffusion (ternary if the immobile porous medium is considered) expression in this approximation is:

$$\bar{N}_i = -\frac{P}{RT} D_i(\text{eff}) \bar{\nabla} x_i + x_i \delta_i \bar{N} - x_i \gamma_i \frac{P}{RT} \frac{B_0}{\mu} \bar{\nabla} P$$

where:

$$\frac{1}{D_i(\text{eff})} = \frac{1}{D_i(\text{Kn})} + \frac{1}{D_y(\text{eff})}$$

$$\delta_i = \frac{D_i(\text{eff})}{D_y(\text{eff})}$$

$$\gamma_i = \frac{D_i(\text{eff})}{D_i(\text{Kn})}$$

$$\frac{1}{D(\text{Kn})} = \frac{x_i}{D_i(\text{Kn})} + \frac{x_j}{D_j(\text{Kn})}$$

$$D_i(\text{Kn}) = \frac{4}{3} K_0 \sqrt{8RT / \pi n_i}$$

$$D_y(\text{eff}) = \frac{\epsilon}{\tau} D_{*ij}$$

ϵ = porosity of the material

τ = tortuosity of pore network

Note that in some cases, it has been found necessary to introduce a slip correction for the coefficient of the pressure gradient term:

$$\frac{B_0}{\mu} + \frac{4}{3} K_0 \frac{\bar{v}}{P}$$

where \bar{v} is the mean molecular velocity.

The parameters in the equation are B_0 , the Poiseuille parameter, and the Knudsen parameter, K_0 . These parameters are properties of the porous material. An accurate evaluation of these parameters would require characterization of the material, which could be very difficult in the case of materials in coated particle fuel, or there would need to be some model of the material. For graphite, the following correlation has been established [3-11].

$$\log_{10} B_0 = -2.6891 + 1.2983 \log_{10} K_0$$

Given the large interconnected porosity in the buffer, the transport of gases in a porous medium (to describe the behavior of fission gases and vapors in the layer) has been examined. Pressure driven diffusion has been studied in porous mediums. References [3-12] and [3-13] provide a comprehensive overview of the subject. In all cases, the molar flux of material through the porous medium is a function of the pressure gradient

across the material. Three different regimes are traditionally considered depending on the mean free path of the gas relative to the characteristic size in the medium, or the Knudsen number ($Kn = \lambda/d_{pore}$, where λ is the mean free path). Characteristic sizes could range from nanopores in a material like an as fabricated buffer to microcracks as might be typical of a cracked buffer.

For $Kn > 1$, the mass transport behavior can be described using free molecular flow and the molar flux, given by:

$$\dot{N}_{Kn} = -\frac{D_{Kn}}{RT} \frac{\epsilon_p}{\tau_{p,Kn}} \nabla p$$

$$D_{Kn} = (4/3) \bar{d}_{pore} \sqrt{RT/2\pi M}$$

where:

- D_{Kn} = the Knudsen diffusivity,
- \bar{d}_{pore} = the average pore size in the medium,
- ϵ_p = the porosity of the medium
- $\tau_{p,Kn}$ = the tortuosity
- M = the molecular weight of the gas
- R = gas constant
- T = absolute temperature.

In the transition region, $0.01 < Kn < 1$, both viscous flow and diffusive flow are considered. They can be summed to determine the overall molar flux. Hence:

$$\dot{N} = \dot{N}_{vis} + \dot{N}_{diff}$$

$$\dot{N}_{diff} = -\frac{D_{eff}}{RT} \frac{\epsilon_p}{\tau_{p,Kn}} \nabla p$$

$$D_{eff} = \left[\frac{1}{D_{Kn}} + \frac{1}{D_{12, gas}} \right]^{-1}$$

$$D_{Kn} = (4/3) \bar{d}_{pore} \sqrt{RT/2\pi M}$$

$$D_{12, gas} = \text{Chapman - Enskog - Theory}$$

$$\dot{N}_{vis} = -\frac{k \bar{p}}{\eta RT} \nabla p$$

The diffusive flux has the same form as in the free molecular flow regime but the diffusivity is an effective diffusivity. The effective diffusivity considers the effects of

Knudsen flow and traditional gas phase mass transport as given by Chapman-Enskog Theory [3-7] in series. The viscous diffusion term depends on the pressure gradient as well as the viscosity of the gas, η , the average pressure of the system, p , and the "apparent" permeability of the material, k .

In the continuum region, where $Kn < 0.01$, the contribution from viscous flow and diffusive flow are summed to determine the overall molar flux. However, in this region, molecular flow effects are very small and the diffusive term takes on traditional form with the diffusivity equal to the traditional gas-phase mass transport value as given by Chapman-Enskog Theory. Thus:

$$\dot{N} = \dot{N}_{vis} + \dot{N}_{diff}$$

$$\dot{N}_{diff} = -\frac{D_{12, gas}}{RT} \frac{\epsilon_p}{\tau_{p, Diff}} \nabla p$$

Scoping calculations for pressure driven diffusion using simple assumptions to understand the magnitude of some of the factors involved these have been performed. These equations have been used to estimate effective diffusivities as a function of pore or crack size. Kr gas at 1000° and 1600°C and pressures in the range of 0.5 MPa to 25 MPa, have been used to represent particle conditions representative of normal operation and accidents. Figure 3-7 then plots the effective diffusivities at 1000 and 1600°C respectively. The results suggest that gas pressure would only be important for characteristic sizes greater than ~ 0.02 microns. Furthermore, a comparison of the two figures suggests that the influence of temperature is moderate. The most important effect is that of the characteristic size of the transport path in the medium. For nanopores, effective diffusivities are on the order of 3 to $53 \times 10^{-7} \text{ m}^2/\text{s}$. By contrast, transport through micropores or micron sized cracks is much faster, with effective diffusivities ranging between 10^{-4} and $10^{-2} \text{ m}^2/\text{s}$ depending on the pressure of the gas involved. By way of comparison, the Germans assumed the diffusivity of all species in the buffer was $10^{-8} \text{ m}^2/\text{s}$ and the US used a value of $10^{-10} \text{ m}^2/\text{s}$ in their evaluations.

Although the actual pore size in the buffer is not well known, these results suggest that rapid transport of fission gases and fission product vapors could be expected through the buffer layer in a coated particle.

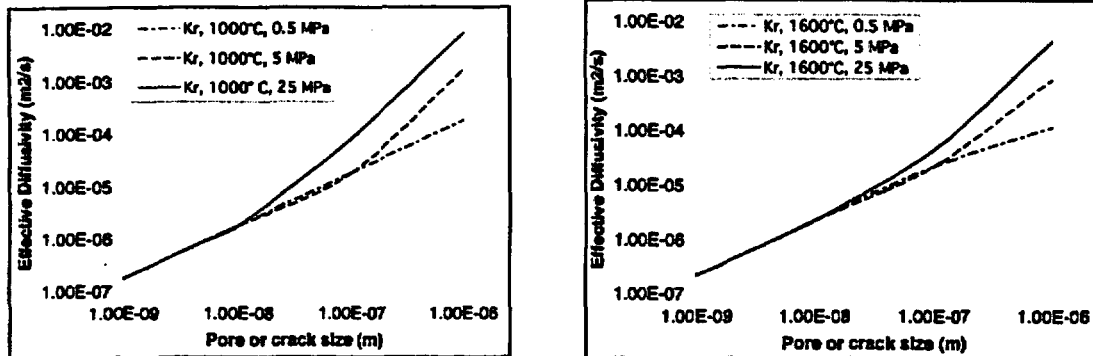


Figure 3-7 Calculated effective diffusivities for Knudsen and viscous diffusion

For these equations, the vapor species transport properties such as binary diffusion coefficients, viscosity and thermal conductivity would be needed for detailed analysis of fission product transport by gas phase mass transport. Very seldom are the properties of gaseous species measured. The transport properties of very high temperature gaseous species also have not been measured. These properties are typically calculated using formulae developed for example either by Chapman and Enskog or the formulae derived by Grad [3-9, 3-10]. In general, these formulae are not strictly applicable to the species of radiological importance because of assumptions related to the nature of collisions among the molecules. Calculations of collision integrals must consider inelastic collisions among the molecules. To do the collision calculations, it is necessary to have some information on the energy potential involved in the interactions of species such as a Lennard-Jones potential or a Sutherland potential. At the very high temperatures associated with coated particle fuel, one approach might be to assume that the vapor species all behave as hard spheres undergoing somewhat inelastic collisions.

For gas phase, mass transport scoping calculations, a formulation involving one gas and estimating the properties of the porous material may be utilized in the evaluation. Accurate modeling would require detailed information about the level of connected porosity and the tortuosity of the material (which can be determined by measurement) as well as an assumption about the nature of the porous material. Three common analytic models for porous materials are found in the literature for transport in graphite and catalysis.

In the parallel straight-channel model, the porous material is assumed to consist of parallel channels of diameter d_c . Then,

$$\frac{\varepsilon}{\tau} = E$$

$$K_0 = \frac{Ed_e}{4}$$

$$B_0 = \frac{Ed_e^2}{32}$$

For the parallel, tortuous channel model, [3-14] the model is the same as that above, except the channels are not straight:

$$B_0 = \frac{\pi d_e^2}{40\tau}$$

$$K_0 = \frac{3\pi \pi d_e}{64 \tau}$$

In the random channel or 'dusty gas' model, the porous solid is assumed to be composed of spherical grains of radius r_g with n_d grains per unit volume:

$$\frac{1}{K_0} = \frac{128 n_d \tau}{9 \varepsilon} r_g^2 (1 + \pi/8)$$

The dusty gas and the tortuous channel models have been applied to graphite. In graphites, it is often found that there is a high degree of correlation between the Knudsen parameter and the Poiseuille parameter. Other models exist in the literature that account for the presence of distributions of voids and channel sizes in the porous materials. Within the catalysis literature, multiple populations of channels with distributions of sizes are considered. To use any of these models completely to calculate the molar flux, the porosity and tortuosity of the buffer need to be known or estimated. Such information has not historically been measured for HTGR fuel particles. Accordingly, the application of these models at this time to coated particle fuel would be limited to scoping calculations.

3.3.3. Thermal Diffusion

The large thermal gradients in the buffer discussed in Section 3.3, can lead to thermal diffusion, which must be added to the traditional concentration gradient driven Fickian diffusion across the layer. The combined diffusive flux for one species can then be written as:

$$J = -D(\nabla C + \frac{C Q^*}{RT^2} \nabla T)$$

where:

D = diffusion coefficient

Q* = heat of transport

T = temperature

J = diffusive flux

C = concentration

The second term on the right hand side of the equation is the thermal diffusion component, or Soret effect. Most of the literature dealing with thermal diffusion (the Soret effect) relates to gases or liquids. There are a few references dealing with solids. The heats of transport, Q^* , for the buffer and condensable fission products combinations are unknown. However, the values of Q^* range from about -210 kJ/mol to $+50$ kJ/mol for various material combinations in the literature [3-15, 3-16, 3-17]. This corresponds to values of Q^*/R from $-25,000$ K to $+6,000$ K. A value of $+20,000$ K can be considered to determine an upper bound for fission product transport through the buffer layer in the presence of a temperature gradient.

The influence of irradiation and thermal gradient on the release of fission products from an intact particle may be scoped out by modeling the kernel and each layer of the coated fuel particle using a one-dimensional diffusional transport code [3-18]. Based on the power per particle and the irradiation temperature, the temperature of each material constituent in the coated particle could be calculated. Based on the power level and time (burnup), the fission product generation can be calculated. Using the diffusivities of cesium in the kernel and layers in the TRISO coating from the German experience [3-5], a diffusivity of 10^{-7} m²/s in the buffer layer and a value of Q^*/R of 20000 K, a calculation of the transport of fission products from the kernel and into the coatings under a specified irradiation history and a subsequent 500 hour isothermal heating at 1600°C may be used to simulate a traditional German accident heating test.

Figure 3-8 summarizes the result of these calculations. Plotted is the fraction of cesium in the OPyC layer at the end of the irradiation and the fraction of cesium released from the particle at both the end of irradiation and the end of the 500-hour high temperature heating for different particle powers. Two different irradiation conditions are considered: a three year constant irradiation at 1225°C and a 10-cycle 3-year pebble bed irradiation where the fuel experiences a change in temperature from 600 to 1200°C ten times over its three year life, as illustrated in Figure 3-4.

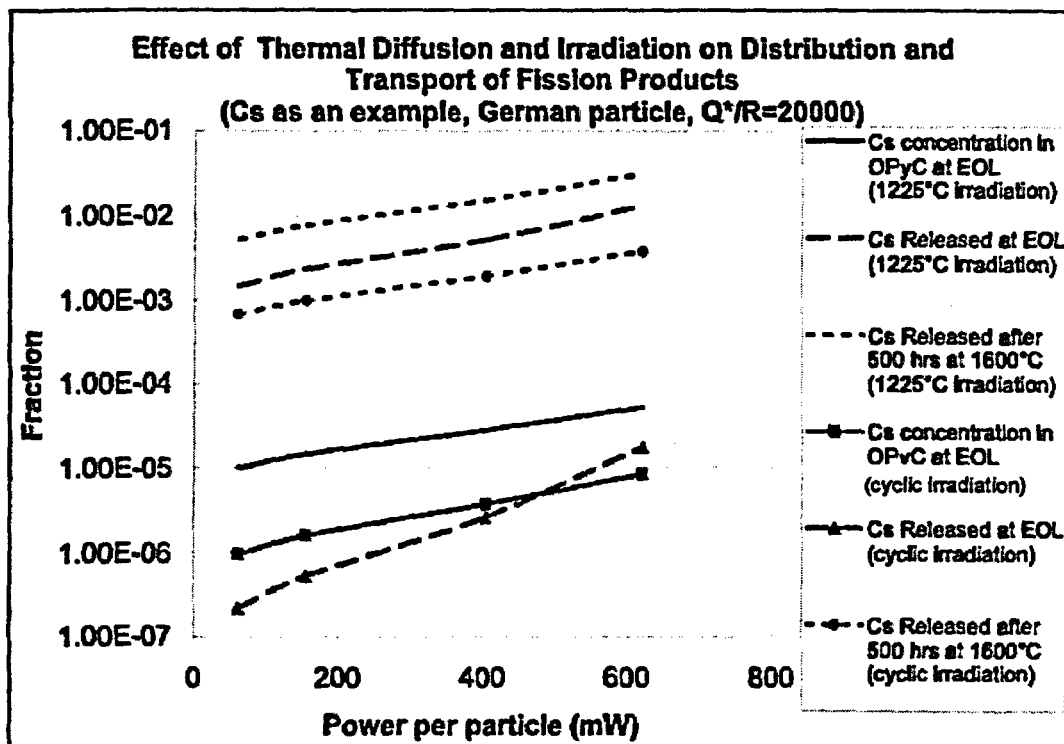


Figure 3-8 Calculated effect of thermal diffusion and irradiation on the distribution and transport of fission products in the coated particle

The calculated results would indicate that the cyclic irradiation has a strong influence on the distribution and transport of fission product cesium. The analysis indicates an order of magnitude more cesium reaching the OPyC layer in the case of the 3-year constant irradiation at 1225°C than in the case of cyclic irradiation, and three to four orders of magnitude more cesium released from the particle at the end of irradiation in the case of constant irradiation at 1225°C than in the case of cyclic irradiation. After the 500-hour high temperature heating, the cesium release from the particle is an order of magnitude greater in the case of constant irradiation at 1225°C than in the case of cyclic irradiation. These results would indicate that the irradiation history has an effect on the concentration of fission products in the layer and the subsequent release from the particle.

The analytical results also indicate that thermal diffusion (Soret effect) can have a moderate influence on the transport and distribution of fission products. A factor of ten increase in power per particle (from 60 mW to 600 mW) would increase the concentration of cesium in the OPyC and the fraction of cesium released after irradiation and after high temperature heating by factors of 5 to 10.

These results indicate the important role of irradiation history on both the distribution of fission products in the coated particle and their release under normal operation and potential accident conditions. Irradiation has a large impact on the fission product

behavior in the accident because of the effects of the initial distribution of fission products in the particle. However, for low power/thermal gradients in German pebbles (and the low level of acceleration in most German irradiations [3-19]), thermal diffusion would be expected to be much less important in (modeling of) fission product release. In cases where the irradiations are of very high power (such as the very accelerated US fuel irradiations that have occurred in U.S. fuel irradiates in the past) thermal diffusion would be expected to be important. However, when the full multicomponent nature of the problem and the effects of pressure diffusion and thermal diffusion are considered together, the results may show a greater effect of thermal diffusion than the simpler calculations presented here.

3.4 The Inner and Outer Pyrocarbon Layers

The inner and outer pyrocarbon layers are dense layered carbon structures. The goal during fabrication is to make the pyrocarbon as isotropic as possible during the deposition to ensure the best radiation stability of the layer, which is needed for particle integrity.

Some data exist on effective diffusivities in the PyC layers. Measured values from BISO particles (without SiC) have been collected and the results shown in Figure 3-9. [5] These data suggest that a dense, intact pyrocarbon layer is a very good barrier to noble gas release with significant diffusional releases not observed until temperatures near 2000°C are reached. The PyC layers do not provide significant barriers to release of cesium, silver and strontium metallic fission products under normal or accident conditions.

The mechanism responsible for the transport of gaseous and metallic fission products in the PyC layer has not been the subject of significant worldwide study. An understanding of the mechanism responsible for noble gas transport in PyC is limited. A comparison of different measurements and calculations are overlaid on the original diffusivity data in Figure 3-10.

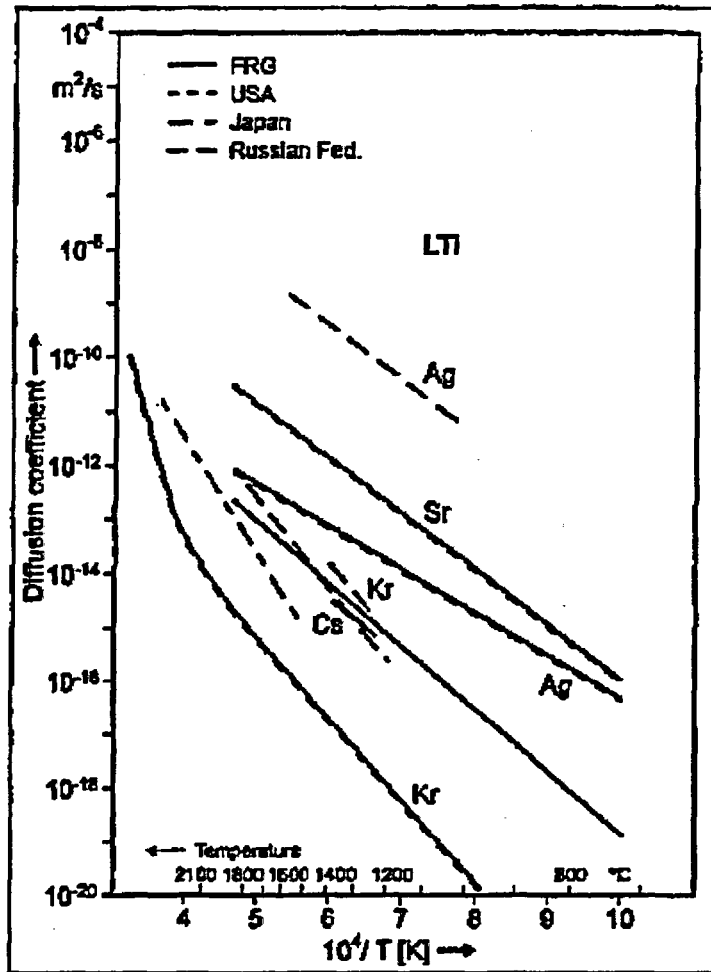


Figure 3-9 Measured fission product diffusivities in low temperature isotopic (LTI) PyC

3.4.1. Gas Phase Fission Product Transport

The measured diffusion coefficients suggest very slow transport through the inner PyC layer. Permeability measurements using He and CO [3-20] indicated in Figure 3-10, suggest very slow transport of these gases consistent with the measured fission product diffusivity. By contrast, diffusion predicted by the Knudsen diffusion model in Section 3.2.3 for nano-porosity or viscous diffusion for micro-porosity if applied to the PyC layer would predict transport rates that are 6 to 10 orders of magnitude faster than the measured data on BISO particles. These results may suggest either (a) Knudsen diffusion of noble gases is extremely small in PyC perhaps because the interconnected porosity is very low or (b) that Knudsen diffusion is not the mechanism responsible for noble gas transport in PyC.

