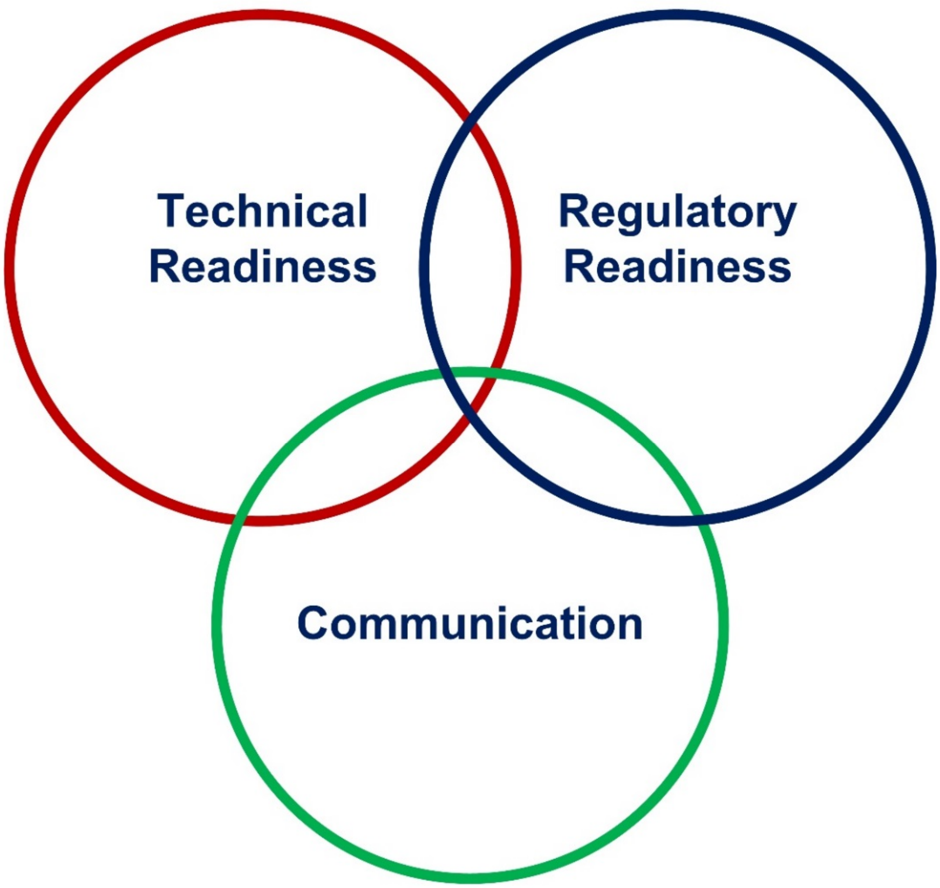
NRC Non-Light Water Reactor (Non-LWR) Vision and Strategy

Volume 3: *Computer Code Development Plans for Severe Accident Progression, Source Term, and Consequence Analysis*



DRAFT - April 1, 2019

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EXECUTIVE SUMMARY

This report summarizes proposed code development efforts to extend NRC's modeling and simulation capabilities for accident progression, source term, and consequence analysis for non-LWR technologies. This report describes the different types of non-LWRs as well as the modeling gaps for NRC's computer codes including MELCOR for accident progression and source term analysis, MACCS for consequence analysis, and SCALE for radionuclide inventories.

Severe accident progression, source term, and consequence analysis are deeply embedded in the NRC's regulatory policy and practices. The licensing process is based on the concept of defense-in-depth, in which power plant design, operation, siting, and emergency planning comprise independent layers of nuclear safety. This approach encourages nuclear plant designers to incorporate several lines of defense in order to maintain the effectiveness of physical barriers between radiation hazards and workers, members of the public, and the environment – for both normal operation and accident conditions. The various regulatory source terms, used in conjunction with the design basis accidents, establish and confirm the design basis of the nuclear facility, including items important to safety, ensuring that the plant design meets the safety and numerical radiological criteria set forth in the U.S. Code of Federal Regulations (CFR) (e.g., 10 CFR 100.11, "Determination of Exclusion Area, Low Population Zone, and Population Center Distance"; 10 CFR 50.67, "Accident Source Term"; 10 CFR 50.34(a)(1)(iv); General Design Criterion 19, "Control Room," of Appendix A, "General Design Criteria for Nuclear Power Plants," to 10 CFR Part 50, "Domestic Licensing of Production and Utilization Facilities") and in subsequent staff guidance.

