Appendix C

Model Pedigree and Quality Extract Table

EXTRACT MATRIX II: MODEL PEDIGREE AND QUALITY

Model	Strengths/Limitations	Surety Considerations
ADAM	**Strengths:** ADAM treats a wide variety of source conditions and accounts for the effects of dense gases, chemical reactions, and latent heat exchanges. **Limitations:** ADAM can be applied to only eight chemicals.	**All quality assurance documentation:** The ADAM model has been reviewed by the U.S. Air Force (Kunkel 1992). The model is known to converge to the U.S. Air Force's AFTOX model for passive releases.
AFTOX	**Strengths:** Has undergone extensive testing and troubleshooting. AFTOX allows 90% confidence bounds to be printed out for toxic corridors and concentrations at a point. **Limitations:** AFTOX is that it does not treat dense gases.	AFTOX was included in the comprehensive model evaluation exercise reported by Hanna et al. (1993).
AI-RISK	**Strengths:** AIRISK is a versatile radiological assessment code capable of handling a variety of postulated accident scenarios common to the DOE complex. **Limitations:** The AIRISK code does not have widespread use outside of LANL. The user is limited to a release containing 40 radionuclides.	No verification and validation documentation available. Documentation describing dose calculations and hard-wired data libraries is light. Some benchmarking performed, but not documented.
ALOHA	**Strengths:** Chemical source terms. **Limitations:** The dispersion model.	Field experiments have been performed.
AQPAC	Several simplifying assumptions are made in the source term model such as constant pool diameter for liquid spills.	Benchmark test and comparison with field experiments have shown good results.
ARAC (MATHEW/ ADPIC)	**Strengths:** The code is very robust and has been applied to thousands of assessments, responses and exercises over a 20-year period. **Limitations:** Limited spatial resolution depending on terrain steepness and the number and size of grid cells used in the domain.	**All quality assurance documentation:** Available **Benchmark runs:** Available **Validation calculations:** Validation is achieved based on a significant number of model verifications or evaluations. **Verification with field experiments that has been performed with respect to this code:** The model has been evaluated against hundreds of tracer data sets from over 20 field programs in a wide variety of settings and scales from a few to thousands of km.
ARCON96	**Strengths:** Several improvements over the commonly-used 1974 Murphy and Campe control room habitability assessment procedure. **Limitations:** Application	**All quality assurance documentation:** Code was developed and tested in accordance with the requirements of ANSI/ASME NQA-1, 1986 edition (ASME 1986), Quality Assurance Program Requirements for Nuclear Facilities.
AXAIRQ	**Strengths:** AXAIRQ strictly follows the guidance in USNRC Regulatory Guide 1.145 and is site specific for SRS. The program is very user friendly and the user-input template is easy to follow. **Limitations:** An ingestion model is planned to be added to AXAIRQ in the next year and transfer to a PC is being considered to overcome those Limitations.	**All quality assurance documentation:** Verification Report listed above Simpkins, A.A. Software Quality Assurance Plan for Environmental Dosimetry, Westinghouse Savannah River Company Report, WSRC-RP-95-1159, Aiken, SC, November, 1994.