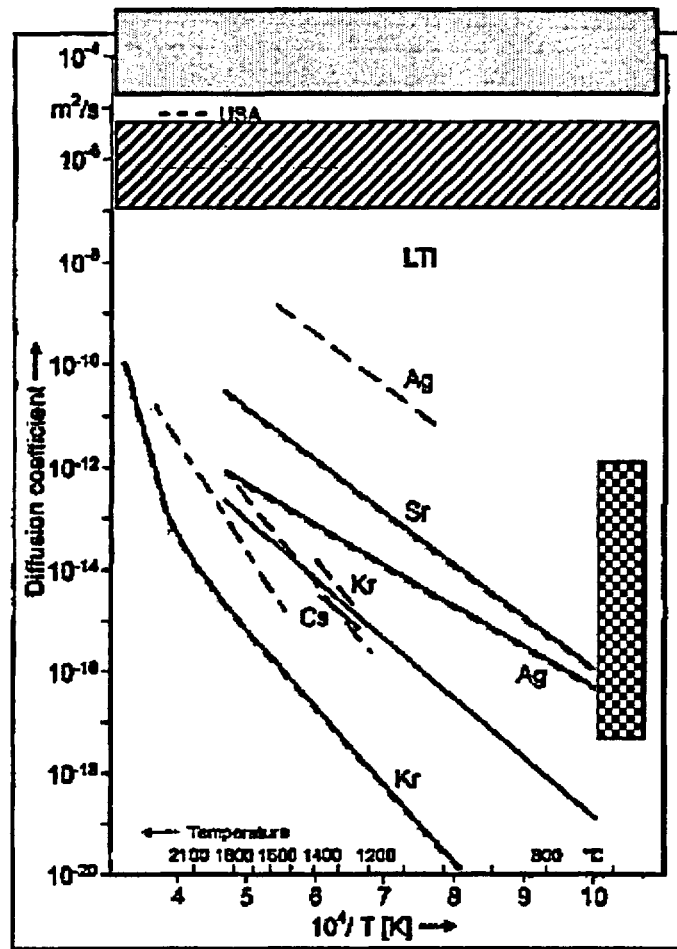


Figure 3-10 Comparison of measured fission product diffusivities in PyC to permeability data, (checkerboard box) Knudsen data, (black and white hatched box) and viscous (gray box) diffusion estimates

3.4.2. Metallic Fission Product Transport and Trapping

For some of the fission metals like cesium and strontium and even iodine, [3-21, 3-22, 3-23, 3-24] transport behavior in intercalated graphite may be important. Intercalation, the insertion of guest atoms into a host structure, has been studied extensively and a diffusion and trapping mechanism has been proposed as the mechanism responsible for the resultant transport behavior in the material [3-25]. Thus, intercalation may be the mechanism responsible for the transport of Cs, Sr and perhaps even iodine and CO in the PyC. A classic diffusion and trapping model has been proposed for modeling the transport, with trapping occurring perhaps at the carbon crystallite edges and defects in the graphitic material. (Trapping is the capture of atoms at the atomic level by physical defects or chemical interaction that impedes transport.)

Diffusion and trapping can be modeled using a simple modification to classical Fickian diffusion as shown in the following equations. [3-18]

$$\begin{aligned}\frac{\partial C}{\partial t} &= D\nabla^2 C - \frac{\partial C_T}{\partial t} \\ \frac{\partial C_T}{\partial t} &= w \frac{x_T}{N} C - r C_T \\ x_T &= x_T^0 - C_T\end{aligned}$$

Trapping impedes diffusion. Many times a concentration dependence of diffusivity is observed, which is an indication that trapping is involved. As the traps get filled at high atom concentrations in the material, the observed transport increases. Thus, one can also write an expression for an apparent diffusivity as follows [3-26]:

$$D_{app} = \frac{D}{\left(1 + \frac{w x_T}{r N}\right)} = \frac{D}{\left(1 + \frac{D_0}{\lambda^2 \nu_0} \exp\left(\frac{E_{trap} - E_{diff}}{kT}\right) \frac{x_T}{N}\right)}$$

Where:

- D_{app} = apparent diffusivity (m^2/s)
- D_0 = pre-exponential of diffusivity (m^2/s)
- D = diffusivity (m^2/s)
- w = trapping rate(/s)
- r = resolution or release rate from the trap(/s)
- λ = jump distance (m)
- ν_0 = Debye frequency (/s)
- x_T = empty trap density (atoms/ m^3)
- E_{trap} = trap energy (ev)
- E_{diff} = diffusion constant activation energy (ev)
- N = number density of host material (atoms/ m^3)

An initial concentration of empty traps is assumed to exist in the material and a mass balance on the traps is performed to determine when all of the trapping sites are occupied. To model the behavior in detail, the trap concentration or trap density is required as well as the energy of the trap, which is important to model release from the traps accurately. Irradiation is known to result in the production of traps via defect formation and thus can increase the complexity of the analysis model.

A few simple parametric and sensitivity calculations can be used to understand the magnitude and importance of trapping in PyC layers of TRISO-coated particle fuel. Figure 3-11 plots the diffusion coefficient of Cs in PyC⁴ and SiC along with the apparent Cs diffusion coefficient in PyC for different trap concentration levels from 10 to 5000 ppm using the measured 4 ev trap energy for graphite.

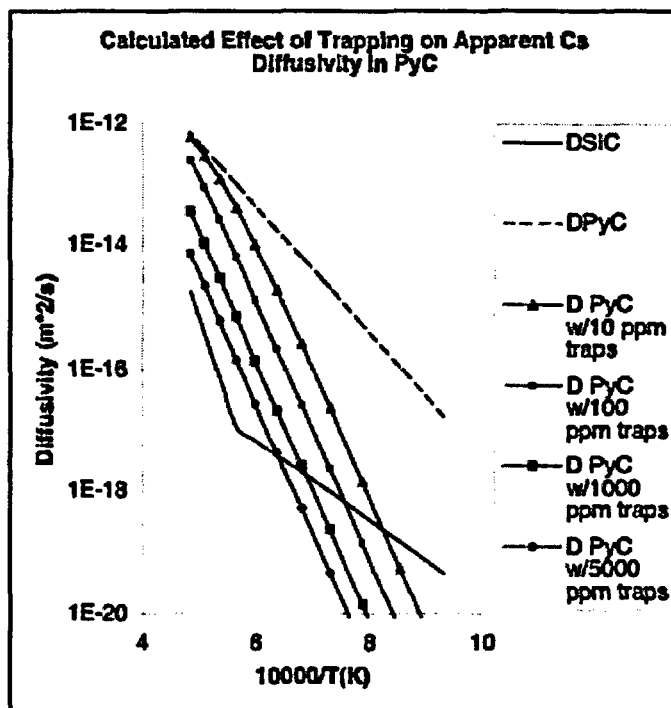


Figure 3-11 Calculated effects of trapping on apparent Cs diffusivity in PyC

The transport through the TRISO coating will then be controlled by the lowest diffusivity in the figure. Under accident conditions, the SiC diffusivity is the lowest suggesting it is the greatest barrier to cesium release. Under normal operating temperature (800-1200°C), trapping can lower the apparent diffusion coefficient in PyC significantly. A comparison of the apparent diffusivities in the PyC with that of PyC with no traps suggests that the apparent diffusion coefficient can be four to five orders of magnitude lower than the intrinsic diffusivity depending on the trap concentration. At the higher temperatures, the release rate from the traps is so large that the effects of trapping is diminished somewhat.

Diffusion and trapping are dynamic factors. As atoms diffuse through the layer, a certain fraction is trapped. As these traps are filled, the apparent diffusivity increases. The

⁴ Existing German data were measured on BISO particles. Concentrations are probably high enough that trapping effects were small and thus the measured diffusion coefficients are representative of transport without trapping.

magnitude of the intrinsic diffusion coefficient in PyC (i.e., without traps is high enough that significant diffusion of cesium into the PyC is expected during normal operation. The Cs concentration in IPyC is expected to be much greater than the trap density, perhaps at the level of 0.5 to 1% atom concentration, so the traps would fill quickly and not in and of itself affect overall transport behavior. In a heat-up event, in which SiC layer might fail, release of Cs inventory from the IPC layer will not be influenced significantly by trapping. Thus, it may be concluded that trapping is not an important effect in the transport behavior in the IPyC layer. However, in the OPyC layer, the Cs concentration in OPyC is much smaller, on the order of the trap concentration expected in graphite. Thus, in the OPyC layer the traps can effectively compete for these Cs atoms, which could result in a much slower transport.

Similar analysis for Sr suggests that given the very low release of Sr from the kernel during operation, the Sr concentration in the IPyC would be at the high end of the trap concentration and thus may not be influenced by trapping. In the OPyC, the Sr concentration is much smaller and trapping effects could be very important.

3.4.3. Influence of PyC Structure on Transport in the Layer

Pyrocarbon has a complex structure made up of different "growth features", the shapes of which can vary depending on the deposition conditions, specifically coating temperature and coating gas composition. Three different types of growth features have been observed: (a) a three dimensional mosaic of tightly packed crystallites with little porosity between the crystallites, (b) small crystallites arranged in the form of long twisted ribbon or fibers which contains a considerable amount of porosity and (c) large crystallites that are layered. Fission product transport at the microscopic level in this layer (intercalation and trapping at the edge of the crystallites for example) depends on the nature of these three types of growth features. A complete understanding of the relationship between structure and transport is lacking. The differences in measured effective diffusion coefficients in the U.S., Germany, Russia and Japan, as shown in Figure 3-9 may reflect differences in the structure of the PyC which may be related to differences in the relative amounts of the different growth features because of differences in PyC coating conditions. Thus, for manufactured TRISO fuel, it is important to establish that the transport-structure relationship implicit in the data in Figure 3-9 is also valid for the newly produced fuel, if the PyC diffusivities shown in the figure are to be used in a fission product transport analysis. This might be accomplished by (a) demonstrating that the PyC produced in the new fuel was fabricated under coating conditions that are the same as that used in the past and has similar structure to that in the literature, and (b) demonstrating by experiment that fission product transport is similar to that measured previously by others. Significant deviations from the historic transport-structure relationship could indicate that the historic experimental database on fission product transport for TRISO-coated particle fuel might not be applicable to the new fuel that is produced.

3.5 The SiC Layer

SiC in TRISO-coated particle, fuel is a high-density polycrystalline beta-SiC. It is the major fission product barrier in the fuel. As with the pyrocarbon layers, data on the effective diffusion coefficients of noble gases, cesium, strontium and silver have been inferred from integral release measurements [3-5]. Figure 3-12 plots the effective diffusion coefficient for noble gases, cesium, strontium and silver.

3.5.1. Transport Mechanisms

The mechanisms responsible for the transport of gaseous and metallic fission products in the SiC layer have not been the subject of significant study worldwide. An understanding of the mechanism(s) responsible for fission product transport in SiC is limited. A Knudsen diffusion mechanism could be postulated for the transport of noble gases and Ag vapor through the SiC layer especially under normal operating conditions. The interconnected porosity of the SiC layer is expected to be quite small because the beta-SiC is very high density (3.21 to 3.23 g/cc is commonly fabricated). Research is being conducted to understand Ag transport through SiC [3-27]. Under accident conditions, bulk diffusion may play an increasing role in the transport.

For the other metallic fission products, a mixture of grain boundary and bulk diffusion has been postulated depending on temperature, with grain boundary diffusion most likely at low temperatures (e.g., <1000°C) and bulk diffusion at high temperatures (e.g., 1400-1800°C) representative of accidents. The magnitudes of the activation energies in Figure 3-12 tend to support this theory. A comparison of the effective diffusion coefficients for fission gases, Cs, Sr and Ag in SiC with more recent measurements on other species in SiC can be used to infer the potential underlying mechanisms. Figure 3-13 overlays the original data with self-diffusion data for C and Si in SiC (hatched box) and grain boundary diffusivities for Fe, Cr (gray box) [3-28, 3-29]. The magnitude and slopes of the grain boundary diffusivities for Fe and Cr are similar to that for Cs and Sr perhaps suggesting that grain boundary diffusion may be the dominant mechanisms for Cs and Sr transport through SiC. The slope of the C and Si diffusion coefficients are similar to that for Xe at high temperature suggesting that a vacancy mechanism may describe noble gas transport in SiC.

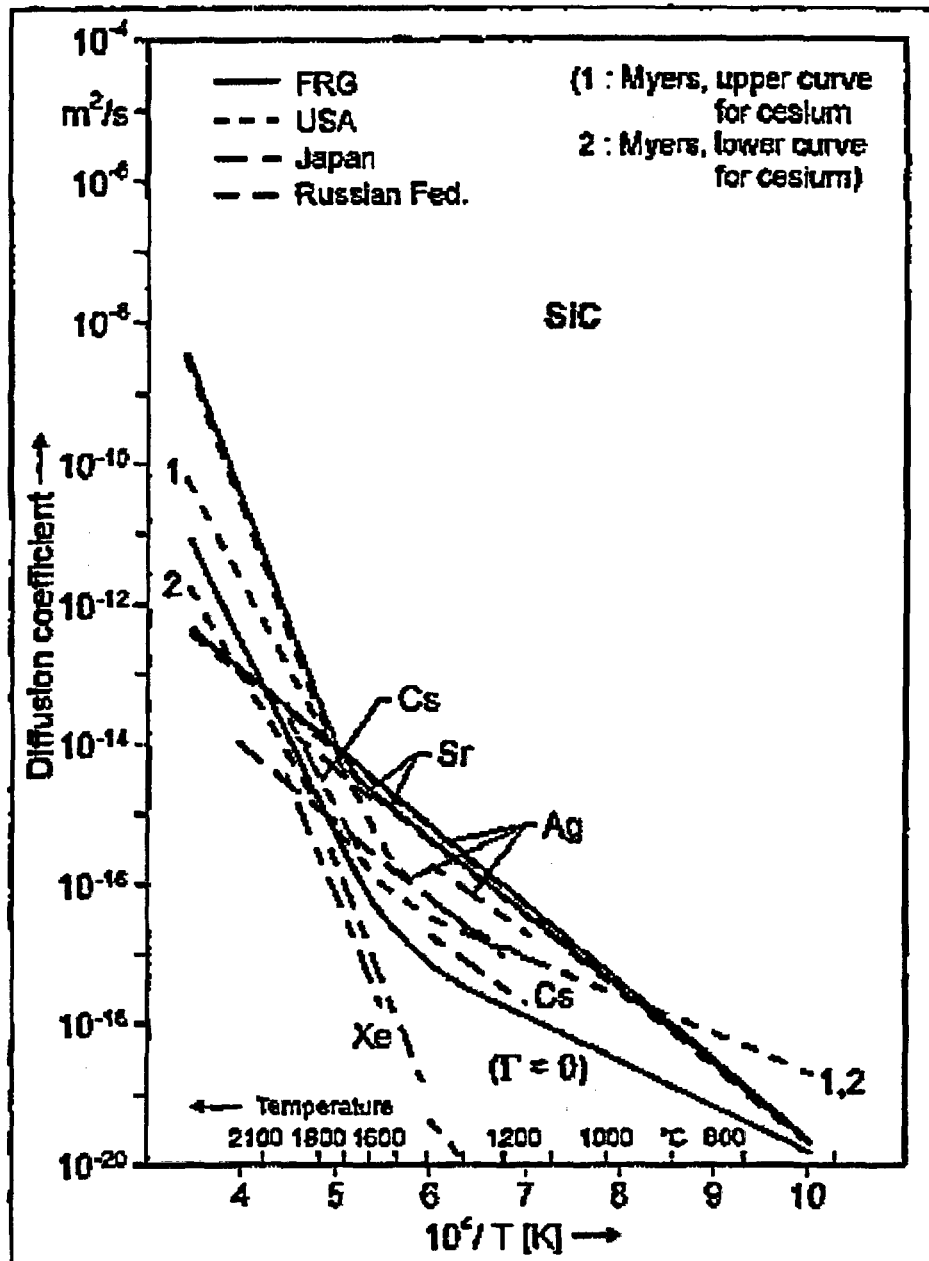


Figure 3-12 Measured diffusion coefficients of Xe, Cs, Sr and Ag in SiC

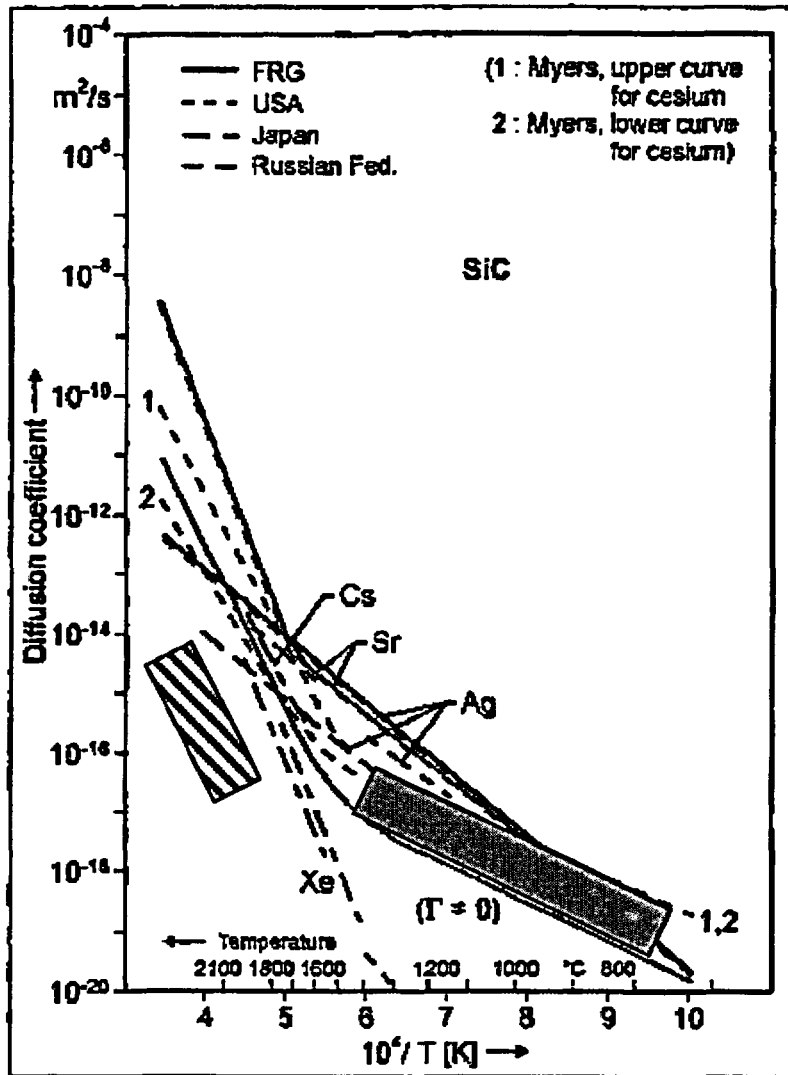


Figure 3-13 Comparison of data for C and Si self-diffusion coefficient (hatched box) and Fe and Cr grain boundary diffusivities (gray box) with fission product diffusivities inferred from integral release measurements on coated particles

3.5.2. Grain Boundary Diffusion

Grain boundary and bulk diffusion may be important in describing fission product transport in coated particle fuel. The importance of each mechanism depends on the temperature, the individual diffusivities in the bulk and along the grain boundaries, and the area fraction occupied by grains and boundaries. Grain boundary diffusion has been studied extensively. It can act as a fast diffusion channel in polycrystalline materials.

Fast diffusion sometimes manifests itself as a very high pre-exponential factor, D_0 , in the measured diffusion coefficients. The classic Arrhenius formalism suggests that D_0 should be on the order of the product of the Debye frequency and the square of the lattice spacing for atomic diffusion. (For many materials this is $\sim 10^{-3} \text{ m}^2/\text{s}$). However, experimental values can be 10^7 greater than this value [3-30] and may be related to the presence of grain boundaries, defects and surface effects. The influence of grain boundaries has been studied extensively and three different kinetic regimes have been found: Type A, B and C [3-31]. Figure 3-14 sets up the analytic picture of a grain boundary of thickness, δ . The grains are of width d and a uniform concentration of the fission product, C_0 , exists across the grains and grain boundary. A segregation coefficient, s , describes the ratio of the concentration in the grain and in the boundary at the surface interface. Solutions are then sought to the classic Fickian diffusion equations in two dimensions in both the grain, denoted by subscript v in the figure, and the grain boundary, denoted by subscript gb , in the figure.

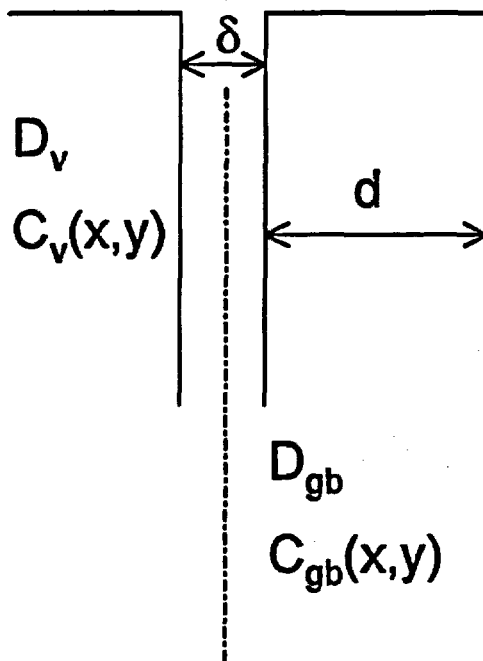


Figure 3-14 Schematic of grains and grain boundary

In Type A grain boundary diffusion, the penetration distance into the grain is much greater than the grain boundary thickness. In this case, both grain boundary and bulk diffusion are operative as would be the case for high temperatures and long heating times as is the case in safety testing of fuel particles. In this case, an effective diffusion coefficient is measured which is a volume weighted average of the bulk and grain boundary diffusion coefficient. The concentration profile is given by a classic complementary error function using the effective diffusivity. For Type A kinetics, these conditions are summarized below.

$$\begin{aligned}
(D_v t)^{1/2} &\gg d \\
c_b &= s c_v \\
D_{eff} &= f D_v + (1-f) D_{gb} \\
\bar{c} &= \operatorname{erfc}\left(\frac{y}{2\sqrt{D_{eff} t}}\right)
\end{aligned}$$

In Type B kinetics, there is much greater penetration along the boundary than into the grains. In this case, what is actually measured is an apparent diffusion coefficient sometimes denoted as P_{gb} , which is the product ($s \delta \square D_{gb}$). This regime may be applicable at high irradiation temperatures. The analytic conditions for Type B kinetics and the resultant solution to the diffusion equations are given by:

$$\begin{aligned}
s\delta &\ll (D_v t)^{1/2} \ll d \\
P_{gb} &= s\delta D_{gb} = 1.322 \sqrt{\frac{D}{t}} \left(-\frac{\partial \ln \bar{c}}{\partial z^{6/5}}\right)^{-5/3}
\end{aligned}$$

where the partial derivative term is the measured concentration profile in the sample.