MELCOR is the state-of-the-art computer code developed by Sandia National Laboratories for NRC to perform nuclear reactor severe accident progression and source term analyses. MELCOR is a flexible, integrated computer code designed to characterize and track the evolution of severe accidents, and the transport of associated radionuclides within a confinement such as a containment or building. It is a knowledge repository comprised of hundreds of millions of dollars' worth of experiments and model development, with particular focus on LWR phenomenology as well as extended capabilities for non-LWR technologies. Specific data and computational needs have been developed and documented in Phenomenon Identification and Ranking Tables (PIRT) such as the Severe Accident (SA) PIRT related to NGNP and also various sodium-cooled fast reactor and molten salt reactor PIRT analyses [1] [2] [3] [4] [5] [6]. Pertinent data needs have been gleaned from these PIRTs and are consolidated in this report. This report provides a high level understanding of the functional status of the code in relation to various non-LWR designs.

MELCOR relies on the SCALE code system to provide fission product and radionuclide inventories, kinetics parameters, power distributions, and decay heat, especially through the ORIGEN code. SCALE is a multi-disciplinary tool developed by Oak Ridge National

Laboratory for NRC to combine nuclear system simulation tools into one cohesive package. This was intended to mitigate human errors from data transfer and manipulation between code packages, consolidate experience, and speed up analysis times. SCALE provides a comprehensive, verified and validated, user-friendly tool set for nuclear data, criticality safety, reactor physics, radiation shielding, radioactive source term characterization, activation, depletion and decay, and sensitivity and uncertainty analysis under a software quality assurance program. Since the 1970s, regulators, licensees, and research institutions around the world have used SCALE for safety analysis.

The MACCS (MELCOR Accident Consequence System) code suite is the NRC's computer code system for probabilistic consequence analysis. MACCS models atmospheric releases of radioactive materials into the environment and the subsequent consequences of such releases. MACCS is the only tool for probabilistic modeling of all the technical elements of the Level 3 PRA Standard including radionuclide release, atmospheric transport and dispersion, meteorology, protective actions and site data, dosimetry, health effects, economic factors, and uncertainty. MACCS has a long, active development history and a broad user base including NRC, DOE, the nuclear industry, academia, and domestic and international research organizations. MACCS applications are numerous and include regulatory cost-benefit analysis, environmental analysis of severe accident mitigation alternatives and design alternatives, level 3 PRA studies, consequence analyses, and other risk-informed activities. MACCS can also be used for calculations of dose exceedance at distance to inform emergency planning and other types of decisions.

Section 1.1 discusses the regulatory need for source term analysis using NRC developed computational tools discussed in this report. Section 1.2 provides an overview of the computer codes and the basis for their selection. Details on the development plans for each code are provided in Sections 2 (MELCOR), 3 (SCALE), and 4 (MACCS). The individual code sections also discuss the current extensive modeling and simulation capabilities and how the modeling gaps are identified and addressed to demonstrate functional readiness for confirmatory analysis. This report also includes several appendices which provide additional information on the non-LWR designs, historical code development efforts, and experiments applicable to non-LWRs.

This document represents the current and best knowledge of technical needs for development of the MELCOR, MACCS, and SCALE codes for application to advanced, non-light water reactor severe accident, source term, and consequence analysis. This is a living document that will be updated as more experience is gained and as new information regarding specific reactor design needs comes to light.