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Model	Strengths/Limitations	Surety Considerations
AXAOTHER XL	**Strengths:** AXAOTHER XL has unique features to analyze adverse weather such as high-velocity straight-line winds and tornadoes. **Limitations:** AXAOTHER XL does not considered daughter ingrowth and only plume shine and inhalation dose pathways are considered.	**All quality assurance documentation:** Verification Report listed above Simpkins, A.A. Software Quality Assurance Plan for Environmental Dosimetry, Westinghouse Savannah River Company Report, WSRC-RP-95-1159, Aiken, SC, November, 1994.
BNLGPM	**Strengths:** Ease of user and application. **Limitations:** Application domain and portability.	No information provided.
CALPUFF	**Strength**: User interface and documentation are easy to use. **Limitations**: Lack of a front end spills model that computes evaporation, jet effects, etc.	**All quality assurance documentation:** The code has been used and reviewed by several different organizations; no formal QA.
CAP88-PC	**Strengths:** Used by over 1,000 registered users around the world.	**All quality assurance documentation:** Available
CASRAM	**Strengths:** Statistical treatment of potential hazardous material accidents both in terms of source strength and meteorology. **Limitations:** Model does not treat dense gas releases.	Pool evaporation calculations have been checked against published data for hydrocarbon evaporation. Dispersion estimates have been validated with numerous field and laboratory data including Project Prairie Grass.
CATS	No information provided.	No information provided.
CCSL	**Strengths:** Easy to initialize. Fast running. Evaluated very well. **Limitations:** Limited to microscale.	**All quality assurance documentation:** User Guide. **Benchmark runs:** Yes **Validation calculations:** Yes **Verification with field experiments that has been performed with respect to this code:** PROJECT WIND; MADONA Field Study
CFAST	**Strengths:** Models multiple fires; includes ventilation systems and a materials data bas. **Limitations:** Requires an a priori specification of the temporal behavior of a fire.	**Quality Assurance:** Available **Benchmarking:** Yes **Code Verification and Validation:** Yes
COMPBRN III	**Strengths:** Has a flame spread model, thermal radiation to targets, and prediction of damage and ignition. **Limitations:** Applicable only to a single room; quasi-steady-state assumptions.	**Quality Assurance:** User Manual **Benchmarking and Verification:** Available. **Validation Against Experimental Data:** Yes
CONTAIN	**Strengths:** No limit to the number of flow path connections to a single control volume. **Limitations:** There is no multi-dimensional capability.	**Quality Assurance:** Available **Benchmarking and V & V:** Available
COSYMA	**Strengths:** Various atmospheric transport and dispersion models. Full tritium dispersion capability. **Limitations:** Lack of extensive experience with the code in the United States.	No information provided
CTDMPLUS	**Strength**: Capability to model dispersion over complex terrain. **Limitations:** Inability to model dense gas dispersion.	None

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Model	Strengths/Limitations	Surety Considerations
DEGADIS	**Strengths:** Can address many types of dense gas releases. **Limitations:** Several	**All quality assurance documentation:** EPA has an extensive quality assurance program. **Benchmark runs:** DEGADIS compares well with other codes of its type. **Validation calculations:** No Information Provided**.** **Verification with field experiments that has been performed with respect to this code:** Yes
DOSEEP	**Strengths:** Requires only a source term, wind speed, and stability. **Limitations:** Simplistic gaussian plume assumptions, specifically designed for releases from underground nuclear tests.	**Verification with field experiments that has been performed with respect to this code:** Verification from planned releases
EMGRESP	**Strengths:** The code processes an extremely large database of physical/chemical properties commonly required for screening level of analysis. **Limitations:** The dispersion results for neutrally buoyant plumes and puffs are generally several times greater in magnitude than results obtained from other neutrally buoyant Gaussian models. No time-varying releases may be modeled. Only instaneous dense gas releases may be modeled.	**Benchmark runs:** Sample cases using a set of large-scale propane release field experiment data were analyzed **Validation calculations:** V&V reports **Verification with field experiments that has been performed with respect to this code:** V&V.
ERAD	**Strengths:** The treatment of vertical dispersion includes current relationships for scaling turbulence within the boundary layer. **Limitations:** Outputs are very limited because the current version was developed for emergency response use.	With few exceptions, cloud top height predictions of the integral plume rise model were within 25% of field observations. Predicted contour areas average within about 50% of the observations. The validation results confirm the model's representation of the physical processes.
ETMOD	**Strengths:** The code is fairly easy to run and provides a lot of output information. **Limitations:** Tritium is the only radionuclide that is available.The conclusion of the validation report even states, "A number of deficiencies have been identified in the ETMOD code."	Although a QA package exists it is very limited and does not contain much detail in the user's manual or verification manual. The verification model does not verify models but simply describes some of them.
FEM3C	**Strengths:** FEM3C has modeling capabilities in the computation of complex turbulent fluid flow in the presence of complex terrain and obstacles to flow. Multiple, simultaneous sources may be accommodated. **Limitations**: The code cannot accept typical vapor/aerosol source terms (e.g., pressurized jets, time-varying vapor emissions). The aerosol mode excludes some of the relevant physical behavior (e.g., droplet evaporation, rainout).	**All quality assurance documentation:** Thorough internal documentation of the source code by means of "comment cards" permits verification of the program. **Benchmark runs: ✔** **Validation calculations:** None **Verification with field experiments that has been performed with respect to this code: ✔**
FIRAC	**Strengths**: Inclusion of source term models for fires; no limit on the number of flow paths. **Limitations:** Momentum balance ignores spatial acceleration term.	**Quality Assurance:** None. **Error Handling/Reporting:** Needs improvement. **Benchmarking and V & V: ✔**
FIRAC/FIRIN	**Strengths:** Widely used throughout the DOE complex for high hazard facilities. **Limitations:** Code is limited since spatial variations can only be handled in an approximate way.	**Quality Assurance: ✔** **Benchmarking and V & V: ✔**