In Type C kinetics, bulk diffusion is “frozen out” and the transport is dominated by grain boundary diffusion $[(D_v t)^{1/2} \ll s\delta]$. This is probably applicable at very low temperatures, conditions that may be representative of average irradiation temperature experiments. In this case, the concentration is given by a Gaussian for a point source and an error function for constant source with the effective diffusivity equal to the grain boundary diffusivity, D_{gb} .

These idealized situations are useful to understand the concepts of grain boundary and bulk diffusion in polycrystalline material. However, in practice the microstructure of the material is more complex. The application of mixed grain boundary and bulk diffusion in SiC would require development of appropriate mixture rules to establish an effective diffusivity through the structure. This is an area of active research [3-32]. Figure 3-15 compares three different idealized microstructures that may bound that expected in SiC as oriented relative to the SiC layer thickness. The large radially oriented columnar structure, which is found in some SiC, is idealized in the left portion of the figure. In this idealized case, the volume weighted mixture rule for the effective diffusivity would appear to be appropriate. At the other extreme is the case of SiC with an idealized circumferentially oriented laminar structure. In this case, a reciprocal series approach to establishing the effective diffusivity may be appropriate. In the middle of the figure is an idealized schematic representation of small-grained SiC, which is the form most sought

after in coated particle fuel. In this case, there is no exact mixture rule to use, but the two extreme cases would appear to bound the actual behavior.

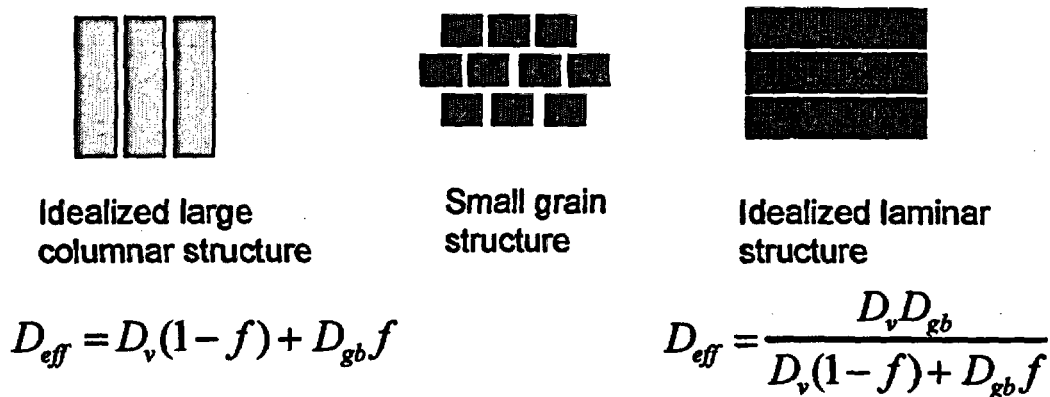


Figure 3-15 Influence of microstructure on apparent diffusivity

3.5.3. Influence of SiC Microstructure on Fission Product Transport

The previous section presented the concept that fission product transport in the SiC in temperature range of interest could be a mixture of bulk and grain boundary diffusion. Grain boundary diffusion is very sensitive to the microstructure of the material (e.g., grain size, fraction of the area occupied by grain boundaries, width of grain boundaries, segregation effects at the grain/grain boundary interface) and as noted earlier large differences in diffusivities have been noted in the literature and attributed to characteristics of the microstructure as well as defects and surface effects. Furthermore, there are little data on individual diffusivities of the important fission products in both single crystals and in polycrystalline material that are needed in these models. In the absence of such data, SiC effective diffusivities have been utilized and have been inferred from fuel element integral release measurements.

There is also a limited understanding of the linkage between transport, microstructure and deposition conditions for SiC. Although most historical work on SiC has focused on optimizing deposition conditions to produce small-grained SiC, the literature is full of examples where changes in deposition conditions, especially coating temperature, can result in large, radial, columnar structures at higher temperatures and laminar structures at lower temperature. At coating temperatures below 1450°C, some alpha-SiC and/or excess silicon is obtained. The structure is striated with no evidence of individual grains. Smaller, fine-grained SiC is obtained using a coating temperature between 1500 and 1550°C. Above 1600°C, large, radial, columnar grains of SiC are obtained, with the crystallite size increasing with increasing temperature. [3-33, 3-34, 3-35] These results suggest that as in the case of pyrocarbon, any new fuel that is produced which would seek to reference the transport behavior shown in Figure 3-12 would have to establish that the transport-structure relationship implicit in the data in Figure 3-12 is also valid for the newly produced fuel. This might be accomplished by (a) demonstrating that the SiC

produced in the new fuel was fabricated under coating conditions that are the same as that used in the past and has similar microstructure (e.g., small grained SiC), and (b) demonstrating by experiment that fission product transport is similar to that measured previously by others. Significant deviations from the historic transport-structure relationship indicate that the historic experimental database on fission product transport for TRISO-coated particle fuel might not be applicable to the new fuel that is produced.

3.6 A Simplified Integral Fission Product Transport Model

In the previous sections, the transport mechanisms in each layer have been reviewed. In this section, a simplified integral model is developed for release from TRISO-coated particle fuel using some of the ideas and data in the previous sections. Some preliminary calculations using the model are also presented.

Morgan and Malinauskas [3-36] developed an analytic solution for depletion of a fission product through a single coating layer given by:

$$FR = 1 - \frac{Ka}{b} \sum_{n=1}^{\infty} \frac{\exp(-D^* t \alpha_n^2 / \delta^2) \sin(\alpha_n)}{[2K\alpha_n + (4b\alpha_n / \delta) \sin^2 \alpha_n] + K \sin(2\alpha_n)}$$

where

$$\cot(\alpha_n) = (b\alpha_n / K\delta) - (\delta / b\alpha_n)$$

$$K = (A/V)s$$

a = the inner radius of the coating,

b = the outer radius of the coating,

A = the surface area of the inside of the coating,

V = the volume inside the coating, and

S = segregation factor (ratio of surface layer concentration to source concentration).

If the TRISO coating is considered a composite layer then the simple resistance concept to model can be used for all three layers as one layer and write the apparent diffusivity D^* as

$$\frac{\delta}{D^*} = \frac{\delta_{IPYC}}{D_{IPYC}^{eff}} + \frac{\delta_{SiC}}{D_{SiC}^{eff}} + \frac{\delta_{OPYC}}{D_{OPYC}^{eff}}$$

Where δ is the total thickness of the three high density TRISO coatings.

This simple model uses effective diffusivities for each layer and can account for trapping if needed, transport through cracks or pores, and different microstructures. The model also accounts for the effects of a depleting source and can consider partitioning(s) between coating layer and kernel.

This model can be used in conjunction with the Booth release model from the kernel to calculate the diffusional releases from the particle during a constant 1600°C heating and a depressurized conduction cool down. Thermal diffusion is not included in the model and no segregation was assumed ($S=1$). (Note that the matrix material sorbs metallic fission products and thus the results are not a complete model for the entire fuel element. As referenced earlier, the model should be viewed as a scoping tool to understand what factors and factors are important to fission product transport in the particle.)

Figure 3-16 and Figure 3-17 plot the calculated fractional release for various fission products during post irradiation heating at 1600°C following a constant three year irradiation at 1200°C typical of a peak fuel particle in a prismatic gas reactor and a ten cycle three-year 600 to 1200°C cyclic irradiation expected in a pebble bed reactor. The results suggest that the irradiation temperature has at best a modest influence on the release at high temperature, given the long time at temperature in these calculations.

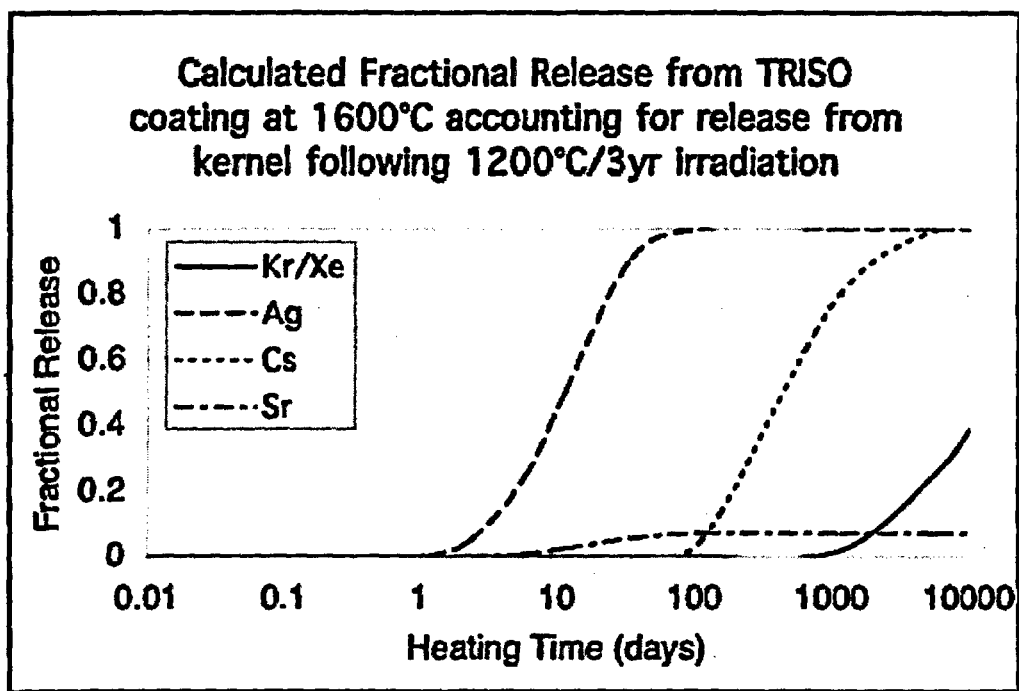


Figure 3-16 Calculated fractional release from a coated fuel particle during 1600°C heating following a three year irradiation at 1200°C

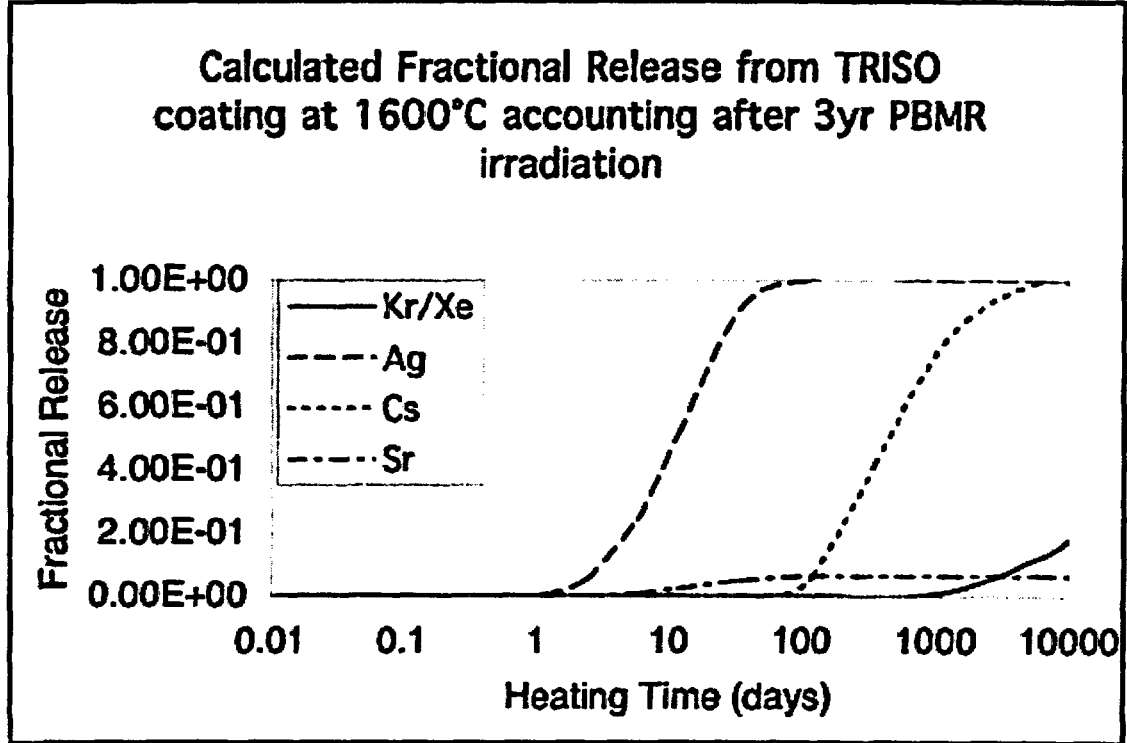


Figure 3-17 Calculated release from a coated fuel particle during 1600°C heating following a three-year ten-cycle PBR irradiation between 600 and 1200°C

The calculated diffusional releases from a conduction cool down (see Figure 3-18) following a PBR irradiation are shown in Figure 3-19. The conduction cool down is characterized by a slow heatup in the maximum fuel element temperature to a peak temperature of ~ 1600°C followed by a gradual temperature decline over the course of hundreds of hours.

By comparison to the releases during a constant high temperature heating in Figures 3-16 and 3-17, only silver and strontium releases from the particle are calculated given the magnitude of the diffusivities in the layers and the time/temperature profile in the accident scenario given in Figure 3-18. These results illustrate the importance of time at temperature on the magnitude and time of the calculated releases.

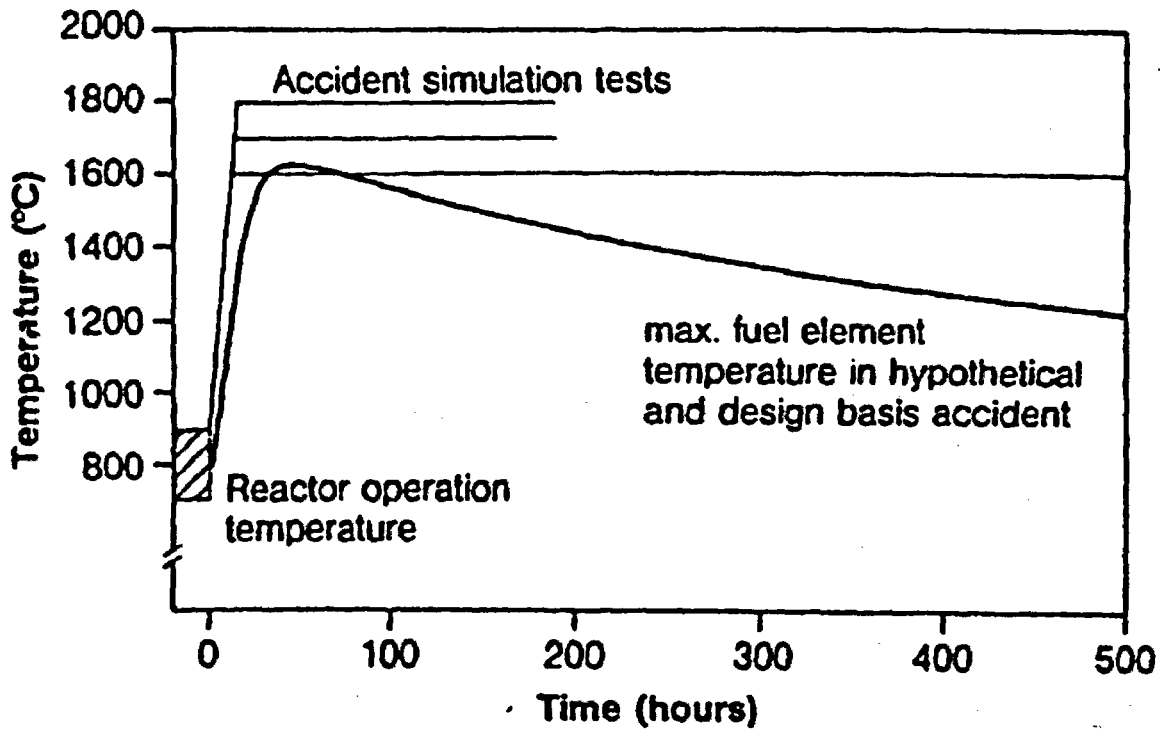


Figure 3-18 Calculated fuel temperature transient during a conduction cooldown

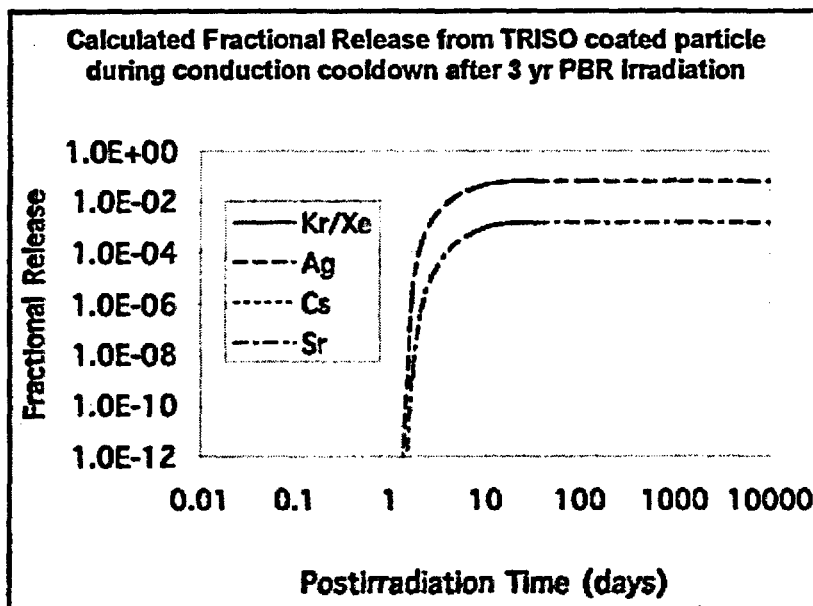


Figure 3-19 Calculated fractional diffusional release from TRISO coated particle during a conduction cooldown following a three-year ten-cycle PBR irradiation

Table 3-3 presents the results of two sensitivity studies: (a) a case where all temperatures are increased by 100°C and a case where the diffusivity in the SiC layer has been increased by a factor of 10 over the base value. The results show a modest impact of between two and six on the overall release for silver and strontium and little impact on either noble gases or cesium.

Table 3-3. Calculated Effect of Increased Temperature and Increased SiC Diffusivity on Fractional Diffusional Releases from TRISO Coated Particles.

Fission Product	Case		
	Base	+100 °C	10X SiC Diff
Kr/Xe	0	0	0
Ag	0.27	0.59	0.98
Cs	0	0	2.54E-05
Sr	0.0098	0.026	0.06

As a final sensitivity study, the influence of the segregation factor on the overall diffusional release from the particle was examined. The segregation factor coefficient can be used to account for the build up of fission products that may occur near cracks because of the fast diffusion at the grain boundary. Figure 3-20 plots the fractional release versus dimensionless time for four different segregation coefficients (1, 5, 10, 50).

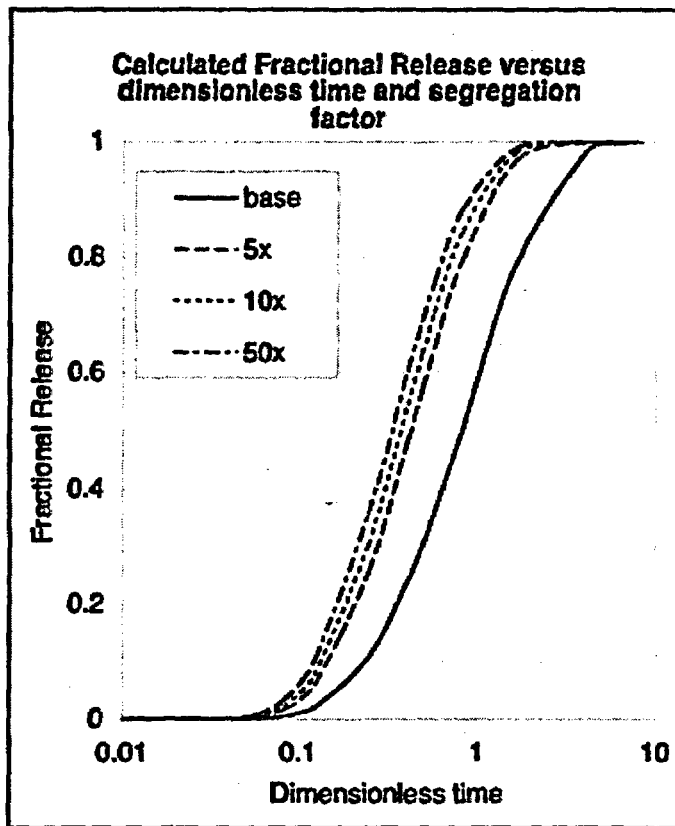


Figure 3-20 Effect of segregation coefficient on fractional release during heating

The results suggest that the fractional release of a fission product at a given time can differ by a factor of two to three depending on the magnitude of the partitioning that exists at the interface. Reference [3-5] suggests that segregation factors between 0.3 and 3 have been measured for some fission products. The simple calculation suggests that segregation or the build up of fission products at the interface between layers may explain some of the variability that has been observed in heating tests of coated particles irradiated to nominally the same conditions. The model presented here, although simple, can help scope out the importance of different reactor parameters on the source term from an ATGR.

3.7 Fission Product Transport in Failed Fuel Particles

Fission product transport in failed fuel particles is expected to be a major contributor to the gas reactor source term. Fission product release from uranium contamination in the fuel element matrix (compact or sphere) as well as from particles with missing layers may also be significant contributors. The transport model depends on the half-life of the fission product and whether it is metallic or gaseous.

3.7.1 Short-lived Fission Gases. For short-lived fission gases, the release is expressed in terms of the release rate to the birth rate (R/B) ratio for the particular fission gas. The R/B is from failed particles and from uranium contamination in the fuel element matrix (compact or sphere) is expressed for gas specie i as:

$$(R/B)_i = f_{fail} (R/B)_{fail,i} + f_{U-contamination} (R/B)_{U-contamination,i}$$

where

f_{fail} = particle failure fraction

$(R/B)_{fail,i}$ = release rate to birth rate ratio per particle failure for gas specie i

$f_{U-contamination}$ = uranium contamination fraction

$(R/B)_{U-contamination,i}$ = release to birth rate for gas specie i due to U contamination.