ABBREVIATIONS

Abbreviation	Definition
AERMOD	American Meteorological Society/Environmental Protection Agency Regulatory Model Program
ALMR	Advanced Liquid Metal Reactor
AniMACCS	MACCS Animations Tool
ANL	Argonne National Laboratories
AOO	Anticipated Operational Occurrence
ARCON96	Atmospheric Relative Concentrations in Building Wakes Program
ARE	Aircraft Reactor Experiment
ATD	Atmospheric Transport and Dispersion
ATWS	Anticipated Transient Without Scram
BDBA	Beyond Design Basis Accident
CF	Control Function
CFD	Computational Fluid Dynamics
CL	Cladding
COMIDA	MACCS Food Chain Preprocessor Code
COR	Core
CSARP	Cooperative Severe Accident Research Program
CSTF	Containment System Test Facility
CV	Control Volume
CVH	Control Volume Hydrodynamics
DBA	Design Basis Accident
DCH	Decay Heat
DOE	U.S. Department of Energy
EBR	Experimental Breeder Reactor
EDF	External Data File
EOS	Equation-of-State
EPZ	Emergency Planning Zone
FFTF	Fast Flux Test Facility
FHR	Fluoride Salt-Cooled High Temperature Reactor
FL	Flow Path
FSD	Fusion Safety Database
FU	Fuel
GCR	Gas-Cooled Reactor
HPR	Heat Pipe Reactor

Abbreviation	Definition
HS	Heat Structure
HTGR	High-Temperature Gas-Cooled Reactor
IFR	Integral Fast Reactor
INL	Idaho National Laboratories
LMR	Liquid Metal Reactor
LWR	Light Water Reactor
MACCS	MELCOR Accident Consequence Code System
MelMACCS	MACCS Source Term Preprocessor Code
MHTGR	Modular High-Temperature Gas-Cooled Reactor
MP	Material Properties
MSR	Molten Salt Reactor
MSRE	Molten Salt Reactor Experiment
NAC	Sodium Chemistry
NEPA	National Environmental Policy Act
NGNP	Next Generation Nuclear Plant
NRC	U.S. Nuclear Regulatory Commission
ORNL	Oak Ridge National Laboratories
P/DLOFC	Pressurized/Depressurized Loss of Forced Circulation
PBR	Pebble Bed Reactor
PCMM	Predictive Capability Maturity Model
PIRT	Phenomena Identification and Ranking Tables
PMR	Prismatic Modular Reactor
PRA	Probabilistic Risk Assessment
PRIME	Plume Rise Model Enhancements
PRISM	Power Reactor Innovative Small Module
QUIC	Quick Urban and Industrial Complex Dispersion Modeling System
RADTRAD	Radionuclide Transport, Removal, and Dose Estimation Program
RASCAL	Radiological Assessment System for Consequence Analysis
RCCS	Reactor Cavity Cooling System
RF	Reflector
RN	Radionuclide
SAFR	Sodium Advanced Fast Reactor
SAMA	Severe Accident Mitigation Alternative
SAMDA	Severe Accident Mitigation Design Alternative
SecPop	Sector Population, Land Fraction, and Economic Estimation Program
SFR	Sodium Fast Reactor

Abbreviation	Definition
SMR	Small Modular Reactor
SNL	Sandia National Laboratories
SOARCA	State-of-the-Art Reactor Consequence Analyses
TF	Tabular Function
TOP	Transient Over-Power
TRISO	Tri-isotropic
U/PLOF	Unprotected/Protected Loss of Flow
U/PLOHS	Unprotected/Protected Loss of Heat Sink
VHTR	Very High-Temperature Reactor

1. INTRODUCTION

This report provides a review of computer code modeling capabilities for non-light water reactors (non-LWRs) for beyond design basis accident analysis and development of regulatory source terms, and describes code developments required for non-LWR safety analysis. Non-LWR nuclear systems use working fluids other than light water on the primary side – typically as a coolant. Four general classes of such non-LWR designs are presently of focus for the U.S. NRC given anticipated licensing needs for the near future. These include:

1) High Temperature Gas-Cooled Reactor (HTGR)
2) Sodium Fast Reactor (SFR)
3) Molten Salt Reactor (MSR)
4) Fluoride Salt-Cooled High Temperature Reactor (FHR)

In addition to these general reactor types, there are a number of design-specific variations and/or hybrids within and across these technologies. For example, several sodium-cooled reactor designs utilizing heat pipe core cooling have been developed for low power, remote applications. Such a system is a significant departure from traditional circulating sodium designs but does share certain characteristics of SFRs. For HTGRs, there are both prismatic (PMR) and pebble bed (PBR) designs with online refueling. Molten salt designs include the circulating salt-cooled, salt-fueled molten salt reactor (MSR) as well as the solid fueled fluoride salt-cooled high temperature reactor (FHR), which is a hybrid design utilizing pebble fuel elements (like pebble bed HTGRs) and a fluoride salt coolant (like salt-cooled MSRs). Some fixed fuel FHR designs (like prismatic HTGRs) have been proposed, but none are currently under commercial consideration.