EXTRACT MATRIX II: MODEL PEDIGREE AND QUALITY

Model	Strengths/Limitations	Surety Considerations
FPETOOL	**Strengths**: FPEtool is a menu-driven code with relatively little computational expense, offering modeling capabilities desired for most Safety Analysis Report applications. **Limitations:** Some of the models have noted limitations in accuracy and do not account for variation in room or fire characteristics in the horizontal dimension.	**Quality Assurance: ✔** **Benchmarking and V & V:** None. **Benchmarking:** No formal benchmarking has been performed. **Verification:** No formal source code verification has been performed. **Validation Against Experimental Data:** None.
GASFLOW	**Strengths**: Full governing equations are utilized. **Limitations:** There is no agglomeration model.	**Quality Assurance: ✔** **Error Handling and Reporting: ✔** **Benchmarking and V & V: ✔**
GAUS1	**Strengths**: Calculates both radiological dose and hazardous material risks. **Limitations**: Runs only on an HP-48 calculator.	**All quality assurance documentation:** User's Guide **Benchmark runs:** Comparison with test problems **Validation calculations:** Test problem comparisons in User's Guide **Verification with field experiments that has been performed with respect to this code:** Only with standard Gaussian Plume results
GENII	**Strengths:** Ease of use **Limitations:** No "risk" calculations; not appropriate for "near-field" atmospheric transport-e.g., worker doses in accidents.	**All quality assurance documentation:** 2 bookcases **Benchmark runs: ✔** **Validation calculations: ✔** **Verification with field experiments:** Participated in IAEA VAMP program
GXQ	**Strength**: Many source term modes **Limitation**:Calculates only atmosphere dispersion; must be used in conjunction with another code.	✔
HARM II	**Strengths:** Contains algorithms to address passive and heavy gases, chemical transformations and removal mechanisms. **Limitations:** Site-specificity and inherent Gaussian structure.	**All quality assurance documentation:** The transport and diffusion codes have been evaluated using data sets from DOE Savannah River Site.
HGSYSTEM	**Strengths**: HGSYSTEM offers the most rigorous treatments of HF source-term and dispersion analysis available for a public domain code. **Limitations:** It is difficult to extend the physical/chemical data base utility DATAPROP to include additional chemical species.	**Quality Assurance**: Unknown to what extent the source code has been verified. **Benchmark Runs (comparison with other codes)**: Compared with nine independent dense gas models. **Comparison with Field Experiments**: Results have been compared with large scale field data.
HOTMAC/ RAPTAD	**Strengths:** The model has true forecast capabilities in three-dimensional space over complex terrain. **Limitations:** Relatively slow computations.	No information provided.
HOTSPOT	**Strengths:** The HOTSPOT code has a well-deserved reputation for ease-of-use in emergency situations. The salient features of this code are contained in its source term modules, which are extensive and well-formulated. **Limitations:** Inappropriate for applications where more complex physical modeling is important; does not provide estimates of groundshine dose.	Validation identified in HOTSPOT PC Health Physics Codes," S.G. Homann, March, 1994, UCRL-MA-106315, with test problems included in documentation.