The uranium contamination is based on the elemental impurity level in the compact matrix material as determined by chemical methods. The sum of the heavy metal contamination and the initial failed particle level is determined by QC measurements on the fuel elements via destructive burn leach measurements. Subtraction of the burn leach results from the chemical results on the fuel element matrix material will provide the initial particle failure fraction. (Subsequent failures under irradiation would add to this source term.) The (R/B) correlations are based upon the Booth equivalent sphere gas release model. These correlations may be generally expressed as [3-37]:

$$(R/B) = (3/x) [\coth(x) - (1/x)]$$

where

$$x = [(\lambda a^2) / D]^{1/2}$$

$$\lambda = \text{decay constant for the fission gas isotope} = \ln 2 / T_{1/2} \text{ (s}^{-1}\text{)}$$

$$T_{1/2} = \text{isotope half life (s)}$$

$$D/a^2 = D' = \text{reduced diffusion coefficient (s}^{-1}\text{)}$$

$$a = \text{radius of equivalent sphere (m)}$$

$$\coth(x) = [\exp(x) + \exp(-x)] / [\exp(x) - \exp(-x)].$$

The equivalent sphere radius, a, is equal to the kernel radius when considering (R/B) for failed particles and is proportional to the raw graphite grain size of the matrix when considering (R/B) from uranium contamination.

Several correlations for reduced diffusion coefficients to be used in (R/B) calculations exist in the literature [3-5]. A few of the frequently referenced correlations are:

The US Model [3-38] which contains a unique reduced diffusion coefficient correlation and also differs from the classic Booth Equivalent Sphere formalism presented above in that it contains a diffusion parameter, multiplicative temperature and burnup functions and an empirical factor.

The British Model [3-2] that incorporates intrinsic diffusion, vacancy diffusion and athermal diffusion (a function of fission rate density) terms in its reduced diffusion coefficient.

The German I and II Models [3-39] that incorporate two separate sets of temperature-dependent reduced diffusion coefficients.

A comparison of the four models for Kr-85m (R/B) per failed particle is presented in Figure 3-21. Input parameters for this comparative calculation are representative of fuel irradiated in the NPR-1A experiment. On-line gas release measurements from the experiment indicated that Kr-85m (R/B) per failed particle was 0.028 at a time-average volume-average temperature of 977 °C. [3-40]. This experimental value compares almost exactly with the calculated German II value of 0.029.

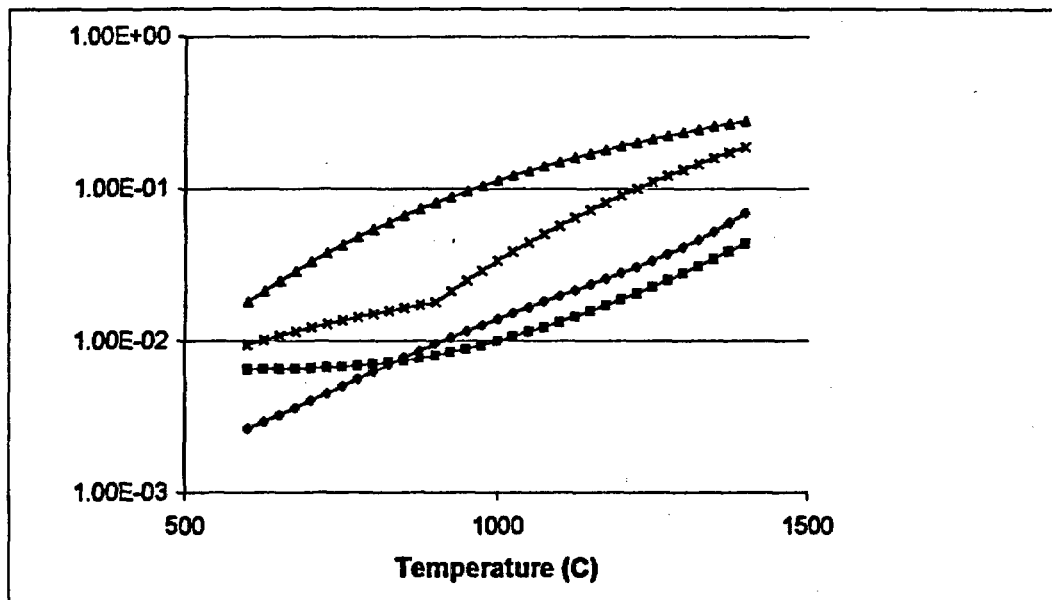


Figure 3-21 Comparison of failed particle model (R/B) results

3.7.2 Long-lived Fission Gases and Fission Metals. The release of long-lived fission gases and metals is modeled using the diffusion models presented earlier in this section using measured values for effective diffusivities for the kernel and each layer in the TRISO-coated particle. When (a fuel performance model predicts that) a given layer has failed, the release is usually calculated assuming that the failed layer offers no resistance to mass transport. This assumption is generally conservative.

It is important to consider mass transport through each layer individually since different fission products have different levels of retentiveness in each layer. For example, a particle with a failed SiC layer but intact PyC layers will release cesium but not noble gases under normal operation because the PyC layers retain noble gases up to very high temperatures. More sophisticated models that account for mass transport through a crack

or via nano-porosity as discussed earlier could also be implemented but historically have not been undertaken given the additional data needed for such mechanistic models.

3.7.3 Water and Air Ingress. In the event of water ingress, release from particles with exposed kernels has been measured (as discussed in Section 2) and some semi-empirical models exist that account for the change in release as a result of the hydrolysis of the kernel during the steam exposure. [3-2, 3-3]. In the event of air ingress, oxidation of the intact particles is considered and simple empirical models exist to predict particle failure based on experimental data [3-2]. However, modeling of the release of fission products is lacking. If a layer of the particle has been consumed in the oxidation, the modeling could conservatively assume that the layer no longer exists. For initially failed particles, the air would convert the UO_2 fuel kernel to higher oxidation states. The accompanying change in the microstructure of the kernel would increase the release.

3.8. Fission Product Transport Factors

Based on the previous sections, there is a wide range of parameters that influence fission product transport in coated particle fuel. These include:

- Parameters on the macroscopic scale such as the burnup of the particle, fast fluence (as a surrogate for radiation damage), the temperature of the layer, and the partial pressure of a gas or vapor.
- Microscopic parameters related to the structure of the material such as the porosity and tortuosity of the porous medium, and the grain boundary microstructure.
- Parameters related to the chemical speciation of the fission products of interest including the stoichiometry of the fuel and its changes during normal and accident conditions, thermochemical data such as free energies of formation, vapor pressures and adsorption isotherms, and transport properties such as binary gas phase diffusivities and heats of transport.
- Physical parameters that result in multidimensional and multicomponent effects including segregation and concentration of fission products as a result of cracking, and azimuthal temperature gradients.

To include all of these factors in the six PIRT tables were judged by the PIRT panel members and the NRC to be somewhat excessive given our state of knowledge about the importance and knowledge levels of some of the more detailed factors. As a result, a few higher level-factors were identified to account for most of the individual factors identified in this section. The factors, identified by the PIRT panel members, and their definitions, are found in Table 3-4. These factors were applied to each of the appropriate layers of the fuel from the kernel out to the fuel element (matrix materials). Not all factors are found in each layer since as discussed in the section, some of the factors may only be unique to one or two of the layers.

Table 3-4 Fission Product Transport Phenomenon Identified by the PIRT Panel

Factor	Definition
Condensed phase diffusion	Transport of condensable fission products by inter-granular diffusion and/or intra-granular solid-state diffusion (grain boundary and/or bulk diffusion)
Gas phase diffusion	Diffusion of gaseous fission products through layer (Knudsen and bulk diffusion through pore structure, and pressure driven permeation through structure including such sub-factors such as holdup, cracking, adsorption, site poisoning, permeability, sintering, and annealing)
Thermodynamics of fission product-SiC system	Chemical form of fission products including the effects of solubility, intermetallics, and chemical activity
Intercalation	Trapping of species between sheets of the graphite structure
Trapping	Adsorption of fission products on defects
Fission product release through failures, e.g., cracking	Passage of fission gas products from the buffer region through regions in the SiC layer that fail during operation or an accident

3.9 Summary

This review suggests that knowledge of the spatial and temporal temperature distribution in the reactor is an important factor for understanding fission product release from TRISO-coated particle fuels. Releases are likely to be dominated by particle failures during the accident. Thus, the source term must consider particle performance and impact of the failed particle configuration on the subsequent transport of fission products.

Different mechanisms are likely responsible for the transport of gases and metals in different layers. Gaseous transport can be described using pressure driven diffusion models through porous media but the use of these models requires information on the connected porosity, the characteristic size of the porosity and the tortuosity of the porous media, which are not well known for the layers of the TRISO coating. Metallic fission product transport is probably a combination of grain boundary and bulk diffusion depending on the temperature and specific fission product of interest.

A preliminary assessment suggests that the power generated in the particle determines conditions in the buffer (cracked versus uncracked). This in turn defines the initial conditions for fission product transport. With the exception of cracking, multi-dimensional effects may be less important. The calculations presented here suggest that Knudsen diffusion is consistent with rapid transport through the buffer and cracks but not intact PyC. Segregation/concentration of fission products at cracks can lead to greater releases and may explain some of the variability seen in accident heating tests. Thermal diffusion as a result of large thermal gradients (Soret effect) across the buffer would tend

to be most important under the cases of high power generation in the particle that leads to larger temperature gradients that typically correspond to very accelerated irradiation conditions that are not typical of gas reactors.

In all of these aforementioned calculations, the factors such as pressure driven and thermal diffusion have been examined individually. However, the literature contains many examples that indicate when all of the factors are modeled simultaneously, counterintuitive results may be obtained [3-6].

Effective diffusivities have been obtained from previous German and U.S. work, but the research did not always focus on the mechanism involved and the researchers did not always reduce the data with a specific mechanism in mind (e.g., Knudsen diffusion parameters, trapping parameters). The measured effective diffusivities in PyC and SiC are consistent with both older and more recent transport measurements. Furthermore, the aforementioned assessments suggest that trapping is important in OPyC layers where concentration of fission products is on the same order as the trap density. Trapping is much less important in IPyC and SiC layers because the trap concentration. Is expected to be much less the fission product concentration in the layers. Sensitivity studies using currently available effective diffusivities and educated guesses on trapping parameters and the simple multi-layer diffusion and trapping model presented here can help scope out these issues in more detail.

Fission product transport at the microscopic level depends strongly on the microstructure of the individual layers in the coated particle and the microstructure depends on the deposition conditions used to fabricate the layer. The understanding of the linkage between transport, microstructure and deposition conditions is not complete. Instead there is an implicit empirical relationship between the measured transport, the underlying layer structure, and the deposition conditions as implied by the measured effective diffusivities for the different layers for a specific manufactured fuel. Thus, for any new fuel that is produced, if the historical fuel fission-product-transport data are referenced, it would be important to establish that the transport-structure relationship implicit in the historic data is also applicable for the newly produced fuel. Significant deviations in the historic transport-structure relationship would raise questions about how much of the historic experimental database on fission product transport for TRISO-coated particle fuel would be valid for the new fuel that is produced.

3.10. References

- 3-1 Littmark, U., and J. F. Ziegler, "Handbook of Range Distributions for Energetic Ions in All Elements," Pergamon Press, 1980.
- 3-2 Booth, A. H., "A Method of Calculating Fission Gas Release from UO₂ Fuel and Its Implication to the X-2-f Loop Test," Atomic Energy of Canada Limited Report - 496, 1957.
- 3-3 Turnbull, J. A., et al., "The Diffusion Coefficient of Gaseous and Volatile Species During the Irradiation of Uranium Dioxide," Journal of Nuclear Materials, Vol. 107, No. 168, 1982.

-
- 3-4 Terry, W. K., (ed.), "Modular Pebble-Bed Reactor Project," Laboratory Directed Research and Development Program FY-2001 Annual Report, INEEL/EXT-2001-623, December 2001.
- 3-5 Fuel Performance and Fission Product Behaviour in Gas Cooled Reactors, IAEA TECDOC-978, Nov. 1997.
- 3-6 Jacox, M. E., J. Phys. Chem. Ref. Data, 32, 2003, p. 1.
- 3-7 Bird, R. B., W. E. Stewart and E. N. Lightfoot, "Transport Phenomena," John Wiley and Sons, 1960.
- 3-8 Toor, H. L., J. AIChE, 3 (1957) 198
- 3-9 Shadanov, V., Yu. Kagan and A. Sazykin, Soviet Physics JETP, 15 (1962) 596.
- 3-10 Mason, E. A., A.P. Malinauskas, and R.B. Evans III, J. Chem. Phys., 46 (1967) 3199.
- 3-11 Jenkins, T. R. and F. Roberts, Proc. Conf. Carbon 5th, Penn State University, Vol. 2, 1961, p. 335.
- 3-12 Kast, W., and C.-R. Hohenthanner, "Mass Transfer with the Gas-Phase of Porous Media," International Journal of Heat and Mass Transfer, Vol. 43, p. 807-823, 2000
- 3-13 Mason, E. A., and A. P. Malinauskas, "Gas Transport in Porous Media: The Dusty Gas Model," Elsevier, Amsterdam, 1983.
- 3-14 Hewitt, G. F., "Gaseous Mass Transport within Graphite" , Chapter 2 in Chemistry and Physics of Carbon - A Series of Advances, Volume 1, P.L. Walker, Jr., Marcel Dekker, 1965.
- 3-15 Korte, C.; Janek, J.; Timm, H. 1997, Transport processes in temperature gradients: Thermal diffusion and Soret effect in crystalline solids. Solid State Ionics ; November, 1997; vol.101-103, no., pp. 465-470
- 3-16 Hofman, G. L., Hayes S. L., Petri M. C. "Temperature gradient driven constituent redistribution in U-Zr alloys," Journal Of Nuclear Materials 227 (3): 277-286 Jan. 1996
- 3-17 Kleykamp, H., 2001,"Phase equilibria in the UO_2 - PuO_2 system under a temperature gradient," Journal of Nuclear Materials; April, 2001; vol.294, no.1-2, pp. 8-12
- 3-18 Longhurst, G. R., et al., "TMAP4 User's Manual," EGG-FSP-10315, May 1998.
- 3-19 Petti, D. A., et al., "Key differences in the fabrication, irradiation and high temperature accident testing of US and German TRISO-coated particle fuel, and their implications on fuel performance," Nuclear Engineering and Design, Vol. 222, p. 281-297, 2003.
- 3-20 Braun, C. et al., "Mesure de la Permeabilite aux Gaz des Revetements de Pyrocarbone Isotrope," Journal of Nuclear Materials, Vol. 89, p. 136-142, 1980.

-
- 3-21 Mathur, R. B., "In-Situ Electrical Resistivity Changes During Bromine Intercalation in Carbon Fibers," *Carbon*, Vol. 34, No. 10, pp. 1215-1220, 1996.
- 3-22 Hollerman, I., et al., "An Infrared Study on CO Intercalated in Solid C60," *J. Chem. Physics*, Vol. 110, No. 4, Jan. 1999.
- 3-23 Palnichenko, A., and S.I. Tanuma, "Effect of Intercalation of Alkali and Halogen Species into the Low Density Carbon Crystal 'Carbolite'," *J. Phys. Chem. Solids*, Vol. 57, No. 6-8, pp. 1163-1166, 1996.
- 3-24 Levi, M. D., and D. Aurbach, "Frumkin Intercalation Isotherm- a Tool for the Description of Lithium Insertion into Host Materials: A Review," *Electrochimica Acta*, Vol. 45, p. 167-185, 1999.
- 3-25 Bisquert, J., and V. S. Bikhrenko, "Analysis of the Kinetics of Ion Intercalation. Two State Model Describing the Coupling of Solid State Ion Diffusion and Ion Binding Processes," *Electrochimica Acta*, Vol. 47, p. 3977-3988, 2002.
- 3-26 Longhurst, G. R., et al., "TMAP4 User's Manual," EGG-FSP-10315, May 1998.
- 3-27 Petti, D. A., et al., "Development of Improved Models and Design of Coated Particle Gas Reactor Fuels: Annual Program Report Under the International Nuclear Energy Research Initiative (I-NERI)," INEEL/EXT-02-0493, Nov. 2002.
- 3-28 Fusamae, F., et al., "Evaluation of Grain-Boundary Groove Profiles and Surface Diffusion Coefficients in SiC Ceramics Using Atomic Force Microscopy," *Ceramic Transactions*, Vol. 71, 1996, p. 463- 472.
- 3-29 Takano, K., et al., "Volume and Dislocation Diffusion of Iron, Chromium, and Cobalt," in *CVD beta-SiC*, "Science and Technology of Advanced Materials, Vol. 2 No. 2 June 2001, p. 381-388.
- 3-30 Wang, X. R., et al., "Apparent Anomalous Prefactor Enhancements for Surface Diffusion due to Surface Defects," *Surface Science*, Vol. 512, p. L361-L366, 2002.
- 3-31 Mishini, Y., and C. Herzig, "Grain Boundary Diffusion: Recent Progress and Future Research," *Materials Science and Engineering*, A260, P. 55-71, 1999.
- 3-32 Zhu, J., et al., "Microstructure Dependence of Diffusional Transport," *Computational Materials Science*, Vol. 20, p. 37-47, 2001.
- 3-33 Gyarmati, E., and H. Nickel, "Stationary and Dynamic Deposition of Silicon Carbide on Coated Fuel Particles," JUL-900-RW, ORNL-TR-2733, November 1972.
- 3-34 Gulden, T. D., "Deposition and Microstructure of Vapor-Deposited Silicon Carbide," *J. American Ceramic Society*, Vol. 51, No. 8, August 1968, p. 424-427
- 3-35 Voice, E. H., and V.C. Scott, "The Formation and Structure of Silicon Carbide Pyrolytically Deposited in a Fluidized Bed of Microspheres," *Proceedings of the 5th Symposium on Special Ceramics*, Stoke on Trent, July 14-16, 1970.

-
- 3-36 Morgan, M. T., and A. P. Malinauskas, "Cesium Release and Transport in BISO-coated Fuel Particles," Nuclear Technology, Vol. 35, p. 457-464, September 1977.
- 3-37 Olander, D. R., "Fundamental Aspects of Nuclear Reactor Fuel Elements", ERDA, TID-26711-P1, 1976.
- 3-38 Martin R. C., "Compilation of Fuel Performance and Fission Product Transport Models and Database for MHTGR Design", ORNL/NPR-91/6, October 1993.
- 3-39 Nabielek, H., "Partikeln und Brennelemente für den HTR", KFA-HTA, January 24, 1991.
- 3-40 Maki, J. T., D. A. Petti, R. R. Hobbins, R. K. McCardell, E. L. Shaber and F. H. Southworth, "NP-MHTGR Fuel Development Program Results", INEEL/EXT-2002-1268, October 2002.

4. TRISO-COATED PARTICLE FUEL PHENOMENON IDENTIFICATION AND RANKING TABLES (PIRTS)

Six summary TRISO-coated particle fuel PIRT tables are presented in this chapter, one each for Manufacturing (Table 4-1), Operations (Table 4-2), Depressurized Heatup Accident (Table 4-3), Reactivity Accident (Table 4-4), Depressurization Accident with Water Ingress (Table 4-5), and Depressurization Accident with Air Ingress (Table 4-6).

The summary information in each PIRT table is presented in an eight-column format.

Column 1 identifies the "Factor, Characteristic, or Phenomenon" for which importance and a knowledge levels were assessed by the TRISO-coated particle fuel PIRT panel.

Column 2 contains the definition prepared by the panel for each entry in Column 1.

Columns 3 and 4 contain an importance rank of either High (H), Medium (M) or Low (L) and knowledge level assessment between 1 and 9 given by the Idaho National Engineering and Environmental Laboratory (INEEL) panel member.

Columns 5 and 6 contain input of the Oak Ridge National Laboratory (ORNL) panel member and Columns 7 and 8 contain the input of the Sandia National Laboratories (SNL) panel member.

An importance rank of "H" indicates that the factor, characteristic or phenomenon had a dominant or controlling impact on the primary evaluation criterion, i.e., fission product release. An importance rank of "L" indicates a small influence. An importance rank of "M" indicates a moderate influence. A knowledge assessment of "1" is used when there is little or no knowledge or understanding of the entry in Column 1 while a knowledge assessment of "9" is used when there is a complete knowledge and understanding. Numbers between 1 and 9 are assigned to indicate intermediate levels of knowledge and understanding.

The summary data for the six PIRT tables presented in this chapter were derived from the detailed PIRT inputs provided by each panel member for each of the six PIRTs. The detailed PIRT input provided by the panel members provides the importance and knowledge assessments as well as the rationales, with varying level of detail, for each. In addition and where possible, the panel members suggested closure efforts that might be undertaken for highly important factors, characteristics and phenomena for which the knowledge and understanding are not sufficiently developed.

Panel member importance and knowledge rankings, detailed rationales for the importance and knowledge rankings, and suggested closure rationales are found in the following appendices.

Appendix A	Manufacturing
Appendix B	Operations
Appendix C	Depressurized Heatup Accident
Appendix D	Reactivity Accident
Appendix E	Depressurization Accident with Water Intrusion
Appendix F	Depressurization Accident with Air Intrusion

Initially, the TRISO-coated particle fuel PIRT panel was tasked to prepare a PIRT for the TRISO-coated particle fuel Design phase. Importance ranks and knowledge levels, as well as the accompanying rationales, were developed by each panel member. The Design PIRT effort was discontinued when the PIRT effort expanded to include additional accident scenarios. Although the panel effort did not proceed to the same degree of completion as the other PIRTs summarized in Tables 4-1 through 4-6, the detailed Design PIRT information prepared by the panel members are thought to include significant insights. Therefore, the detailed INEEL, ORNL, and SNL PIRT inputs are provided in Appendix H.