Figure 1-1 illustrates the evaluation model (EM) developed for the Next Generation Nuclear Plant (NGNP) project (PBR and PMR) as presented to the NRC's Advisory Committee on Reactor Safeguards (ACRS) in a subcommittee meeting on future plant designs on April 5, 2011. This historical EM outlines requisite steps to perform a confirmatory safety analysis for a given licensing basis event (LBE). As per Regulatory Guide 1.203, "Transient and Accident Analysis Methods", an EM is "the calculational framework for evaluating the behavior of the reactor system during a postulated transient or design-basis accident. As such, the EM may include one or more computer programs, special models, and all other information needed to apply the calculational framework to a specific event." This figure is provided to illustrate that the EMs currently proposed for non-LWR analysis throughout this report are not new and have been the subject of research over a long period of time.

This report focuses on the development of evaluation models for non-LWR designs and the role of the computer codes MELCOR, MACCS, and SCALE. The long-term goal is development of regulatory source term (see section 1.1) and capabilities for analysis of severe accident progression and offsite consequences for various design types.

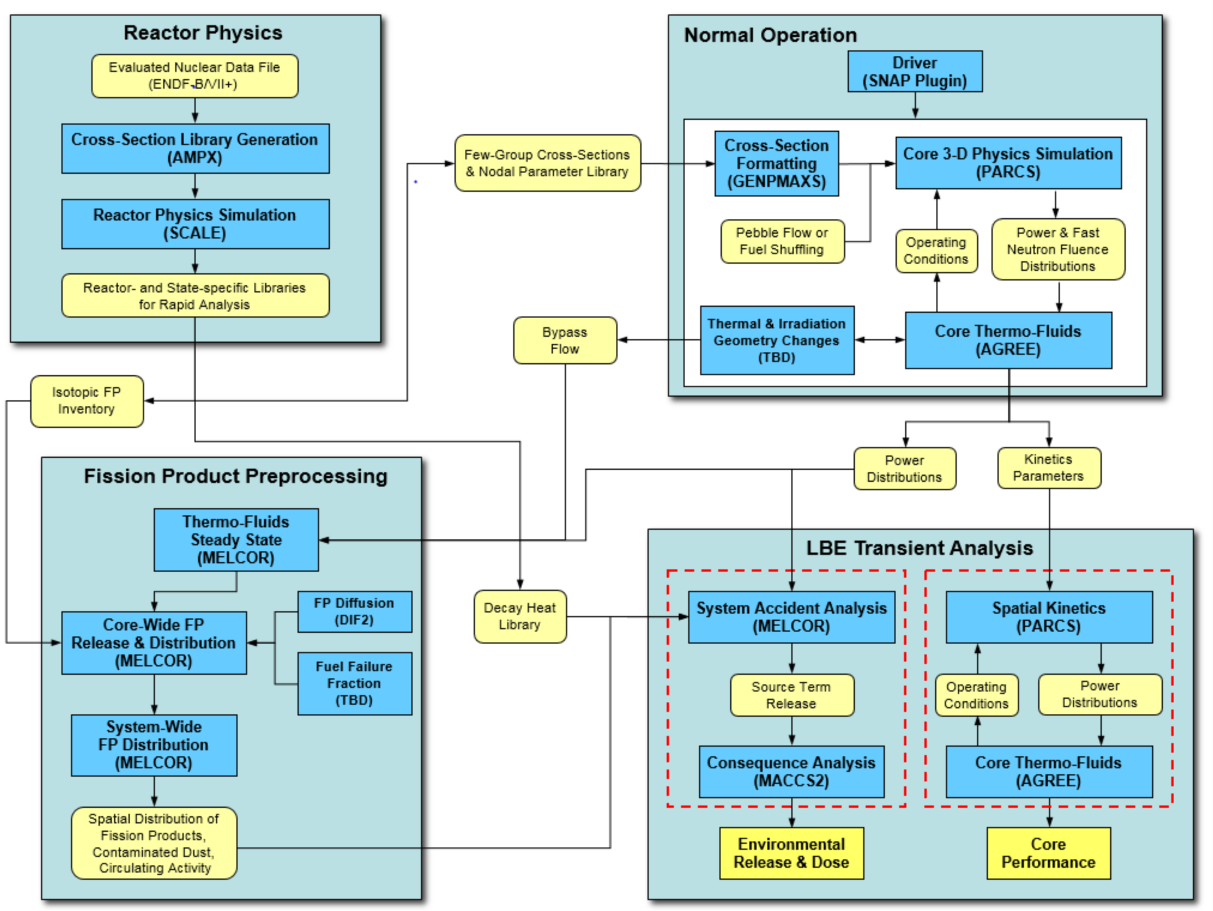

Figure 1-1. NRC Evaluation Model for NGNP (from April 2011)

The important objectives addressed in this report include:

1) **Code Development Plan**. Provide a development plan to address those gaps in modeling that are needed to demonstrate functional readiness.
2) **Model Maturity Evaluation**. Review readiness of the codes for non-LWR licensing calculations, including discussions of important non-LWR phenomena as determined by previous PIRTs and expert elicitations. For each phenomenon, existing capabilities/provisions and unresolved modeling gaps are outlined.
3) **Model Validation**. Discuss validation needs and existing validation efforts.
4) **Data Needs**. Discuss code input/output requirements, identify the role of experiments in filling data needs, and identify missing data.

Section 1.1 discusses the regulatory need for source term analysis using NRC developed computational tools discussed in this report. Section 1.2 provides an overview of the computer codes and the basis for their selection. The codes' development plans listing the specific tasks for each reactor type are given in Section 1.2. Details on the development plans for each code are provided in Sections 2 (MELCOR), 3 (SCALE), and 4 (MACCS). A review of the current extensive modeling and simulation capabilities and how the modeling gaps are identified and addressed to demonstrate functional readiness for confirmatory analysis are discussed in the individual codes' sections.