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Model	Strengths/Limitations	Surety Considerations
HPAC	HPAC has the following strengths: **!** Dispersion methodology is based on second order turbulence closure scheme. **!** The probabilistic prediction is based on fluctuation variance. **!** Accurately incorporates wind shear. **!** SCIPUFF includes a rational description of time-averaging effects. **!** Utilizes an integrated description of dynamic effects.	**All quality assurance documentation:** ✔ **Benchmark runs:** 17 Test Cases are used with various options turned on and off to ensure verification standards between versions. **Validation calculations:** DSWA has an active and extensive HPAC Verification and Validation Program. **Verification with field experiments that has been performed with respect to this code:** 770+ events with thousands of data points have been compared to HPAC predictions.
HRW	**Strengths:** Evaluated very well. **Limitations:** Limited to microscale.	**All quality assurance documentation:** User Guide **Benchmark runs:** ✔ **Validation calculations:** ✔ **Verification with field experiments that has been performed with respect to this code:** MADONA PROJECT WIND
HYSPLIT	**Strengths:** Flexible code structure permits easy modification to perform a variety of different simulations. **Limitations:** Meteorology is not directly coupled with the concentration grid.	**All quality assurance documentation:** ✔ **Benchmark runs:** Distribution comes with sample data set. **Validation calculations:** In User's guide. **Verification with field experiments that has been performed with respect to this code:** ✔
INPUFF	**Strengths**: Has capability of handling time-dependent release rates and multiple release locations. **Limitations**: Inability to model dense-gas dispersion.	No Information provided**.**
KBERT	**Strengths:** Fast running, easy to use, and provides dose consequence directly. **Limitations:** All flow rates must be known for all times for the accident, but other codes can be used to supply flows; no turbulence and diffusion modeling within a control volume.	**All quality assurance documentation:** ✔ **Benchmark runs:** ✔ **Validation calculations:** ✔ **Verification:** ✔
MACCS2	**Strengths:** Estimates of consequences of releases of all known radionuclides that may be available in nuclear reactor accidents. **Limitations:** The straight-line Gaussian plume model of atmospheric transport and diffusion.	**All quality assurance documentation:** Standard software development procedures at Sandia National Laboratories. **Benchmark runs:** ✔ **Validation calculations:** ✔ **Verification with field experiments:** None
MAILS	**Strengths:** Simplicity, fast operation, direct applicability of output for intended purpose. **Limitations:** Inflexibility.	**All quality assurance documentation:** Unknown **Benchmark runs:** Versus ISCST **Validation calculations:** Versus ISCST (see user guide) **Verification with field experiments:** None

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Model	Strengths/Limitations	Surety Considerations
MARSS	**Strengths:** Addresses specialty chemicals located at the Kennedy Space Center. Interactive graphics system. Dispersion coefficients based on field tracer studies. **Limitations:** The OB/DG and LOMPUFF models are restricted to cold spills behaving as a neutrally buoyant gas, considers only wind direction in its treatment of effluent transport, calculates a centerline value and only roughly estimates plume footprint using 2-sigma width.	**All quality assurance documentation:** Unknown **Benchmark runs:** Unknown **Validation calculations:** No Information Provided **Verification with field experiments that has been performed with respect to this code:** No information provided
MELCOR	**Strengths:** Fast running, versatile code. **Limitations:** Multi-dimensional capability, ventilation system components must be built by user input.	**Quality Assurance**: Software development plan and requirements. **Error handling/Reporting:** ✔ **Benchmarking and V&V:** ✔
OMEGA/ ADM v3.5	**Strengths:** The model is a state-of-the-art weather prediction model, so all scales (both spatial and temporal) are considered. **Limitations:** No urban canyons or other city-scape features, mitigation features, or casualty or human effects modules.	**Benchmark runs:** Installed as part of the system. **Validation calculations:** ✔ **Verification with field experiments:** ✔
PAVAN	PAVAN is the baseline model for calculation of site-specific unit air concentration values (X/Q).	Documentation is adequate for most users.
PIKE	**Strengths:** Readily available meteorology, simple input parameters, portability of code, quick estimates of exposures, conservative values for safety. **Limitations:** Lack of areal meteorology, terrain effects very crudely accounted for, no dynamic interactions, basic analog may be unrealistic.	**All quality assurance documentation:** Published reports **Benchmark runs:** Done on PIKE, other events **Validation calculations:**.Verified against PIKE Analyses **Verification with field experiments:** Verified against several tests that had ventings.
PUFF-PLUME	**Strengths:** Speed and simplicity, and modeling of tritium and tritium oxide deposition. **Limitations:** Inability to accommodate a two or three dimensional wind field, unable to model dense-gas dispersion.	**All quality assurance documentation:** ✔ **Verification with field experiments that has been performed with respect to this code:** ✔
RSAC-5	**Strengths:** Calculates and fractionates fission product inventories. **Limitations:** Fission product calculations are valid primarily for high-enriched fuels.	**All quality assurance documentation:** Configuration control is maintained. **Benchmark runs:** See V&V reports. **Validation calculations:** See V&V reports. **Verification with field experiments :** See V&V reports.
RTVSM	**Strengths:** Site-specific dispersion parameterization based on tracer studies. Ability to address a wide spectrum of source terms. **Limitations:** Gaussian model. Inability to address submicron particulate sources.	**All quality assurance documentation:** The transport and diffusion components have been validated using data from Dugway Proving Ground chemical/biological agent and stimulant and smoke/obscurant field tests.