Analyses and summaries of the PIRT results presented in Tables 4-1 through 4-6 and Appendices A through F are found in Chapter 5, TRISO-coated particle fuel PIRT Analysis and Summary.

The extensive phenomena accounted for in the TRISO-coated particle fuels PIRT tables may be viewed as an inventory of all of the basic phenomena that the PIRT panel considers to play a role in TRISO-coated particle fuel performance and the transport of fission products within the fuel components. However, the PIRT panel does not intend to imply that each and every factor, characteristic or phenomenon that has been identified must be explicitly and individually accounted for in the modeling or analysis of gas-cooled reactor fuel performance and fission product transport. The panel recognizes that it may prove feasible to model some of these phenomena to assess performance and fission product transport in the fuel in a way that adequately and effectively combines some of the individual phenomena into an integrated parameter(s). In such cases these PIRT tables will serve as a valuable "checklist" to support the assessment of the approach in which the basic TRISO PIRT phenomena are addressed.

Table 4-1 TRISO-Coated Particle Fuel Manufacturing Summary PIRT

Factor, Characteristic, or Phenomenon	Definition	INEEL		ORNL		SNL**	
		Rank	KL*	Rank	KL	Rank	KL
Layer coating process specifications: Gases (levitation gas and coating gas)	Gases used to levitate and coat to create layer	M	8	H	8	-	-
Layer coating process specifications: Ratio of gases	Ratio of active gas to total gas, including concentration	H	7	H	7	-	-
Layer coating process specifications: Temperature	Temperature of coater	H	8	H	7	-	-
Layer coating process specifications: Coating Rate	The average deposition rate over space and time of the layer	H	8	H	6	-	-
Layer coating process specifications: Pressure	Pressure inside coater	L	3	L	4	-	-
Layer coating process specifications: Coater Size	Size is measured by the diameter of the coater	H	6	H	6	-	-
Layer coating process	Continuous vapor deposition TRISO coating without unloading of particles	H	6	H	4	-	-
Process control:	Correlation between measured process parameters and irradiation performance	H	6	H	6	-	-
Product control:	Correlation between measured product parameters and irradiation performance	M	6	H	5	-	-
Fuel Element: Particle overcoating (fuel form dependent)	Layer on outside of outer PyC added after coating	H	8	H	7	-	-
Fuel Element: Matrix and Binder	Filler mixed with resin	H	6	H	7	-	-
Fuel Element: Bonding strength (PyC to matrix)	Interfacial strength at the interface	L	6	M	7	-	-
Fuel Element: Compacting	Process of forming fuel element involving molding and pressing	H	7	H	7	-	-

Table 4-1 TRISO-Coated Particle Fuel Manufacturing Summary PIRT (continued)

Factor, Characteristic, or Phenomenon	Definition	INEEL		ORNL		SNL**	
		Rank	KL*	Rank	KL	Rank	KL
Fuel Element: Carbonization	Baking full fuel element to drive off volatiles	L	6	M	7	-	-
Fuel Element: Heat Treatment	High temperature annealing to stabilize fuel form	L	7	M	7	-	-
Fuel Element: Impurities Control	Minimization of contamination of fuel form by process equipment (e.g., iron, chrome, etc)	H	7	H	7	-	-
Fuel Element: Tramp Uranium	Uranium introduced by raw materials, e.g., resin	H	8	H	8	-	-
Fuel Element: Strength	An overall measure of fuel element resistance to stresses that might occur during operation or accidents	H	8	H	8	-	-
Fuel Element: Initial particle defect fraction due to manufacture	Exposed kernel fraction	H	6	H	7	-	-
Outer PyC layer: Anisotropy (initial)	Difference in grain orientation along principal directions as measured by the BAF	H	8 FRG 6 US	H	5	-	-
Outer PyC layer: Porosity	Interconnected void accessible to the surface	M	8	M	7	-	-
SiC layer: Grain size and microstructure, e.g., alignment	Size and orientation of the grains and the pores	H	8	H	6	-	-
SiC layer: Fracture strength	Mean tensile strength (Weibull parameter or equivalent)	H	6	H	6	-	-
SiC layer: Density	Mass per unit volume	H	8	H	8	-	-
SiC layer: Bonding strength (SiC to outer PyC)	Interfacial strength at the interface	L	6	L	2	-	-
SiC layer: Stoichiometry	Ratio of silicon to carbon (absence of gold spots, i.e., elemental Si)	H	6	H	6	-	-

Table 4-1 TRISO-Coated Particle Fuel Manufacturing Summary PIRT (continued)

Factor, Characteristic, or Phenomenon	Definition	INEEL		ORNL		SNL**	
		Rank	KL*	Rank	KL	Rank	KL
SiC layer: Heavy metal dispersion	Amount of heavy metals dispersed in the layer present after manufacture	M	7	H	7	-	-
SiC layer: Defects	Initial undetected pinhole or other defects resulting from the manufacturing process	H	5	H	5	-	-
Inner PyC layer: Anisotropy (initial)	Difference in crystal orientation along principal directions as measured by the BAF	H	5	H	5	-	-
Inner PyC layer: Bonding strength (inner PyC to SiC)	Interfacial strength at the interface	H	6	H	3	-	-
Inner PyC layer: Porosity	Interconnected void accessible to the surface	M	5	H	7	-	-
Buffer layer: Thin or missing	Layer thickness less than specified or missing layer	H	7	H	7	-	-
Buffer layer: Density and open porosity	Mass per unit volume and interconnected void accessible to the surface	M	8	H	7	-	-
Kernel: Density	Mass per unit volume in final form	M	9	M	8	-	-
Kernel: Microstructure (UO ₂)	Grain size, pore structure (interconnectivity) and orientation in kernel	M	8	M	7	-	-

* KL = Knowledge Level

** Panel member declined to provide input due to lack of manufacturing background.

Table 4-2 TRISO-Coated Particle Fuel Operations Summary PIRT

Factor, Characteristic, or Phenomenon	Definition	INEEL		ORNL		SNL	
		Rank	KL*	Rank	KL	Rank	KL
Fuel element: Temperature	Local temperature in the fuel element	H	8	H	7	M	8
Fuel element: Fast fluence	Accumulated fast neutron fluence greater than 0.18 MeV	M	5	M	7	M	5
Fuel element: Power density	Power per pebble or compact (W)	L	6	M	7	M	6
Fuel element: Temperature difference	Temperature between center or centerline and surface in °C	M	7	M	7	H	7
Fuel element: Temperature-time histories	Local temporal temperature of fuel element over its lifetime	H	7	H	7	M	7
Fuel element: Condensed phase diffusion	Inter-granular diffusion and/or intra-granular solid-state diffusion	H	5	H	6	H	4
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)	M	7	H	7	H	5
Fuel element: Corrosion by coolant impurities	Corrosion of the fuel element outer surface by part per million level of gaseous impurities in the helium coolant	M	6	M	7	M	4
Kernel: CO production	Formation of CO from excess oxygen released in fission	H UO ₂ L UCO	8 UO ₂ 5 UCO	H	7	H	2
Kernel: Burnup	Fission of initial metal atoms	H	7	H	7	L	2
Kernel: Kernel swelling	Volumetric expansion of kernel resulting from fissioning	L	6	L	6	L	5
Kernel: Microstructure changes	Change in structure in kernel with burnup, including fission gas bubbles, grain growth and grain disintegration	L	6	M	6	H	5

Table 4-2 TRISO-Coated Particle Fuel Operations Summary PIRT (continued)

Factor, Characteristic, or Phenomenon	Definition	INEEL		ORNL		SNL	
		Rank	KL*	Rank	KL	Rank	KL
Kernel: Fission product chemical form	Chemical speciation of fission products as a function of burnup and temperature	H	7	H	6	L	5
Kernel: Buffer interaction	Mechanical and chemical interactions between the kernel and buffer, e.g., chemical reactions at interface and displacement of buffer by kernel growth.	M	6	L	6	H	3
Kernel: Kernel migration (fuel dependent)	Kernel migration (fuel dependent)	M UO ₂ L UCO	8 UO ₂ 8 UCO	H	7	H	3
Kernel: Fission product generation	Yield of fission products from uranium and plutonium fission	H	9	H	8	L	9
Kernel: Temperature gradient	Temperature gradient across the kernel	L	6	H	7	H	3
Kernel: Isotopic half life	The time lapse during which a mass of a particular isotope loses half of its radioactivity	M	9	M	8	L	9
Buffer Layer: Pressure	Gas pressure generated in the void volume associated with the buffer layer	H H	6 UO ₂ 7 UCO	H	6	H	4
Buffer Layer: Shrinkage	Radiation or otherwise induced dimensional change	M	6	M	6	M	2
Buffer Layer: Cracking	Shrinkage cracks produced in layer during operation	H	5	H	6	H	3
Buffer Layer: Carbonyl vapor species	M-CO species partial pressures	M	3	L	1	H	4
Buffer Layer: Temperature gradient	Temperature difference across the buffer layer	H	5	H	6	H	3
Buffer Layer: Condensed phase diffusion	Inter-granular diffusion and/or intra-granular solid-state diffusion	M	5	M	5	H	2

Table 4-2 TRISO-Coated Particle Fuel Operations Summary PIRT (continued)

Factor, Characteristic, or Phenomenon	Definition	INEEL		ORNL		SNL	
		Rank	KL*	Rank	KL	Rank	KL
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)	M	5	M	6	H	5
Buffer Layer: Recoil effects	Buffer damage arising from capture of high-energy fission products	M	7	M	5	L	5
Inner PyC layer: Radiation induced creep	Strain release as a result of radiation induced dimensional change	H	5	H	5	L	4
Inner PyC layer: Fast fluence	Accumulated fast neutron fluence greater than 0.18 MeV	H	8	H	6	M	5
Inner PyC layer: Dimensional change	Unrestrained radial and tangential changes with fast fluence	H	7	H	5	M	4
Inner PyC layer: Anisotropy	Operation-induced (thermal + radiation) change in grain orientation along principal directions as measured by the BAF	H	8 FRG 8 US	H	5	L	3
Inner PyC layer: Cracking	Lengths, widths, and numbers of cracks produced in layer during operation	H	6	H	5	H	3
Inner PyC layer: Debonding	Separation of PyC layer from SiC layer	M	5	M	3	L	3
Inner PyC layer: Condensed phase diffusion	Inter-granular diffusion and/or intra-granular solid-state diffusion	H	7	H	6	H	1
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)	H	7	H	7	H	4
SiC layer: Kernel interaction with SiC layer	Kernel migration (amoeba effect)	M	8	H	7	H	6

Table 4-2 TRISO-Coated Particle Fuel Operations Summary PIRT (continued)

Factor, Characteristic, or Phenomenon	Definition	INEEL		ORNL		SNL	
		Rank	KL*	Rank	KL	Rank	KL
SiC layer: Fission product corrosion	Attack of layer by fission products, e.g., Pd	H	6	H	6	H	4
SiC layer: Heavy metal attack	Damage to layer due to fissioning of heavy metals dispersed in the layer	L	6	L	7	L	6
SiC layer: Cracking	Lengths, widths and numbers of cracks produced in layer during operation	H	7	H	6	H	1
SiC layer: Condensed phase diffusion	Inter-granular diffusion and/or intra-granular solid-state diffusion	H	7	H	6	H	1
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)	H	7	H	7	H	4
Outer PyC layer: Radiation induced creep	Strain release as a result of radiation induced dimensional change	L	6	M	5	L	3
Outer PyC layer: Dimensional change	Unrestrained radial and tangential changes with fast fluence	M	7	M	5	L	2
Outer PyC layer: Anisotropy	Operation-induced (thermal + radiation) change in grain orientation along principal directions as measured by the BAF	M	7	M	5	L	7
Outer PyC layer: Condensed phase diffusion	Solid state diffusion	H	7	H	6	M	1
Outer PyC layer: Gas phase diffusion	Transport through pores and void structures by vapors, e.g., noble gases	H	7	H	7	H	4

Table 4-2 TRISO-Coated Particle Fuel Operations Summary PIRT (continued)

Factor, Characteristic, or Phenomenon	Definition	INEEL		ORNL		SNL	
		Rank	KL*	Rank	KL	Rank	KL
Outer PyC layer: Cracking	Lengths, widths and numbers of cracks produced in layer during operation	M	3	M	5	H	1

- KL = Knowledge Level

Table 4-3 TRISO-Coated Particle Fuel Depressurized Heatup Accident Summary PIRT

Factor, Characteristic, or Phenomenon	Definition	INEEL		ORNL		SNL	
		Rank	KL* (1)/(2)	Rank	KL* (1)/(2)	Rank	KL* (1)/(2)
Fuel Element: Irradiation history	The temperature, burnup and fast fluence history of the layer	H	5/5	H	7/5	H	3
Fuel Element: Condensed phase diffusion	Inter-granular diffusion and/or intra-granular solid-state diffusion	M	5/5	H	6/5	M	2
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	M	5/5	H	7/7	H	4
Fuel Element: Transport of metallic FPs through fuel element – Chemical form	Chemical stoichiometry of the chemical species that includes the radioisotope of interest	H	5/5	H	5/5	H	3
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)	H	7/7	H	7/7	H	4
Outer PyC Layer: Condensed-phase diffusion	Inter-granular diffusion and/or intra-granular solid-state diffusion	H	7/7	H	7/7	M	2
Outer PyC Layer: Layer oxidation	Uptake of oxygen by the layer through a chemical reaction	L	6/6	L	6/6	L	8
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	L	5/5	M	6/6	M	4
Outer PyC Layer: Intercalation	Trapping of species between sheets of the graphite structure	M	4/4	L	2/1	L	3

Table 4-3 TRISO-Coated Particle Fuel Depressurized Heatup Accident Summary PIRT (continued)

Factor, Characteristic, or Phenomenon	Definition	INEEL		ORNL		SNL	
		Rank	KL* (1)/(2)	Rank	KL* (1)/(2)	Rank	KL* (1)/(2)
Outer PyC Layer: Trapping	Adsorption of fission products on defects	M	4/4	L	2/1	L	3
Outer PyC Layer: Cracking	Lengths, widths and numbers of cracks produced in layer during operation or an accident	H	5/5	H	5/5	H	2
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)	H	7/7	H	7/5	H	4
SiC Layer: Condensed-phase diffusion	Inter-granular diffusion and/or intra-granular solid-state diffusion	H	7/7	H	7/5	M	2
SiC Layer: Thermal deterioration/decomposition	Decline in the quality of the layer due to thermal loading	H	8/6	H	7/5	M	3
SiC Layer: Fission product corrosion	Attack of layer by fission products, e.g., Pd	H	7/5	H	7/5	L	3
SiC Layer: Heavy metal diffusion	Diffusion of heavy metals through the intact layer	L	3/3	L	5/5	M	2
SiC Layer: Layer oxidation	Uptake of oxygen by the layer through a chemical reaction	M	6/6	M	5/5	L	3
SiC Layer: Fission product release through undetected defects	Passage of fission products from the buffer region through defects in the SiC layer	H	6/6	H	5/5	H	3
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	H	7/6	H	6/5	H	3
SiC Layer: Thermodynamics of the SiC-fission product system	Chemical form of fission products including the effects of solubility, intermetallics, and chemical activity	H	7/7	H	7/5	H	4

Table 4-3 TRISO-Coated Particle Fuel Depressurized Heatup Accident Summary PIRT (continued)

Factor, Characteristic, or Phenomenon	Definition	INEEL		ORNL		SNL	
		Rank	KL* (1)/(2)	Rank	KL* (1)/(2)	Rank	KL* (1)/(2)
SiC Layer: Sintering	Change of SiC microstructure as a function of temperature	L	5/5	L	7/7	M	6
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)	H	7/7	H	7/6	H	6
Inner PyC Layer: Condensed-phase diffusion	Inter-granular diffusion and/or intra-granular solid-state diffusion	H	7/7	H	7/7	M	2
Inner PyC Layer: Pressure loading (Fission products)	Stress loading of the layer by increased pressure from fission products	M	8/8	M	7/7	L	2
Inner PyC Layer: Pressure loading (Carbon monoxide)	Stress loading of the layer by carbon monoxide by increased pressure	H UO ₂ L UCO	7/7	H	7/7	H	2
Inner PyC Layer: Layer oxidation	Reaction of pyrolytic graphite with oxygen released from the kernel	L	5/5	L	7/7	M	3
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	M	6/6	M	7/7	L	2
Inner PyC Layer: Cracking	Lengths, widths and numbers of cracks produced in layer during accident	H	5/5	H	6/6	H	1
Inner PyC Layer: Intercalation	Trapping of species between the basal planes of the structure	M	6/6	L	1/1	M	2
Inner PyC Layer: Trapping	Adsorption of fission products on defects	L	6/6	L	2/1	No entry	No entry

Table 4-3 TRISO-Coated Particle Fuel Depressurized Heatup Accident Summary PIRT (continued)

Factor, Characteristic, or Phenomenon	Definition	INEEL		ORNL		SNL	
		Rank	KL* (1)/(2)	Rank	KL* (1)/(2)	Rank	KL* (1)/(2)
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)	H	7/7	H	7/7	H	4
Buffer Layer: Condensed-phase diffusion	Inter-granular diffusion and/or intra-granular solid-state diffusion	H	7/7	H	7/7	L	1
Buffer Layer: Response to kernel swelling	Mechanical reaction of the layer to the growth of the kernel via swelling	L	4/4	L	7/7	M	4
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	L	2/2	L	7/7	L	2
Buffer Layer: Layer oxidation	Reaction of buffer layer with-oxide materials in the kernel	H	6/6	L	7/7	H	3
Buffer Layer: Thermal gradient	Change in temperature with distance	L	6/6	L	7/7	H	2
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	L	7/7	L	6/6	L	5
Kernel: Maximum fuel temperature	Maximum fuel temperature attained by the fuel kernel during the accident	H	7/7	H	7/7	H	5
Kernel: Temperature vs. time transient conditions	The time-dependent variation of fuel temperature with time	H	7/7	H	7/7	H	4
Kernel: Energy Transport: Conduction within kernel	Flow of heat within a medium from a region of high temperature to a region of low temperature	M	6/6	L	7/7	M	3

Table 4-3 TRISO-Coated Particle Fuel Depressurized Heatup Accident Summary PIRT (continued)

Factor, Characteristic, or Phenomenon	Definition	INEEL		ORNL		SNL	
		Rank	KL* (1)/(2)	Rank	KL* (1)/(2)	Rank	KL* (1)/(2)
Kernel: Thermodynamic state of fission products	Chemical and physical state of fission products	H	7/7	H	6/6	H	5
Kernel: Gas-phase diffusion	Diffusion of gaseous fission products through layer (Knudsen and bulk diffusion through pore structure, and pressure driven permeation through structure)	H	7/7	H	6/6	H	3
Kernel: Condensed-phase diffusion	Inter-granular diffusion and/or intra-granular solid-state diffusion	H	7/7	H	6/4	H	3
Kernel: Oxygen flux	Mass transport of oxygen per unit surface area per unit time	M UO ₂ L UCO	6/6	L	3/3	H	3
Kernel: Grain growth	Enlargement of grains as a result of diffusion	L	4/4	L	3/3	L	8
Kernel: Buffer carbon-kernel interaction	Chemical reaction between carbon and the fuel (UO ₂) to form UC ₂ and CO (gas)	H	6/6	L	5/5	H	3

* KL = Knowledge Level

- (1) First entry is knowledge level for fuel temperatures ≤ 1600 °C
- (2) Second entry is knowledge level for fuel temperatures > 1600 °C

Table 4-4 TRISO-Coated Particle Fuel Reactivity Accident Summary PIRT

Factor, Characteristic, or Phenomenon	Definition	INEEL		ORNL		SNL	
		Rank	KL*	Rank	KL*	Rank	KL*
Fuel Element: Irradiation history	The temperature, burnup and fast fluence history of the layer	M	8	H	7	H	1
Fuel Element: Condensed-phase diffusion	Inter-granular diffusion and/or intra-granular solid-state diffusion	H	6	H	6	L	2
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	H	5	H	7	H	2
Fuel Element: Transport of metallic FPs through fuel element – Chemical form	Chemical stoichiometry of the chemical species that includes the radioisotope of interest	H	5	M	5	M	8
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)	L	8	H	7	L	3
Outer PyC Layer: Condensed-phase diffusion	Inter-granular diffusion and/or intra-granular solid-state diffusion	L	8	L	7	L	2
Outer PyC Layer: Layer oxidation	Uptake of oxygen by the layer through a chemical reaction	M	6	L	6	L	3
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	M	7	L	6	L	2
Outer PyC Layer: Intercalation	Trapping of species between sheets of the graphite structure	L	No entry	L	1	L	3

Table 4-4 TRISO-Coated Particle Fuel Reactivity Accident Summary PIRT (continued)

Factor, Characteristic, or Phenomenon	Definition	INEEL		ORNL		SNL	
		Rank	KL*	Rank	KL*	Rank	KL*
Outer PyC Layer: Trapping	Adsorption of fission products on defects	L	No entry	L	2	L	3
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)	L	No entry	L	7	L	2
SiC Layer: Condensed-phase diffusion	Inter-granular diffusion and/or intra-granular solid-state diffusion	L	No entry	L	7	L	2
SiC Layer: Thermal deterioration/decomposition	Decline in the quality of the layer due to thermal loading	L	No entry	L	7	L	4
SiC Layer: Fission product corrosion	Attack of layer by fission products, e.g., Pd	L	No entry	L	7	H	6
SiC Layer: Heavy metal diffusion	Diffusion of heavy metals through layer	L	5	M	5	L	2
SiC Layer: Layer oxidation	Uptake of oxygen by the layer through a chemical reaction	M	5	L	5	L	5
SiC Layer: Fission product release through undetected defects, e.g., cracking	Passage of fission products from the buffer region through regions in the SiC layer that fail during operation or an accident	L	5	L	7	L	2
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	H	6	H	5	H	7
SiC Layer: Thermodynamics of the SiC-fission product system	Chemical form of fission products including the effects of solubility, intermetallics, and chemical activity	L	5	L	7	L	4
SiC Layer: Sintering	Change of graphite microstructure as a function of temperature	L	5	L	7	L	6