1.1. Regulatory Need for Source Term Analysis

Regulatory source terms are deeply embedded in the NRC's regulatory policy and practices, as the current licensing process has evolved over the past 50 years. This approach encourages nuclear plant designers to incorporate several lines of defense in order to maintain the effectiveness of physical barriers between radiation hazards and workers, members of the public, and the environment – for both normal operation and accident conditions. The approach centers on the concept of design basis accidents (DBAs), which aim to determine the effectiveness of each line of defense. The DBAs establish and confirm the design basis of the nuclear facility, including its safety-related structures, systems, and components and items important to safety. This ensures that the plant design meets the safety and numerical radiological criteria set forth in regulations and subsequent guidance. From this foundation, specific safety requirements have evolved through a number of criteria, procedures, and evaluations as reflected in the regulations, guides, standard review plans, technical specifications, and license conditions, as well as TID, WASH, and NUREG documents.

The various regulatory source terms, used in conjunction with the DBAs, establish and confirm the design basis of the nuclear facility, including items important to safety, ensuring that the plant design meets the safety criteria set forth in the U.S. Code of Federal Regulations (CFR) (e.g., 10 CFR 100.11, "Determination of Exclusion Area, Low Population Zone, and Population Center Distance"; 10 CFR 50.67, "Accident Source Term"; 10 CFR 50.34(a)(1)(iv); General Design Criterion 19, "Control Room," of Appendix A, "General Design Criteria for Nuclear Power Plants," to 10 CFR Part 50, "Domestic Licensing of Production and Utilization Facilities") and in subsequent staff guidance. For non-LWR safety analyses, potentially impacted regulatory requirements and guidance include the following:

- Regulations (10 CFR Part 50; 10 CFR Part 52, "Licenses, Certifications, and Approvals for Nuclear Power Plants"; and 10 CFR Part 100)
- Regulatory guides
- Technical specifications
- Emergency preparedness procedures
- Evaluation methods for assessing the environmental impacts of accidents