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Model	Strengths/Limitations	Surety Considerations
SCIPUFF	**Strengths:** Particularly suitable for assessing radiological impacts associated with nuclear reactor accidents. **Limitations:** Several, and the so-called "operator friendly" model input interface is very awkward and user unfriendly.	**All quality assurance documentation:** ✔ **Benchmark runs:** Would be difficult to benchmark against other models. **Verification with field experiments that has been performed with respect to this code:** ✔
SLAB	SLAB is recognized as the easiest-to-use dense gas model in the public domain. It agrees well with available field data. It does not calculate source emission rates.	**All quality assurance documentation:** Unclear whether the SLAB code has been subject to formal procedures of quality assurance. **Verification with field experiments that has been performed with respect to this code:** SLAB was included in the comprehensive model evaluation exercise reported by Hanna et al. (1993).
SUDU	**Strengths:** Downwind dose estimates are obtained quickly. **Limitations:** Pre-windows technology, old dose factors, and simple straight-line model.	**All quality assurance documentation:** Derived from HUDU Code **Benchmark runs:** Comparison to HUDU and GENII **Validation calculations:** Comparison to HUDU and GENII **Verification with field experiments:** None
TRAC RA/HA	**Strengths**: A state-of-the-art model that addresses the three-dimensional complex flows commonly occurring at the front range of the Rocky Mountains, and at other mountain-valley locations; calculates offsite and onsite doses out to 100 km.	**Software Quality Assurance:** Documentation has been recently developed. **Verification and Validation:**The code has been accepted by the State of Colorado.
TRIAD 2-1	**Strengths:** Accounts for effects of fast chemical reactions, dry deposition and gravitational settling, variable source emission rates, on-site dispersion schemes, variable windfield, and differences in elevations of sources. **Limitations:** Does not account for the effects of the vertical variation of wind direction shear on puff transport exists.	**All quality assurance documentation:** Peer-reviewed documentation. **Benchmark runs:** Included in User's Manual **Validation calculations:** Applied in different climatic conditions. **Verification with field experiments:** Documented in peer-reviewed journal publications.
TSCREEN	**Strengths:** Easy to use, fast to set up, little training necessary, fast calculation time, covers several source configurations. **Limitations:** Can only evaluate scenarios that match workbook.	**All quality assurance documentation:** No specific quality assurance records are available. **Benchmark runs:** Not discussed in the documentation.
UFOTRI	**Strengths:** Behavior of tritium is described dynamically in atmosphere, soil and plants (time step of one hour). **Limitations:** The soil submodel seems to be too conservative.	**Validation calculations:** Tested in the frame of BIOMOVS (biological model Validation Study phase II) **Verification with field experiments:** Limited
VAFTAD	**Strengths:** User run in 1-2 minutes for any location globally with various gridded wind input options. Output charts of the forecast visual ash cloud, not ash concentrations, are preferred for aircraft operations. **Limitations:** Applies only to aircraft operating in the vicinity of volcanic ash.	No Information Provided.

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Model	Strengths/Limitations	Surety Considerations
VDI	**Strengths:** The dense gas model has the option of modeling (a) the effect of the presence of obstacles to flow, and (b) the dispersion from a line, area, and volumetric neutrally buoyant vapor source. **Limitations:** The method used for modeling line, area, and volumetric neutrally buoyant vapor sources is not an accurate solution to the diffusion equation. The dense gas program assumes no initial dilution of the vapor cloud	Unknown
VENTSAR XL	**Strengths:** The program is very user friendly and the user-input template is easy to follow. Output is easily converted to graphs. **Limitations:** Daughter ingrowth is not considered**.**	**All quality assurance documentation:** Software Quality Assurance Plan for Environmental Dosimetry. **Benchmark runs:** Runs are maintained by the Environmental Dosimetry Group and SRS. **Validation and Verification: ✔**
VLSTRACK	**Strengths:** Applications for munitions. **Limitations:** Difficult to apply to common chemical spills of the type generally evaluated by DOE.	**All quality assurance documentation:** VLSTRACK 1.6 is being verified, documented, and validated against experimental data in a similar manner to VLSTRACK 1.2 and 1.5.1. Details were not provided.
VULCAN	**Strengths:** Applicable to a wide-range of problems/fires; able to predict, a priori, how a fire will develop and spread heat and smoke. **Limitations:** Limited to cartesian coordinate systems, 1 or 2 fuel types of hydrocarbon-based fuels, and several restrictions.	No information provided.