Table 4-4 TRISO-Coated Particle Fuel Reactivity Accident Summary PIRT (continued)

Factor, Characteristic, or Phenomenon	Definition	INEEL		ORNL		SNL	
		Rank	KL*	Rank	KL*	Rank	KL*
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)	H	6	H	7	H	2
Inner PyC Layer: Condensed-phase diffusion	Inter-granular diffusion and/or intra-granular solid-state diffusion	L	7	L	7	L	2
Inner PyC Layer: Pressure loading (Fission products)	Stress loading of the layer by increased pressure from fission products	H	7	H	4	H	5
Inner PyC Layer: Pressure loading (Carbon monoxide)	Stress loading of the layer by carbon monoxide by increased pressure	H	7	H	4	H	3
Inner PyC Layer: Layer oxidation	Reaction of pyrolytic graphite with oxygen released from the kernel	M	5	L	7	L	4
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	M	7	L	4	H	2
Inner PyC Layer: Intercalation	Trapping of species between the basal planes of the structure	M	5	L	1	L	4
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)	H	7	H	6	H	4
Buffer Layer: Condensed-phase diffusion	Inter-granular diffusion and/or intra-granular solid-state diffusion	H	7	H	7	L	2
Buffer Layer: Response to kernel swelling	Mechanical reaction of the layer to the growth of the kernel via swelling	H	4	H	3	H	7

Table 4-4 TRISO-Coated Particle Fuel Reactivity Accident Summary PIRT (continued)

Factor, Characteristic, or Phenomenon	Definition	INEEL		ORNL		SNL	
		Rank	KL*	Rank	KL*	Rank	KL*
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	H	4	H	5	M	2
Buffer Layer: Layer oxidation	Reaction of buffer layer with-oxide materials in the kernel	L	5	L	7	L	4
Buffer Layer: Thermal gradient	Change in temperature with distance	M	7	H	2	L	5
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	L	7	M	5	L	7
Kernel: Maximum fuel temperature	Maximum fuel temperature attained by the fuel kernel during the accident	H	7	H	6	H	8
Kernel: Temperature vs. time transient conditions	The time-dependent variation of fuel temperature with time	H	7	H	7	H	8
Kernel: Energy deposition (total)	Amount of fission energy generated in kernel during reactivity event (j/gm heavy metal because of Pu)	H	7	H	4	H	7
Kernel: Energy deposition rate	Rate at which fission energy is generated in kernel	H	7	M	8	M	6
Kernel: Energy Transport: Conduction within kernel	Flow of heat within a medium from a region of high temperature to a region of low temperature	M	7	H	5	H	6
Kernel: Thermodynamic state of fission products	Chemical and physical state of fission products	H	7	H	6	H	7

Table 4-4 TRISO-Coated Particle Fuel Reactivity Accident Summary PIRT (continued)

Factor, Characteristic, or Phenomenon	Definition	INEEL		ORNL		SNL	
		Rank	KL*	Rank	KL*	Rank	KL*
Kernel: Gas-phase diffusion	Diffusion of gaseous fission products through layer (Knudsen and bulk diffusion through pore structure, and pressure driven permeation through structure)	H	5	H	5	M	6
Kernel: Condensed-phase diffusion	Inter-granular diffusion and/or intra-granular solid-state diffusion	H	5	H	6	H	6
Kernel: Oxygen flux	Mass transport of oxygen per unit surface area per unit time	L	No entry	L	3	M	5
Kernel: Grain growth	Enlargement of grains as a result of diffusion	M	5	L	5	L	7
Kernel: Buffer carbon-kernel interaction	Chemical reaction between carbon and the fuel (UO ₂) to form UC ₂ and CO (gas)	L	6	L	5	H	2

* KL = Knowledge Level

Table 4-5 TRISO-Coated Particle Fuel Depressurization Accident with Water Ingress Summary PIRT

Factor, Characteristic, or Phenomenon	Definition	INEEL		ORNL		SNL	
		Rank	KL*	Rank	KL	Rank	KL
Fuel Element: Irradiation history	The temperature, burnup and fast fluence history of the layer	M	7	H	7	H	3
Fuel Element: Condensed phase diffusion	Inter-granular diffusion and/or intra-granular solid-state diffusion	H	6	H	4	M	1
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	H	5	H	7	H	4
Fuel Element: Transport of metallic FPs through fuel element – Chemical form	Chemical stoichiometry of the chemical species that includes the radioisotope of interest	H	7	H	5	H	4
Fuel Element: Chemical attack by water – Kinetics	Rate of reaction per unit surface area as a function of temperature and partial pressure of steam	H	6	H	4	H	4
Fuel Element: Chemical attack by water – Catalysis	Modification of the reaction rate by fission products or impurities	M	5	M	4	H	4
Fuel Element: Chemical attack by water – changes in chemical form of fission products	Changes in chemical form resulting from oxidizing or reducing fission products	H	7	H	4	H	5
Fuel Element: Chemical attack by water – Changes in graphite properties	Changes in diffusivity, porosity, adsorptivity, etc.	M	6	H	4	H	2
Fuel Element: Chemical attack by water – Holdup reversals	Release of graphite FP inventory	M	6	H	4	L	5

Table 4-5 TRISO-Coated Particle Fuel Depressurization Accident with Water Ingress Summary PIRT (continued)

Factor, Characteristic, or Phenomenon	Definition	INEEL		ORNL		SNL	
		Rank	KL*	Rank	KL	Rank	KL
Fuel Element: Chemical attack by water – Temperature distributions	Impact of graphite oxidation on temperature distribution through material	H	8	H	4	H	5
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)	M	6	M	5	H	6
Outer PyC Layer: Condensed-phase diffusion	Inter-granular diffusion and/or intra-granular solid-state diffusion	M	6	M	7	M	2
Outer PyC Layer: Layer oxidation	Uptake of oxygen by the layer through a chemical reaction	H	7	H	4	H	2
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	L	8	M	6	L	2
Outer PyC Layer: Intercalation	Trapping of species between sheets of the graphite structure	M	4	L	2	L	2
Outer PyC Layer: Trapping	Adsorption of fission products on defects	M	4	L	3	L	2
Outer PyC Layer: Cracking	Lengths, widths and numbers of cracks produced in layer during operation or an accident	M	6	H	5	H	1
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	H	7	H	3	H	6
Outer PyC Layer: Chemical attack by water – Catalysis	Modification of the reaction rate by fission products or impurities	M	4	M	4	H	3
Outer PyC Layer: Chemical attack by water – Changes in chemical form of fission products	Changes in chemical form resulting from oxidizing or reducing fission products	H	7	H	4	H	5

Table 4-5 TRISO-Coated Particle Fuel Depressurization Accident with Water Ingress Summary PIRT (continued)

Factor, Characteristic, or Phenomenon	Definition	INEEL		ORNL		SNL	
		Rank	KL*	Rank	KL	Rank	KL
Outer PyC Layer: Chemical attack by water – Changes in graphite properties	Changes in diffusivity, porosity, adsorptivity, etc.	M	6	L	1	H	3
Outer PyC Layer: Chemical attack by water – Holdup reversals	Release of graphite FP inventory	M	6	M	3	L	4
Outer PyC Layer: Chemical attack by water – Temperature distributions	Impact of graphite oxidation on temperature distribution through material	H	8	H	5	H	3
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)	H	7	H	4	H	6
SiC Layer: Condensed-phase diffusion	Inter-granular diffusion and/or intra-granular solid-state diffusion	H	7	H	4	M	2
SiC Layer: Thermal deterioration/decomposition	Decline in the quality of the layer due to thermal loading	M	8	M	4	M	3
SiC Layer: Fission product corrosion	Attack of layer by fission products, e.g., Pd	M	7	M	7	L	3
SiC Layer: Heavy metal diffusion	Diffusion of heavy metals through the intact layer	L	3	L	5	M	2
SiC Layer: Layer oxidation	Uptake of oxygen by the layer through a chemical reaction	H	5	M	4	L	5
SiC Layer: Fission product release through undetected defects	Passage of fission products from the buffer region through regions in the SiC layer that fail during operation or an accident	M	5	M	7	H	1
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	H	7	H	4	H	4

Table 4-5 TRISO-Coated Particle Fuel Depressurization Accident with Water Ingress Summary PIRT (continued)

Factor, Characteristic, or Phenomenon	Definition	INEEL		ORNL		SNL	
		Rank	KL*	Rank	KL	Rank	KL
SiC Layer: Thermodynamics of the SiC-fission product system	Chemical form of fission products including the effects of solubility, intermetallics, and chemical activity	H	7	H	7	M	2
SiC Layer: Sintering	Change of SiC microstructure as a function of temperature	L	2	L	7	L	6
SiC Layer: Chemical attack by water – Kinetics	Rate of reaction per unit surface area as a function of temperature and partial pressure of steam	H	6	M	1	H	1
SiC Layer: Chemical attack by water – Catalysis	Modification of the reaction rate by fission products or impurities	M	5	L	1	M	1
SiC Layer: Chemical attack by water – Changes in chemical form of fission products	Changes in chemical form resulting from oxidizing or reducing fission products	H	7	H	4	H	5
SiC Layer: Chemical attack by water – Changes in SiC properties	Changes in diffusivity, porosity, adsorptivity, etc.	M	2	M	1	H	1
SiC Layer: Chemical attack by water – Holdup reversals	Release of graphite FP inventory	M	6	L	3	L	1
SiC Layer: Chemical attack by water – Temperature distributions	Impact of graphite oxidation on temperature distribution through material	H	8	H	5	H	5
Inner PyC Layer: Gas-phase diffusion	Diffusion of gaseous fission products through layer (Knaus and bulk diffusion through pore structure, and pressure driven permeation through structure)	M	6	H	4	H	6
Inner PyC Layer: Condensed-phase diffusion	Inter-granular diffusion and/or intra-granular solid-state diffusion	M	6	M	4	M	2
Inner PyC Layer: Pressure loading (Fission products)	Stress loading of the layer by increased pressure from fission products	H	8	H	7	L	2

Table 4-5 TRISO-Coated Particle Fuel Depressurization Accident with Water Ingress Summary PIRT (continued)

Factor, Characteristic, or Phenomenon	Definition	INEEL		ORNL		SNL	
		Rank	KL*	Rank	KL	Rank	KL
Inner PyC Layer: Pressure loading (Carbon monoxide)	Stress loading of the layer by carbon monoxide by increased pressure	H UO ₂ L UCO	8	H	7	H	2
Inner PyC Layer: Layer oxidation	Reaction of pyrolytic graphite with oxygen released from the kernel	H	3	H	3	H	2
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	L	8	H	7	L	2
Inner PyC Layer: Cracking	Lengths, widths and numbers of cracks produced in layer during accident	H	5	H	4	H	1
Inner PyC Layer: Intercalation	Trapping of species between sheets of the graphite structure	M	6	L	2	M	2
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	H	7	H	3	H	6
Inner PyC Layer: Chemical attack by water – Catalysis	Modification of the reaction rate by fission products or impurities	M	4	M	4	H	3
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	H	7	H	4	H	5
Inner PyC Layer: Chemical attack by water – Changes in graphite properties	Changes in diffusivity, porosity, adsorptivity, etc.	M	6	L	1	H	3
Inner PyC Layer: Chemical attack by water – Holdup reversals	Release of graphite FP inventory	M	6	L	3	L	4
Inner PyC Layer: Chemical attack by water – Temperature distributions	Impact of graphite oxidation on temperature distribution through material	H	8	H	5	H	3

Table 4-5 TRISO-Coated Particle Fuel Depressurization Accident with Water Ingress Summary PIRT (continued)

Factor, Characteristic, or Phenomenon	Definition	INEEL		ORNL		SNL	
		Rank	KL*	Rank	KL	Rank	KL
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)	L	7	H	7	H	4
Buffer Layer: Condensed-phase diffusion	Inter-granular diffusion and/or intra-granular solid-state diffusion	L	7	H	7	L	1
Buffer Layer: Response to kernel swelling	Mechanical reaction of the layer to the growth of the kernel via swelling	M	4	M	7	M	4
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	L	2	H	7	L	3
Buffer Layer: Layer oxidation	Reaction of buffer layer with oxide materials in the kernel	H	5	L	7	H	2
Buffer Layer: Thermal gradient	Change in temperature with distance	L	6	L	7	H	4
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	M	7	M	6	L	5
Buffer Layer: Chemical attack by water – Kinetics	Rate of reaction per unit surface area as a function of temperature and partial pressure of steam	M	7	M	4	L	6
Buffer Layer: Chemical attack by water – Catalysis	Modification of the reaction rate by fission products or impurities	L	3	L	4	L	4
Buffer Layer: Chemical attack by water – Changes in chemical form of fission products	Changes in chemical form resulting from oxidizing or reducing fission products	H	7	H	4	M	3

Table 4-5 TRISO-Coated Particle Fuel Depressurization Accident with Water Ingress Summary PIRT (continued)

Factor, Characteristic, or Phenomenon	Definition	INEEL		ORNL		SNL	
		Rank	KL*	Rank	KL	Rank	KL
Inner PyC Layer: Chemical attack by water – Changes in graphite properties	Changes in diffusivity, porosity, adsorptivity, etc.	L	3	L	1	L	3
Buffer Layer: Chemical attack by water – Holdup reversals	Release of graphite FP inventory	L	3	L	4	L	4
Buffer Layer: Chemical attack by water – Temperature distributions	Impact of graphite oxidation on temperature distribution through material	M	8	M	5	M	3
Kernel: Maximum fuel temperature	Maximum fuel temperature attained by the fuel kernel during the accident	H	7	H	7	H	6
Kernel: Temperature vs. time transient conditions	The time-dependent variation of fuel temperature with time	H	7	H	7	H	4
Kernel: Energy Transport: Conduction within kernel	Flow of heat within a medium from a region of high temperature to a region of low temperature	M	6	M	7	M	3
Kernel: Thermodynamic state of fission products	Chemical and physical state of fission products	H	7	H	4	H	5
Kernel: Oxygen flux	Mass transport of oxygen per unit surface area per unit time	L	6	L	3	M	3
Kernel: Grain growth	Enlargement of grains as a result of diffusion	L	4	L	3	L	8
Kernel: Buffer carbon-kernel interaction	Chemical reaction between carbon and the fuel (UO ₂) to form UC ₂ and CO (gas)	H	6	L	5	H	3
Kernel: Chemical attack by water – Kinetics	Rate of reaction per unit surface area as a function of temperature and partial pressure of steam	H	7	H	4	L	8
Kernel: Chemical attack by water – Catalysis	Modification of the reaction rate by fission products or impurities	M	5	M	1	L	8

Table 4-5 TRISO-Coated Particle Fuel Depressurization Accident with Water Ingress Summary PIRT (continued)

Factor, Characteristic, or Phenomenon	Definition	INEEL		ORNL		SNL	
		Rank	KL*	Rank	KL	Rank	KL
Kernel: Chemical attack by water – Changes in chemical form of fission products	Changes in chemical form resulting from oxidizing or reducing fission products	H	7	H	4	L	8
Kernel: Chemical attack by water – Changes in kernel properties	Changes in diffusivity, porosity, adsorptivity, etc.	M	5	H	5	No Entry	No entry

- KL = Knowledge Level

Table 4-6 TRISO-Coated Particle Fuel Depressurization Accident with Air Ingress Summary PIRT

Factor, Characteristic, or Phenomenon	Definition	INEEL		ORNL		SNL	
		Rank	KL*	Rank	KL	Rank	KL
Fuel Element: Irradiation history	The temperature, burnup and fast fluence history of the layer	M	7	H	7	H	3
Fuel Element: Condensed phase diffusion	Inter-granular diffusion and/or intra-granular solid-state diffusion	H	6	H	4	M	1
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	H	5	H	7	H	4
Fuel Element: Transport of metallic FPs through fuel element – Chemical form	Chemical stoichiometry of the chemical species that includes the radioisotope of interest	H	7	H	5	H	4
Fuel Element: Chemical attack by air – Kinetics	Rate of reaction per unit surface area as a function of temperature and partial pressure of air	H	7	H	5	H	4
Fuel Element: Chemical attack by air – Catalysis	Modification of the reaction rate by fission products or impurities	M	5	H	4	H	5
Fuel Element: Chemical attack by air – Changes in chemical form of fission products	Changes in chemical form resulting from oxidizing or reducing fission products	H	6	H	4	H	4
Fuel Element: Chemical attack by air – Changes in graphite properties	Changes in diffusivity, porosity, adsorptivity, etc.	H	6	H	4	H	2
Fuel Element: Chemical attack by air – Holdup reversals	Release of graphite FP inventory	M	6	H	4	L	5

Table 4-6 TRISO-Coated Particle Fuel Depressurization Accident with Air Ingress Summary PIRT (continued)

Factor, Characteristic, or Phenomenon	Definition	INEEL		ORNL		SNL	
		Rank	KL*	Rank	KL	Rank	KL
Fuel Element: Chemical attack by air – Temperature distributions	Impact of graphite oxidation on temperature distribution through material	H	8	H	4	H	6
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)	H	6	H	5	H	6
Outer PyC Layer: Condensed-phase diffusion	Inter-granular diffusion and/or intra-granular solid-state diffusion	H	6	H	7	M	2
Outer PyC Layer: Layer oxidation	Uptake of oxygen by the layer through a chemical reaction	H	7	H	4	H	2
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	L	8	M	6	L	2
Outer PyC Layer: Intercalation	Trapping of species between sheets of the graphite structure	M	4	L	2	L	2
Outer PyC Layer: Trapping	Adsorption of fission products on defects	M	4	L	3	L	2
Outer PyC Layer: Cracking	Lengths, widths and numbers of cracks produced in layer during operation or an accident	M	6	H	5	H	1
Outer PyC Layer: Chemical attack by air – Kinetics	Modification of the reaction rate by fission products or impurities	H	7	H	4	H	2
Outer PyC Layer: Chemical attack by air – Catalysis	Modification of the reaction rate by fission products or impurities	M	4	M	3	H	4
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	H	7	H	4	H	5
Outer PyC Layer: Chemical attack by air – Changes in graphite properties	Changes in diffusivity, porosity, adsorptivity, etc.	M	6	M	1	H	3

Table 4-6 TRISO-Coated Particle Fuel Depressurization Accident with Air Ingress Summary PIRT (continued)

Factor, Characteristic, or Phenomenon	Definition	INEEL		ORNL		SNL	
		Rank	KL*	Rank	KL	Rank	KL
Outer PyC Layer: Chemical attack by air – Holdup reversal	Release of graphite FP inventory	M	6	L	3	L	4
Outer PyC Layer: Chemical attack by air – Temperature distributions	Impact of graphite oxidation on temperature distribution through material	H	8	H	5	H	3
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)	H	7	H	4	H	6
SiC Layer: Condensed-phase diffusion	Inter-granular diffusion and/or intra-granular solid-state diffusion	H	7	H	4	M	2
SiC Layer: Thermal deterioration/decomposition	Decline in the quality of the layer due to thermal loading	M	8	H	4	M	3
SiC Layer: Fission product corrosion	Attack of layer by fission products, e.g., Pd	M	7	H	7	L	3
SiC Layer: Heavy metal diffusion	Diffusion of heavy metals through the intact layer	L	3	L	5	M	2
SiC Layer: Layer oxidation	Uptake of oxygen by the layer through a chemical reaction	H	5	H	4	L	5
SiC Layer: Fission product release through undetected defects	Passage of fission products from the buffer region through regions in the SiC layer that fail during operation or an accident	M	5	M	7	H	1
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	H	7	H	4	H	4
SiC Layer: Thermodynamics of the SiC-fission product system	Chemical form of fission products including the effects of solubility, intermetallics, and chemical activity	H	7	H	7	M	2

Table 4-6 TRISO-Coated Particle Fuel Depressurization Accident with Air Ingress Summary PIRT (continued)

Factor, Characteristic, or Phenomenon	Definition	INEEL		ORNL		SNL	
		Rank	KL*	Rank	KL	Rank	KL
SiC Layer: Sintering	Change of SiC microstructure as a function of temperature	L	2	L	7	L	6
SiC Layer: Chemical attack by air – Kinetics	Modification of the reaction rate by fission products or impurities	H	5	H	4	H	4
SiC Layer: Chemical attack by air – Catalysis	Modification of the reaction rate by fission products or impurities	M	5	L	1	L	2
SiC Layer: Chemical attack by air – Changes in chemical form of fission products	Changes in chemical form resulting from oxidizing or reducing fission products	H	7	H	4	H	6
SiC Layer: Chemical attack by air – Changes in SiC properties	Changes in diffusivity, porosity, adsorptivity, etc.	M	4	H	1	M	2
SiC Layer: Chemical attack by air – Holdup reversal	Release of graphite FP inventory	M	4	L	3	L	1
SiC Layer: Chemical attack by air – Temperature distributions	Impact of graphite oxidation on temperature distribution through material	H	8	H	5	H	6
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)	H	6	H	4	H	6
Inner PyC Layer: Condensed-phase diffusion	Inter-granular diffusion and/or intra-granular solid-state diffusion	M	6	M	4	M	2
Inner PyC Layer: Pressure loading (Fission products)	Stress loading of the layer by increased pressure from fission products	H	8	H	7	L	2
Inner PyC Layer: Pressure loading (Carbon monoxide)	Stress loading of the layer by carbon monoxide by increased pressure	H L UCO	8	H	7	L	2