The NUREG-0800 Standard Review Plan (SRP) for the review of safety analysis reports for nuclear power plants contains specific examples of the various regulatory source terms and provides information on the staff's regulatory guides. The various regulatory source terms discussed in the SRP include the following:

- Accident source term is based on DBAs to establish and confirm the design basis of the nuclear facility and items important to safety while ensuring that the plant design meets the safety and numerical radiological criteria set forth in the CFR (e.g., 10 CFR 100.11, 10 CFR 50.67, 10 CFR 50.34(a)(1)(iv), GDC 19, and subsequent staff guidance). SRP Chapter 15 addresses this topic.

- Equipment qualification source term is used to assess dose and dose rates to equipment. SRP Section 3.11, "Environmental Qualification of Mechanical and Electrical Equipment"; SRP Section 12.2, "Radiation Sources"; Regulatory Guide 1.89, "Environmental Qualification of Certain Electric Equipment Important to Safety for Nuclear Power Plants"; and Regulatory Guide 1.183, "Alternative Radiological Source Terms for Evaluating Design Basis Accidents at Nuclear Power Reactors," Appendix I, address this topic.
- Post-accident shielding source term is used to assess vital area access, including work in the area. SRP Section 12.2; Item II.B.2 of NUREG-0737, "Clarification of TMI Action Plan Requirements," issued November 1980; RG 1.89; and RG 1.183 address this area.
- Design-basis source term is based on 0.25–1-percent fuel defects to determine the adequacy of shielding and ventilation design features. SRP Section 12.2 provides further guidance.
- Anticipated operational occurrences source term is based on the technical specifications or the design-basis source term, whichever is more limiting, to determine the effects of events like primary-to-secondary leakage and reactor steam source term. SRP Section 11.1, "Coolant Source Terms," gives reactor coolant (primary and secondary) and reactor steam design details.
- Normal operational source term is based on operational reactor experience, as described in American National Standards Institute/American Nuclear Society N18.1, "Selection and Training of Nuclear Power Plant Personnel." SRP Section 11.1 and Section 11.2, "Liquid Waste Management System," give further guidance for reactor coolant (primary and secondary) and reactor steam design details, and SRP Section 11.3, "Gaseous Waste Management System," gives system design features used to process and treat liquid and gaseous effluents before being released or recycled.

This process of developing source terms was initially very prescriptive and defined in TID-18444 "Calculations of Distance Factors for Power and Test Reactor Sites". It was replaced by a mechanistic process as defined in NUREG-1465, "Accident Source Terms for Light-Water Nuclear Power Plants." Both source term characterizations are focused on LWRs and are therefore not appropriate for direct application to non-LWRs. Even so, the mechanistic source term described in NUREG/CR-1465 provides the framework for developing methods and codes such as MELCOR for severe accident analysis.

The NRC staff has concluded that an ongoing code development process is appropriate for incorporating new information on non-LWR accident source terms especially as priorities regarding the different technologies emerge. An applicant may propose changes in source term parameters (timing, release magnitude, and chemical form) from those contained in the applicable guidance, based on and justified by design-specific features. Regulatory Position 2 of Regulatory Guide 1.183 provides attributes of an acceptable alternative source term.

To generate an acceptable source term, certain modeling capabilities must be either adapted from current light water capabilities, added for new phenomena specific to new technologies, or ignored for those physics models specific to LWR application. Figure 1-2 below depicts the radionuclide (RN) transport path from release from the fuel to release to the environment for an LWR. Deposition and resuspension of aerosols on surfaces, evaporation and condensation on aerosols and structures, agglomeration of aerosols, chemisorption on surfaces, and bubble transport through coolant are examples of existing phenomena developed for LWR analysis that are also important in non-LWR applications though the state domain, properties, and boundary conditions are different. For sodium-moderated reactors, sodium fire modeling becomes important in characterizing aerosol released which is a phenomenon that is not important for LWR analysis. Similarly, for TRISO fuels, which may be used in HTGRs and possibly MSRs, zonal diffusion through a TRISO particle is important. As a consequence, the RN release/transport path diagram is different for each general reactor type. Modified versions of this diagram are provided in the discussions that follow for each general reactor type.