Table 4-6 TRISO-Coated Particle Fuel Depressurization Accident with Air Ingress Summary PIRT (continued)

Factor, Characteristic, or Phenomenon	Definition	INEEL		ORNL		SNL	
		Rank	KL*	Rank	KL	Rank	KL
Inner PyC Layer: Layer oxidation	Reaction of pyrolytic graphite with oxygen released from the kernel	H	3	H	3	H	2
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	L	8	H	7	L	2
Inner PyC Layer: Cracking	Lengths, widths and numbers of cracks produced in layer during accident	H	5	H	4	H	1
Inner PyC Layer: Intercalation	Trapping of species between sheets of the graphite structure	M	6	L	2	M	2
Inner PyC Layer: Chemical attack by air – Kinetics	Modification of the reaction rate by fission products or impurities	H	7	H	4	H	5
Inner PyC Layer: Chemical attack by air – Catalysis	Modification of the reaction rate by fission products or impurities	M	4	M	1	H	3
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	H	7	H	4	H	5
Inner PyC Layer: Chemical attack by air – Changes in graphite properties	Changes in diffusivity, porosity, adsorptivity, etc.	M	6	M	2	H	1
Inner PyC Layer: Chemical attack by air – Holdup reversal	Release of graphite FP inventory	M	6	L	2	L	2
Inner PyC Layer: Chemical attack by air – Temperature distributions	Impact of graphite oxidation on temperature distribution through material	H	8	H	4	H	3
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)	L	7	H	7	H	4
Buffer Layer: Condensed-phase diffusion	Inter-granular diffusion and/or intra-granular solid-state diffusion	L	7	H	7	L	1

Table 4-6 TRISO-Coated Particle Fuel Depressurization Accident with Air Ingress Summary PIRT (continued)

Factor, Characteristic, or Phenomenon	Definition	INEEL		ORNL		SNL	
		Rank	KL*	Rank	KL	Rank	KL
Buffer Layer: Response to kernel swelling	Mechanical reaction of the layer to the growth of the kernel via swelling	M	4	H	5	M	4
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	L	2	H	7	L	3
Buffer Layer: Layer oxidation	Reaction of buffer layer with oxide materials in the kernel	H	5	L	7	H	2
Buffer Layer: Thermal gradient	Change in temperature with distance	L	6	L	7	H	4
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	M	7	M	6	L	5
Buffer Layer: Chemical attack by air – Kinetics	Modification of the reaction rate by fission products or impurities	M	7	M	3	L	2
Buffer Layer: Chemical attack by air – Catalysis	Modification of the reaction rate by fission products or impurities	L	3	M	1	L	4
Buffer Layer: Chemical attack by air – Changes in chemical form of fission products	Changes in chemical form resulting from oxidizing or reducing fission products	H	7	H	4	L	6
Buffer Layer: Chemical attack by air – Changes in graphite properties	Changes in diffusivity, porosity, adsorptivity, etc.	L	3	L	2	L	3
Buffer Layer: Chemical attack by air – Holdup reversal	Release of graphite FP inventory	L	3	L	2	L	2
Buffer Layer: Chemical attack by air – Temperature distributions	Impact of graphite oxidation on temperature distribution through material	H	8	H	4	M	4

Table 4-6 TRISO-Coated Particle Fuel Depressurization Accident with Air Ingress Summary PIRT (continued)

Factor, Characteristic, or Phenomenon	Definition	INEEL		ORNL		SNL	
		Rank	KL*	Rank	KL	Rank	KL
Kernel: Maximum fuel temperature	Maximum fuel temperature attained by the fuel kernel during the accident	H	7	H	7	H	6
Kernel: Temperature vs. time transient conditions	The time-dependent variation of fuel temperature with time	H	7	H	7	H	4
Kernel: Energy Transport: Conduction within kernel	Flow of heat within a medium from a region of high temperature to a region of low temperature	M	6	M	7	M	3
Kernel: Thermodynamic state of fission products	Chemical and physical state of fission products	H	7	H	4	H	5
Kernel: Oxygen flux	Mass transport of oxygen per unit surface area per unit time	L	6	L	3	M	3
Kernel: Grain growth	Enlargement of grains as a result of diffusion	L	4	L	3	L	8
Kernel: Buffer carbon-kernel interaction	Chemical reaction between carbon and the fuel (UO ₂) to form UC ₂ and CO (gas)	H	6	L	5	H	3
Kernel: Chemical attack by air – Kinetics	Modification of the reaction rate by fission products or impurities	H	7 UO ₂ 6 UCO	H	3	L	9
Kernel: Chemical attack by air – Catalysis	Modification of the reaction rate by fission products or impurities	M	3	L	1	L	1
Kernel: Chemical attack by air – Changes in chemical form of fission products	Changes in chemical form resulting from oxidizing or reducing fission products	H	7	H	4	L	5
Kernel: Chemical attack by air – Changes in kernel properties	Changes in diffusivity, porosity, adsorptivity, etc.	M	5	M	4	L	8

- KL = Knowledge Level

5. TRISO-COATED PARTICLE FUEL PIRT ANALYSES AND SUMMARY

The PIRT analysis and summary information presented in this chapter is based on two sources. The first source is the summary TRISO-coated particle fuel PIRT tables presented for Manufacturing, Operations, Depressurized Heatup Accident, Reactivity Accident, Depressurization Accident With Water Ingress, and Depressurization Accident With Air Ingress PIRT Analysis presented in Chapter 4. The second source is the detailed PIRT inputs submitted by the TRISO-coated particle fuel PIRT panel members as found in Appendices A-F. A PIRT effort was started for the Design phase of the TRISO-coated particle fuel life cycle but it was not continued to completion. Preliminary panel findings on the Design PIRT are provided in Appendix H.

General technical findings from the TRISO-coated particle fuel PIRTs are presented in Section 5.1. Analyses of the findings for each individual PIRT are provided in Sections 5.2 through 5.7. As with each PIRT effort, lessons are learned that may prove beneficial to subsequent PIRT efforts. Programmatic lessons learned from the TRISO-coated particle fuel PIRT effort are provided in Section 5.8.

5.1 General TRISO-Coated Particle Fuel PIRT Findings

In this section, key findings of the TRISO-coated particle fuel PIRT panel are identified, analyzed and summarized.

Each of the six summary PIRTs presented in Chapter 4 were examined and each factor, characteristic or phenomenon determined to be of High importance by all PIRT panel members was identified. The resulting consensus TRISO-coated particle fuel factors, characteristics, and phenomena ranked high are presented in Table 5-1.

The factors, characteristics or phenomena entered in Table 5-1 for Manufacturing do not appear in any of the remaining five PIRT tables.

The Depressurization Heatup Accident with Air Ingress was characterized by a large number of highly ranked phenomena (25). Approximately one-half of these were directly related to phenomena associated with the interaction of air with the various components of TRISO-coated particle fuel. Interactions of air with the kernel and buffer layer were not ranked high by the PIRT panel. However, changes in the chemical form of fission products, kinetics, and temperature distributions associated with a chemical attack by air were ranked High for the remaining layers of the TRISO-coated particle fuel. Two of the panel members generally concluded that the knowledge level regarding these phenomena were either Low or Mid-range while the third panel member concluded the knowledge level was High. Phenomena associated with interactions of air with the TRISO-coated particle fuel may require additional research effort if the majority perspective on importance is confirmed.

Similar conclusions apply for the Depressurization Accident with Water Ingress. The primary difference is that phenomena associated with the interaction of water with the various components of TRISO-coated particle fuel are only ranked High for the fuel element and outer PyC layers. As with air ingress, two of the panel members generally concluded that the knowledge level regarding these phenomena were either Low or Mid-range while the third panel member concluded the knowledge level was High. Phenomena associated with interactions of water with the TRISO-coated particle fuel

may require additional research effort if the Depressurization Accident with Water Ingress is to be included among events considered within the licensing basis or as a severe core damage accident.

In addition to the observations regarding the air- and water-ingress accidents, the factors, characteristics and phenomena in Table 5-1 were further evaluated using several screening criteria. Although helpful in focusing attention on specific factors, characteristics and phenomena, the criteria are, in fact, arbitrary. Those who plan to utilize the TRISO-coated particle fuel PIRT should examine each of the factors, characteristics and phenomena carrying a consensus importance ranking of High and those factors, characteristics, and phenomena viewed by a majority of the panel members as having High importance. Table 5-1 identifies only those factors, characteristics, and phenomena viewed by all panel members as having High importance. These screening criteria identify additional factors, characteristics and phenomena of potential importance.

The first screening criterion was a consensus importance ranking of High in three or more of the six conditions considered. The first screening aggregated the results for each component of the TRISO-coated particle fuel, i.e., kernel, buffer layer, inner pyrolytic carbon (PyC) layer, silicon carbide (SiC) layer, Outer PyC layer, and fuel element. Ten factors, characteristics and phenomena were identified by this screening criterion. The knowledge level assessed by the PIRT panel for each of the ten was then considered. The resulting analyses for the ten factors identified by the first screening criterion are presented below.

1. Temperature related phenomena in the kernel, i.e., maximum fuel temperature and temperature versus time transient conditions, were judged to be important for each of the four accident conditions considered. The knowledge level was judged to be High by two of the panel members while the third judged it to be at the upper end of the Mid-range. These two factors do not require additional research efforts.
2. The thermodynamic state of the fission products in the kernel was judged to be important for each of the four accident conditions considered. The knowledge level was judged to be Mid-range by two of the panel members while the third judged it to be High. This factor may require additional research for the water- and air-ingress accidents, if these events are to be included among the events considered within the licensing basis or as a severe core damage accident.
3. The knowledge level for cracking of the inner PyC layer was judged by all panel members to be either in the Low or Mid-range. Research to achieve better understanding of this phenomenon, i.e., increased knowledge level, is needed for this phenomenon.
4. The knowledge level for gas phase diffusion through the inner PyC layer was judged to be High by two of the panel members for the different conditions and Mid-range or Low by the other panel member. This phenomenon may require additional research.

Table 5-1 TRISO-Coated Particle Fuel Factors, Characteristics, and Phenomena Ranked High

Factor, Characteristic or Phenomenon	Condition					
	Manufacture	Operation	Depressurization Accident	Reactivity Accident	Water Ingress Accident	Air Ingress Accident
Kernel: CO production		X				
Kernel: Condensed-phase diffusion			X	X		
Kernel: Energy deposition (total)				X		
Kernel: Gas-phase diffusion			X			
Kernel: Maximum fuel temperature			X	X	X	X
Kernel: Temperature vs. time transient conditions			X	X	X	X
Kernel: Thermodynamic state of fission products			X	X	X	X
Buffer Layer: Cracking		X				
Buffer Layer: Gas-phase diffusion			X	X		
Buffer Layer: Pressure		X				
Buffer Layer: Response to kernel swelling				X		
Buffer Layer: Temperature gradient		X				
Buffer Layer: Thin or missing	X					
Inner PyC Layer: Chemical attack by air or water – Changes in chemical form of fission products					X	X
Inner PyC Layer: Chemical attack by air or water – Kinetics					X	X
Inner PyC Layer: Chemical attack by air or water – Temperature distributions					X	X
Inner PyC layer: Condensed phase diffusion		X				
Inner PyC layer: Cracking		X	X		X	X
Inner PyC layer: Gas phase diffusion		X	X	X		X
Inner PyC Layer: Layer oxidation					X	X
Inner PyC Layer: Pressure loading (Carbon monoxide)			X	X	X	
Inner PyC Layer: Pressure loading (Fission products)				X		
Inner PyC layer: Anisotropy (initial)	X					
Inner PyC layer: Bonding strength (inner PyC to SiC)	X					

Table 5-1 TRISO-Coated Particle Fuel Factors, Characteristics, and Phenomena Ranked High (continued)

Factor, Characteristic or Phenomenon	Condition					
	Manufacture	Operation	Depressurization Accident	Reactivity Accident	Water Ingress Accident	Air Ingress Accident
SiC Layer: Chemical attack by air or water- Changes in chemical form of fission products					X	X
SiC Layer: Chemical attack by air or water - Kinetics						X
SiC Layer: Chemical attack by air or water - Temperature distributions					X	X
SiC layer: Condensed phase diffusion		X				
SiC layer: Cracking		X				
SiC layer: Defects	X					
SiC layer: Density	X					
SiC layer: Fission product corrosion		X				
SiC Layer: Fission product release through failures, e.g., cracking			X	X	X	X
SiC Layer: Fission product release through undetected defects			X			
SiC layer: Fracture strength	X					
SiC layer: Gas phase diffusion		X	X		X	X
SiC layer: Grain size and microstructure, e.g., alignment	X					
SiC layer: Stoichiometry	X					
SiC Layer: Thermodynamics of the SiC-fission product system			X			
Outer PyC layer: Anisotropy (initial)	X					
Outer PyC Layer: Chemical attack by air or water - Changes in chemical form of fission products					X	X
Outer PyC Layer: Chemical attack by air or water - Kinetics					X	X
Outer PyC Layer: Chemical attack by air or water - Temperature distributions					X	X
Outer PyC Layer: Cracking			X			
Outer PyC layer: Gas phase diffusion		X	X			X
Outer PyC Layer: Layer oxidation					X	X

Table 5-1 TRISO-Coated Particle Fuel Factors, Characteristics, and Phenomena Ranked High (continued)

Factor, Characteristic or Phenomenon	Condition					
	Manufacture	Operation	Depressurization Accident	Reactivity Accident	Water Ingress Accident	Air Ingress Accident
Fuel Element: Chemical attack by air or water – Changes in chemical form of fission products					X	X
Fuel Element: Chemical attack by air or water – Changes in graphite properties						X
Fuel Element: Chemical attack by air or water – Kinetics					X	X
Fuel Element: Chemical attack by air or water – Temperature distributions					X	X
Fuel Element: Compacting	X					
Fuel element: Condensed phase diffusion		X				
Fuel Element: Gas-phase diffusion				X	X	X
Fuel Element: Impurities Control	X					
Fuel Element: Initial particle defect fraction due to manufacture	X					
Fuel Element: Irradiation history			X			
Fuel Element: Matrix and Binder	X					
Fuel Element: Particle overcoating (fuel form dependent)	X					
Fuel Element: Strength	X					
Fuel Element: Tramp Uranium	X					
Fuel Element: Transport of metallic fission products– Chemical form			X		X	X
Layer coating process specifications: Ratio of gases	X					
Layer coating process specifications: Temperature	X					
Layer coating process specifications: Coating Rate	X					
Layer coating process specifications: Coater Size	X					
Layer coating process	X					
Process control:	X					

5. The importance of pressure loading of the inner PyC layer by carbon monoxide was judged to be High by two of the panel members and Low by the other panel member.
6. The panel members assessed the knowledge level for fission product release through SiC layer failures as primarily Mid-range or High.
7. The knowledge level for gas phase diffusion through the SiC layer was judged to be Mid-range or High by the panel members.
8. The knowledge level for gas phase diffusion through the fuel element as assessed by the panel members spanned the range from Low to High. This phenomenon may require additional research.
9. The panel members assessed the knowledge level for the chemical form of the metallic fission products transported through the fuel element to primarily be in Mid-range. A better understanding of this phenomenon, (i.e., increased knowledge level), is needed for this phenomenon.

The second screening criterion was the appearance of a phenomenon three or more times in Table 5-1 when considering all conditions and all components of the TRISO-coated particle fuel. This screening criterion identified four phenomena. The knowledge level assessed by the PIRT panel for each of the four was then considered. The resulting analyses for the four factors identified by the first screening criterion are presented below.

1. Condensed-phase diffusion appeared four times in Table 5-1. With one exception, the knowledge level for condensed-phase diffusion was judged to be Mid-range or High by the panel members. Three of the four rankings of High importance were associated with Operations. This phenomenon appears to be most important during the operational phase of the TRISO-coated particle fuel life cycle.
2. Gas-phase diffusion appeared 15 times in Table 5-1. Gas-phase diffusion is considered an important phenomenon that must be well understood. Knowledge levels were generally assessed as either Mid-range or High but there were instances where the knowledge level was assessed as low. This phenomenon may require additional research effort.
3. Particle layer cracking appeared 10 times in Table 5-1. Layer cracking is considered an important phenomenon that must be well understood. Knowledge levels were generally assessed as either Low or Mid-range. Seven of the ten cracking entries in Table 5-1 were associated with the inner PyC and SiC layers. Research to achieve a better understanding of this phenomenon, (i.e., increased knowledge level), appears to be needed for this phenomenon.
4. Pressure or pressure loading on particle layers appeared five times in Table 5-1. Pressure loading is considered a phenomenon that must be well understood. Knowledge levels were generally assessed as either Mid-range or High but there were instances where the knowledge level was assessed as low. The pressure-related entries in Table 5-1 were primarily associated with the inner PyC layer. This phenomenon may require additional research.

5.2 Manufacturing PIRT Analysis

The Manufacturing PIRT presented in this section differs in several important ways from the remaining PIRTs presented in Sections 5.3 – 5.7. First, several process specifications were identified and ranked for importance and the level of knowledge assessed. Second, several process or process control factors were identified and ranked for importance and the level of knowledge assessed. Third, only two members of the PIRT panel provided input for the Manufacturing PIRT, the remaining panel member declining due to a lack of manufacturing experience.

Several summary statistics regarding the manufacturing of TRISO-coated particle fuel are provided in Table 5-2. The statistical summary is presented to draw attention to (1) the number of factors identified by consensus to be of High importance relative to the total number of factors, (2) the number of factors identified to be of High importance by a majority of the panel, and (3) the number of factors identified by a majority, but not consensus, to be of High importance, and (4) the number of factors for which the range of importance assessed by the panel members was so large that the PIRT findings are inconclusive. The factors in each of the above categories are listed following Table 5-2.

Table 5-2 Significant Importance and Knowledge Level Statistics for Manufacturing

Total Number of Factors¹	35
--	----

¹Factor: factor, characteristic, or phenomenon identified for Manufacturing

Consensus Assessment²	High Importance	Knowledge Level		
		Low 1-3	Mid-range 4-6	High 7-9
Not applicable	22	0	8	9

²Consensus Assessment: All panel members had identical assessment of importance and knowledge level.

Majority Assessment³	High Importance	Knowledge Level
		Low or mid-range 1-6
		Not Applicable

³Majority Assessment: Two members of the three-member panel

Divergent Assessment⁴	Importance⁵	Knowledge Level⁴
All fuel temperatures	5	

⁴Divergent Assessment: A range of High to Low importance assessed by individual panel members.

⁵Knowledge level deemed secondary to the divergent importance rankings amongst the panel members.

The two participating panel members concluded that 22 of the 35 Manufacturing factors, characteristics and phenomena are of “High” importance. The fraction of factors ranked High for Manufacturing is larger than for the other five PIRTs. One reason may be that the panel identified only important or near important factors when it created the PIRT table. Of the 22 High-importance factors, characteristics and phenomena, these panel members agreed that the knowledge levels of nine are High (7-9). These nine items follow.

Kernel	None
Buffer layer	Thin or missing
Inner pyrolytic carbon layer	None
SiC layer	Density
Outer PyC layer	None
Fuel element	Particle overcoating (fuel form dependent) Compacting Impurities control Tramp uranium Strength
Other	Layer coating process specifications – ratio of gases Layer coating process specifications – temperature

Of the 22 High-importance factors, characteristics and phenomena, the two participating panel members agreed that the knowledge levels of eight are Mid-range (4-6). These eight items follow.

Kernel	None
Buffer layer	None
Inner PyC layer	Anisotropy (initial)
SiC layer	Fracture strength Stoichiometry Defects
Outer PyC layer	Anisotropy (initial)
Fuel element	None
Other	Layer coating process specifications – coater size Layer coating process Process control

The two participating panel members agreed that there are no factors, characteristics, or phenomena for which the importance is High and the knowledge level Low (1-3).

There are no factors, characteristics, or phenomena for which one of the two participating panel members ranked the importance High and one as Low.

5.3 Operations PIRT Analysis

Several summary statistics regarding the Operation of TRISO-coated particle fuel are provided in Table 5-3. A brief discussion of each is provided following Table 5-3.

Table 5-3 Significant Importance and Knowledge Level Statistics for Operations

Total Number of Factors¹	46
--	----

¹Factor: factor, characteristic, or phenomenon identified for Operations

Consensus Assessment²	High Importance	Knowledge Level		
		Low 1-3	Mid-range 4-6	High 7-9
	13	0	3	0

²Consensus Assessment: All panel members had identical assessment of importance and knowledge level.

Majority Assessment ³	High Importance	Knowledge Level
	3	Low or mid-range 1-6
		3

³Majority Assessment: Two members of the three-member panel

Divergent Assessment ⁴	Importance ⁵	Knowledge Level ⁴
All fuel temperatures	8	

⁴Divergent Assessment: A range of High to Low importance assessed by individual panel members.

⁵Knowledge level deemed secondary to the divergent importance rankings amongst the panel members.

The panel determined that 13 of the 46 Operation factors, characteristics and phenomena are of "High" importance. The thirteen factors are:

Kernel	Carbon monoxide production
Buffer layer	Pressure Cracking Temperature gradient
Inner PyC layer	Cracking Condensed phase diffusion Gas phase diffusion
SiC layer	Fission product corrosion Cracking Condensed phase diffusion Gas phase diffusion
Outer PyC layer	Gas phase diffusion
Fuel element	Condensed phase diffusion

There is a consensus among the panel members that the level of knowledge is Mid-range (4-6) for buffer layer pressure, SiC layer fission product corrosion, and fuel element condensed phase diffusion.

There is one factor, characteristic or phenomenon ranked of High importance by a majority of the panel (two members) and the knowledge level assessed as either Low or Mid-Range. The factor is radiation induced creep in the inner PyC layer.

There are nine factors, characteristics, or phenomena for which the range of panel importance assessments varies from High to Low. These nine items should be the focus of particular attention by the international peer review group, with the objective of developing a clear majority assessment of importance. The nine items are:

Kernel	Burnup Microstructure changes Fission product chemical form Kernel-buffer interaction Fission product generation Temperature gradient
Buffer layer	Carbonyl vapor species
Inner PyC layer	Anisotropy

	Radiation induced creep
SiC layer	None
Outer PyC layer	None
Fuel element	None

5.4 Depressurization Heatup Accident PIRT Analysis

Several summary statistics regarding the Depressurization Heatup Accident PIRT results for two temperature ranges, i.e., fuel temperatures $T_{fuel} \leq 1600$ °C and $T_{fuel} > 1600$ °C, are provided in Table 5-4. A brief discussion of each is provided following Table 5-4.

Table 5-4 Significant Importance and Knowledge Level Statistics for the Depressurization Heatup Accident

Total Number of Factors ¹	46
---	----

¹Factor: factor, characteristic, or phenomenon identified for Depressurization Heatup Accident

Consensus Assessment ²	High Importance	Knowledge Level		
		Low 1-3	Mid-range 4-6	High 7-9
All fuel temperatures	17	0	0	0

²Consensus Assessment: All panel members had identical assessment of importance and knowledge level.

Majority Assessment ³	High Importance	Knowledge Level
		Low or mid-range 1-6
$T_{fuel} \leq 1600$ °C	8	8

³Majority Assessment: Two members of the three-member panel

Majority Assessment ⁴	High Importance	Knowledge Level
		Low or mid-range 1-6
$T_{fuel} > 1600$ °C	12	12

⁴Majority Assessment: Two members of the three-member panel

Divergent Assessment ⁵	Importance ⁶	Knowledge Level ⁵
All fuel temperatures	6	

⁵Divergent Assessment: A range of High to Low importance assessed by individual panel members.

⁶Knowledge level deemed secondary to the divergent importance rankings amongst the panel members.

The panel determined that 17 of the 46 Depressurization Heatup Accident factors, characteristics and phenomena are of High importance. The seventeen factors are:

Kernel	Condensed phase diffusion Gas-phase diffusion Maximum fuel temperature Temperature vs. time transient conditions Thermodynamic state of fission products
Buffer layer	Gas-phase diffusion
Inner PyC layer	Cracking Gas phase diffusion Pressure loading (carbon monoxide)
SiC layer	Fission product release through failures, e.g., cracking Fission product release through undetected failures Gas-phase diffusion Thermodynamics of the SiC fission product system
Outer PyC layer	Cracking Gas phase diffusion
Fuel element	Irradiation history Transport of metallic fission products – chemical form

There is no consensus agreement among the panel members on the level of knowledge for any of the 17 High-ranked factors, characteristics and phenomena. However, there are four factors, characteristics and phenomena for which all three panel members agreed that the knowledge level is Low or Mid-range for $T_{fuel} \leq 1600$ °C (Fuel Element: Transport of metallic FPs through fuel element – Chemical form, Outer PyC Layer: Cracking, SiC Layer: Fission product release through undetected defects, and Inner PyC Layer: Cracking) and six factors, characteristics and phenomena for $T_{fuel} > 1600$ °C (Fuel Element: Irradiation history, Fuel Element: Transport of metallic FPs through fuel element – Chemical form, Outer PyC Layer: Cracking, SiC Layer: Fission product release through undetected defects, SiC Layer: Fission product release through failures, e.g., cracking, and Inner PyC Layer: Cracking).

There are two factors, characteristics or phenomena ranked of High importance by a majority of the panel (two members) and the knowledge level is assessed as either Low or Mid-Range for fuel temperatures ≤ 1600 °C and four factors, characteristics and phenomena for which the knowledge level assessed as either Low or Mid-Range for fuel temperatures > 1600 °C. The factors are:

	$T_{fuel} \leq 1600$ °C	$T_{fuel} > 1600$ °C
Kernel	Buffer carbon-kernel interaction	Buffer carbon-kernel interaction
Buffer layer	Layer oxidation	Layer oxidation
Inner PyC layer	None	None
SiC layer		Thermal deterioration or decomposition Fission product corrosion
Outer PyC layer	None	None
Fuel element	None	None

There are six factors, characteristics, or phenomena for which the range of panel importance assessments varies from High to Low. These six items should be the focus of

particular attention by the international peer review group, with the objective of developing a clear majority assessment of importance. The six items are:

Kernel	Oxygen flux Buffer carbon-kernel interaction
Buffer layer	Condensed phase diffusion Layer oxidation Thermal gradient
Inner PyC layer	None
SiC layer	Fission product corrosion
Outer PyC layer	None
Fuel element	None

5.5 Reactivity Accident PIRT Analysis

Several summary statistics regarding the Reactivity Accident PIRT results are provided in Table 5-5. A brief discussion of each is provided following Table 5-5.

Table 5-5 Significant Importance and Knowledge Level Statistics for the Reactivity Accident

Total Number of Factors ¹	45
---	----

¹Factor: factor, characteristic, or phenomenon identified for Reactivity Accident

Consensus Assessment ²	High Importance	Knowledge Level		
		Low 1-3	Mid-range 4-6	High 7-9
	12	0	1	1

²Consensus Assessment: All panel members had identical assessment of importance and knowledge level.

Majority Assessment ³	High Importance	Knowledge Level
		Low or mid-range 1-6
	4	4

³Majority Assessment: Two members of the three-member panel

Divergent Assessment ⁴	Importance ⁵	Knowledge Level ⁴
All fuel temperatures	5	

⁴Divergent Assessment: A range of High to Low importance assessed by individual panel members.

⁵Knowledge level deemed secondary to the divergent importance rankings amongst the panel members.

The panel determined that 12 of the 46 Reactivity Accident factors, characteristics and phenomena are of "High" importance. The twelve factors are:

Kernel	Temperature vs. time transient conditions Condensed phase diffusion Maximum fuel temperature Energy deposition (total) Thermodynamic state of fission products
--------	--

Buffer layer	Gas phase diffusion Response to kernel swelling
Inner PyC layer	Gas phase diffusion Pressure loading (fission products) Pressure loading (carbon monoxide)
SiC layer	Fission product release through failures, e.g., cracking
Outer PyC layer	None
Fuel element	Gas phase diffusion

There is a consensus among the panel members that the level of knowledge is High (7-9) for kernel temperature vs. time transient conditions and Mid-range (4-6) for kernel condensed phase diffusion.

There are no factors, characteristics and phenomena for which all three panel members agreed that the knowledge level is Low or Mid-range.

There are four factors, characteristics and phenomena ranked of High importance by a majority of the panel (two members) and the knowledge level assessed as either Low or Mid-Range. The four factors are:

Kernel	Gas phase diffusion Energy transport: conduction within the kernel
Buffer layer	Maximum fuel gaseous fission product uptake
Inner PyC layer	None
SiC layer	None
Outer PyC layer	None
Fuel element	Condensed phase diffusion

There were five factors, characteristics, or phenomena for which the range of panel importance assessments varies from High to Low. These five items should be the focus of particular attention by the international peer review group, with the objective of developing a clear majority assessment of importance. The five items are:

Kernel	Buffer carbon-kernel interaction
Buffer layer	Condensed phase diffusion Thermal gradient
Inner PyC layer	Stress state (compression/tension)
SiC layer	None
Outer PyC layer	Gas-phase diffusion
Fuel element	None

5.6 Depressurization Accident With Water Ingress PIRT Analysis

Several summary statistics regarding the Depressurization Accident with Water Intrusion PIRT results are provided in Table 5-6. A brief discussion of each is provided following Table 5-6.

Table 5-6 Significant Importance and Knowledge Level Statistics for the Depressurization Accident With Water Ingress

Total Number of Factors ¹	77
---	----

¹Factor: factor, characteristic, or phenomenon identified for Depressurization Accident With Water Ingress

Consensus Assessment ²	High Importance	Knowledge Level		
		Low 1-3	Mid-range 4-6	High 7-9
	22	1	1	0

²Consensus Assessment: All panel members had identical assessment of importance and knowledge level.

Majority Assessment ³	High Importance	Knowledge Level
		Low or mid-range 1-6
	7	7

³Majority Assessment; Two members of the three-member panel

Divergent Assessment ⁴	Importance ⁵	Knowledge Level ⁴
All fuel temperatures	12	

⁴Divergent Assessment: A range of High to Low importance assessed by individual panel members.

⁵Knowledge level deemed secondary to the divergent importance rankings amongst the panel members.

The panel determined that 22 of the 77 Water Intrusion Accident factors, characteristics and phenomena are of "High" importance. The twenty-two factors are:

Kernel	Temperature vs. time transient conditions Maximum fuel temperature Thermodynamic state of fission products
Buffer layer	None
Inner PyC layer	Oxidation Cracking Pressure loading (carbon monoxide) Chemical attack by water: kinetics Chemical attack by water: changes in chemical form of fission products Chemical attack by water: temperature distributions
SiC layer	Gas-phase diffusion Fission product release through failures, e.g., cracking Chemical attack by water: changes in chemical form of fission products Chemical attack by water: temperature distributions
Outer PyC layer	Layer oxidation Chemical attack by water: kinetics Chemical attack by water: temperature distributions Chemical attack by water: changes in chemical form of fission products
Fuel element	Gas phase diffusion Transport of metallic fission products through fuel element – chemical form

	Chemical attack by water: kinetics Chemical attack by water: changes in chemical form of fission products Chemical attack by water: temperature distributions
--	---

There is a consensus among the panel members that the level of knowledge is Mid-range (4-6) for fuel element chemical attack by water: kinetics and Low (1-3) for inner PyC layer oxidation.

There is one phenomenon for which all three panel members agreed that the importance is High and the knowledge level is Low or Mid-range (Inner PyC Layer: Cracking).

There are seven factors, characteristics and phenomena ranked of High importance by a majority of the panel (two members) and the knowledge level assessed as either Low or Mid-Range. The factors are:

Kernel	Buffer carbon-kernel interaction
Buffer layer	Layer oxidation
Inner PyC layer	Gas phase diffusion
SiC layer	Chemical attack by water - kinetics
Outer PyC layer	Cracking
Fuel element	Condensed phase diffusion Chemical attack by water – changes in graphite properties

There are twelve factors, characteristics, or phenomena for which the ranges of panel importance assessments vary from High to Low. These twelve items should be the focus of particular attention by the international peer review group, with the objective of developing a clear majority assessment of importance. The twelve items are:

Kernel	Chemical attack by water: kinetics Chemical attack by water: changes in chemical form of fission products
Buffer layer	Gas phase diffusion Condensed phase diffusion Maximum fuel gaseous fission product uptake Thermal gradient
Inner PyC layer	Pressure loading (fission products) Stress state (compression/tension) Chemical attack by water: changes in graphite properties
SiC layer	Layer oxidation
Outer PyC layer	Chemical attack by water: changes in graphite properties
Fuel element	Chemical attack by water: holdup reversals

5.7 Depressurization Accident With Air Ingress PIRT Analysis

Several summary statistics regarding the Depressurization Accident with Air Ingress PIRT results are provided in Table 5-7. A brief discussion of each is provided following Table 5-7.

Table 5-7 Significant Importance and Knowledge Level Statistics for the Depressurization Accident With Air Ingress

Total Number of Factors¹	77
--	----

¹Factor: factor, characteristic, or phenomenon identified for Depressurization Accident With Air Ingress

Consensus Assessment²	High Importance	Knowledge Level		
		Low 1-3	Mid-range 4-6	High 7-9
	25	1	4	0

²Consensus Assessment: All panel members had identical assessment of importance and knowledge level.

Majority Assessment³	High Importance	Knowledge Level	
		Low or mid-range 1-6	
	7	8	

³Majority Assessment: Two members of the three-member panel

Divergent Assessment⁴	Importance⁵	Knowledge Level⁴
All fuel temperatures	13	

⁴Divergent Assessment: A range of High to Low importance assessed by individual panel members.

⁵Knowledge level deemed secondary to the divergent importance rankings amongst the panel members.

The panel determined that 25 of the 77 Air Intrusion Accident factors, characteristics and phenomena are of "High" importance. The twenty-five factors are:

Kernel	Temperature vs. time transient conditions Maximum fuel temperature Thermodynamic state of fission products
Buffer layer	None
Inner PyC layer	Oxidation Cracking Gas phase diffusion Chemical attack by air: kinetics Chemical attack by air: changes in chemical form of fission products Chemical attack by air: temperature distributions
SiC layer	Gas-phase diffusion Fission product release through failures, e.g., cracking Chemical attack by air: changes in chemical form of fission products Chemical attack by air: temperature distributions Chemical attack by air: kinetics
Outer PyC layer	Gas phase diffusion Layer oxidation Chemical attack by air: kinetics Chemical attack by air: temperature distributions Chemical attack by air: changes in chemical form of fission products

Fuel element	Gas phase diffusion Transport of metallic fission products through fuel element - chemical form Chemical attack by air: kinetics Chemical attack by air: changes in chemical form of fission products Chemical attack by air: changes in graphite properties Chemical attack by air: temperature distributions
--------------	---

There is a consensus among the panel members that the level of knowledge is Mid-range (4-6) for chemical attack by air - changes in form of fission products, outer PyC layer-gas-phase diffusion, SiC layer chemical attack by air - kinetics, and inner PyC layer - gas phase diffusion. There was a consensus that the level of knowledge was Low for inner PyC layer oxidation.

There are no factors, characteristics, or phenomena for which all three panel members agreed that the importance is High and the knowledge level is Low or Mid-range.

There are six factors, characteristics and phenomena ranked of High importance by a majority of the panel (two members) and the knowledge level assessed as either Low or Mid-Range. The factors are:

Kernel	Buffer carbon-kernel interaction
Buffer layer	Layer oxidation
Inner PyC layer	None
SiC layer	Layer oxidation
Outer PyC layer	Cracking
Fuel element	Condensed phase diffusion Chemical attack by air - catalysis

There are thirteen factors, characteristics, or phenomena for which the range of panel importance assessments varies from High to Low. These thirteen items should be the focus of particular attention by the international peer review group, with the objective of developing a clear majority assessment of importance. The thirteen items are:

Kernel	Chemical attack by air: kinetics Chemical attack by air: changes in chemical form of fission products
Buffer layer	Gas phase diffusion Condensed phase diffusion Maximum fuel gaseous fission product uptake Layer oxidation Thermal gradient Chemical attack by air: changes in chemical form of fission products
Inner PyC layer	Pressure loading (fission products) Pressure loading (carbon monoxide) Stress state (compression/tension)
SiC layer	Fission product corrosion
Outer PyC layer	None
Fuel element	Chemical attack by air: holdup reversals

5.8 Lessons Learned

The PIRT process is still evolving with each new application. Given this evolution, it is worthwhile to record any lessons learned for the benefit of subsequent PIRT efforts. There were three such lessons learned from the TRISO-coated particle fuel PIRT effort. They are described in the following sections.

5.8.1 Development of PIRT Objectives

The importance of developing a clear objective statement for each PIRT effort is presented in Section 1.2. The following description of this step in the PIRT process is provided. *“Step 2: Define the specific objectives of the PIRT. The PIRT objectives are usually specified by the sponsoring agency. A clear statement of PIRT objectives is important because it defines the focus, content, and intended applications of the PIRT product. The PIRT objectives should include a description of the final products to be prepared.”*

The specific objectives of the TRISO-coated particle fuel PIRT evolved during the course of the first panel meeting. The number of PIRTs originally envisioned was four: (1) Design, (2) Manufacturing, (3) Operations, and (4) Accident, with the latter being a single accident. The final TRISO-coated particle fuel PIRT objectives focused on (1) Manufacturing, (2) Operations, (3) Depressurized Heatup Accident, (4) Reactivity Accident, (5) Depressurization Accident with Water Ingress, and (6) Depressurization Accident with Air Ingress. A PIRT effort was started for the Design phase (Appendix H) of the TRISO-coated particle fuel life cycle but it was not continued to completion.

The importance of developing a precise and definitive objective statement for each PIRT effort is emphasized. Having such a statement does not preclude changes in the objectives, as was the case with the TRISO-coated particle fuel PIRT. However, such a statement should minimize such occurrences. Generally, the objective statements are to be developed by the institution sponsoring the PIRT effort. If the PIRT effort involves several institutions, e.g., the NRC and industry, every effort should be made to reach agreement on the objectives before the initial PIRT meeting.

5.8.2 PIRT Panel Size

PIRT panels have been created utilizing between three and twenty-five expert panel members. The TRISO-coated particle fuel PIRT panel had three expert members.

Significant challenges were encountered with this small number of PIRT panel members. For the most part, these challenges arise when the panel members do not develop a consensus regarding the importance and knowledge level of a particular PIRT phenomenon.

For example, if two panel members believe a phenomenon is of High importance and the remaining panel member concludes that the importance is Medium or Low, the two-to-one vote cannot be considered to be conclusive.

More importantly, if each of the panel members evaluates importance differently, i.e., one ranks the importance High, one Medium, and one Low, little can be concluded other than that phenomenon should be the focus of additional consideration by a wider group of

experts. The use of the PIRT as a tool for informing the evaluation of experimental data, experimental facilities, analytical methods and resource allocation is compromised.

Similar statements can be made with the panel members do not reach consensus or near consensus on the level of knowledge.

Based upon the experience with panels having as many as 25 members and panels with intermediate numbers of panel members, the optimal panel size appears to be approximately five to seven members. With PIRT panel membership of this intermediate size, it is still possible to have extensive in-meeting discussion, make assignments for out-of-meeting contributions, and reach consensus. Should a consensus not be reached, it is more likely that a clear majority (near-consensus) will evolve. With this near majority, it is feasible to apply the PIRT as a tool for informing the evaluation of experimental data, experimental facilities, analytical methods and resource allocation is compromised.

Having made this point, it is recognized that care should be taken that minority opinions are not dismissed without careful consideration of the rationales provided for importance and knowledge level.

5.8.3 Documentation of Rationales

The recording of written rationales for importance and knowledge level has become an important part of a quality PIRT effort. When questions arise regarding the basis for the importance and knowledge levels assigned, the PIRT user can consider the written rationales appearing in the PIRT report. Thus, the written rationales can and do enhance the PIRT applicability and utility.

In previous PIRT efforts, written rationales have been developed in several ways. For example, rationales have been developed and recorded during the course of PIRT meetings. The advantage of this approach is that the rationales are discussed, adopted, and recorded immediately. This approach limits the out-of-meeting time requirements of the PIRT panel members. However, the rationales tend to be brief. Other than the brief rationale statement, supporting evidence is rarely cited or documented.

For the TRISO-coated particle fuel PIRT effort, ranking and rationale development proceeded largely outside the meeting and at the panel member's home base. Thus, the rationales were developed largely on an individual basis. Importance rankings, knowledge levels, and the rationales were then discussed in PIRT panel meetings. The effort required to prepare the requested written rationales was large and frequently repetitive. However, the written rationales cited supporting evidence, included figures and tables on occasion, and were often detailed. Thus, one of the prime contributions of the TRISO-coated particle fuel PIRT panel, given the limitations of a three-member panel (see Section 5.8.2) is the very detailed panel member inputs provided for each of the six PIRTs summarized in Chapter 4. This information should prove useful to the international peer review group. These detailed PIRT inputs are provided in Appendices A-F of this report.

BIBLIOGRAPHIC DATA SHEET

(See instructions on the reverse)

1. REPORT NUMBER
(Assigned by NRC, Add Vol., Supp., Rev.,
and Addendum Numbers, if any.)

NUREG-6844 Volume 1

2. TITLE AND SUBTITLE

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

Main Report

3. DATE REPORT PUBLISHED

MONTH | YEAR
July | 2004

4. FIN OR GRANT NUMBER
Y6704

5. AUTHOR(S)

R. N. Morris*, D. A. Petti**, D. A. Powers***, and B. E. Boyack****

6. TYPE OF REPORT

Technical

7. PERIOD COVERED (Inclusive Dates)

8/25/02 - 10/31/03

8. PERFORMING ORGANIZATION - NAME AND ADDRESS (If NRC, provide Division, Office or Region, U.S. Nuclear Regulatory Commission, and mailing address; if contractor, provide name and mailing address.)

* Oak Ridge National Laboratory UT-Battelle, MS 6295, P.O. Box 2008, Oak Ridge, TN 37831-6295

** Idaho National Engineering and Environmental Laboratory, Fission and Fusion Systems Dept., P.O. Box 1625, Idaho Falls, ID 83415-3860

*** Nuclear and Risk Technologies Center, MS-0727, Sandia National Laboratories, P.O. Box 5800, Albuquerque, NM 87185

**** Consultant

9. SPONSORING ORGANIZATION - NAME AND ADDRESS (If NRC, type "Same as above"; if contractor, provide NRC Division, Office or Region, U.S. Nuclear Regulatory Commission, and mailing address.)

Division of Systems Analysis and Regulatory Effectiveness
Office of Nuclear Regulatory Research
U. S. Nuclear Regulatory Commission
Washington, DC 20555-0001

10. SUPPLEMENTARY NOTES

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.

12. KEY WORDS/DESCRIPTORS (List words or phrases that will assist researchers in locating the report.)

TRISO-coated particle fuel, PIRT, fission product transport, fuel particle failure, HTGR

13. AVAILABILITY STATEMENT

unlimited

14. SECURITY CLASSIFICATION

(This Page)

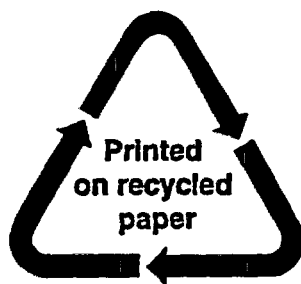
unclassified

(This Report)

unclassified

15. NUMBER OF PAGES

16. PRICE



Federal Recycling Program

**UNITED STATES
NUCLEAR REGULATORY COMMISSION
WASHINGTON, DC 20555-0001**

OFFICIAL BUSINESS