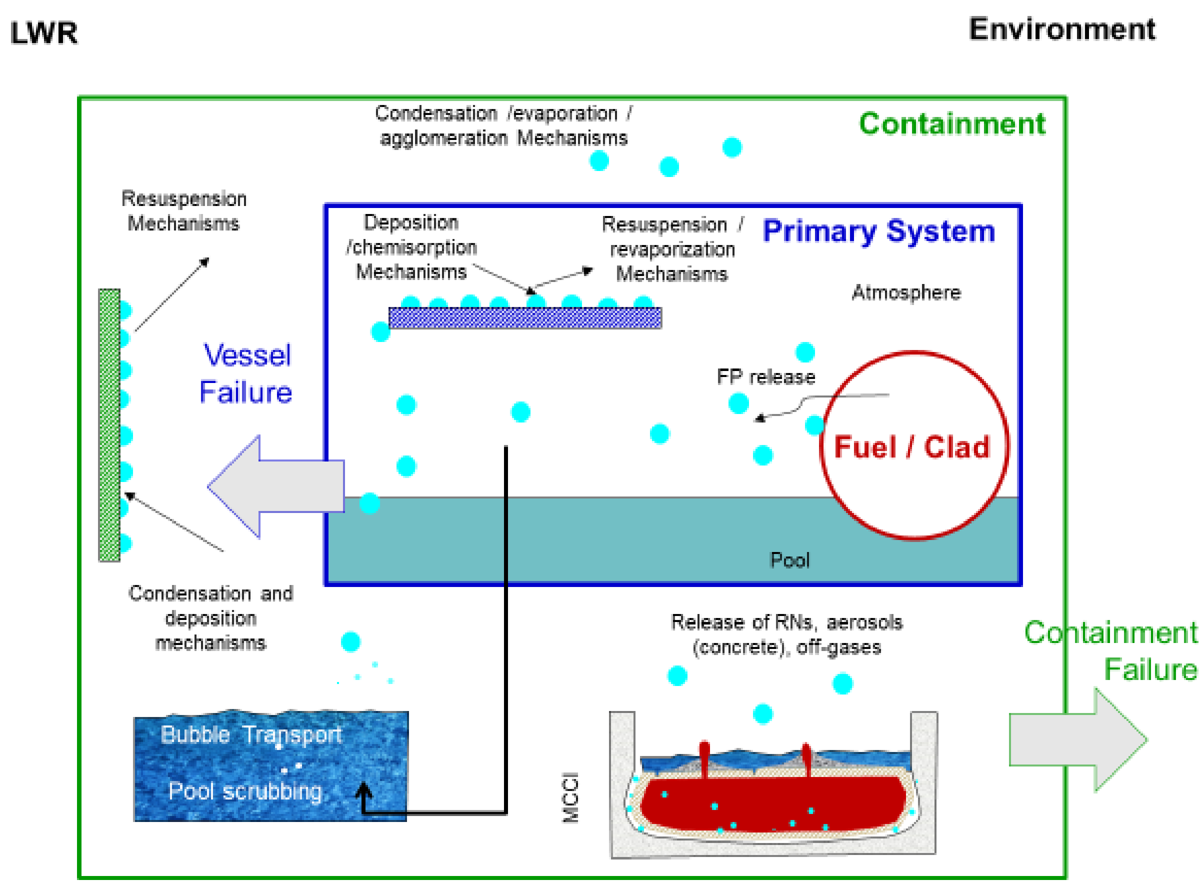

Figure 1-2. Radionuclide transport paths for LWR designs.

The role of the computer codes used to generate accident source term and consequences is depicted in Figure 1-3. NRC's Office of Nuclear Regulatory Research (RES) is responsible for the development of the computer codes and follows the information flow shown in Figure 1-3.

The figure also shows an overview of regulatory uses of the codes by the Office of New Reactors (NRO) who is responsible for siting and licensing of new reactor designs. Future uses of the information by the Office of Nuclear Material Safety and Safeguards (NMSS) are also shown. For consequence analysis, this report volume focuses on the MACCS code; other related codes shown in Figure 1-3 including RADTRAD and RASCAL are discussed separately in Volume 4 of this report series.

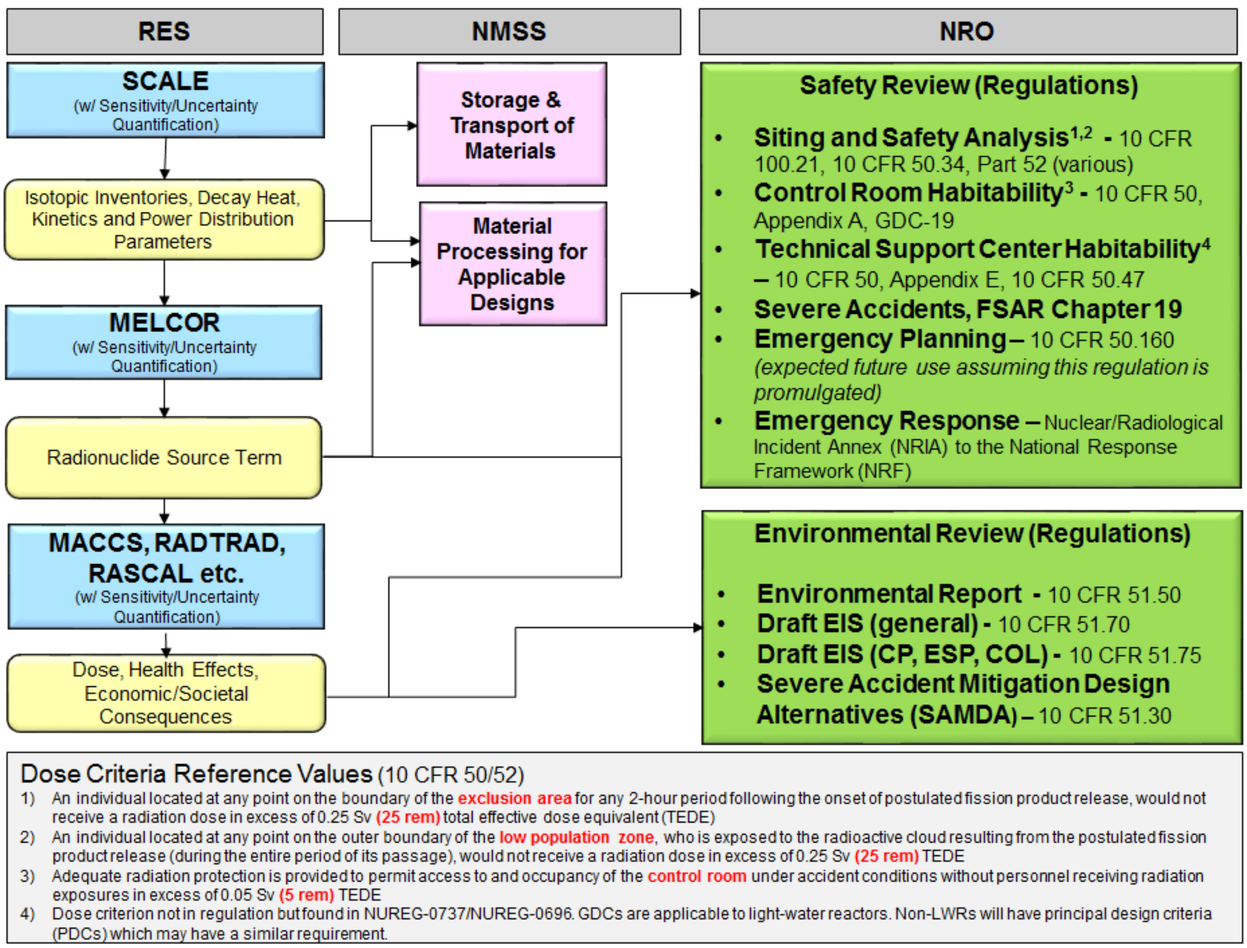

Figure 1-3. Role of Accident Progression, Source Term, and Consequence Analysis Computer Codes and Applicable Regulatory Requirements

1.2. Description of Computer Codes

This section provides a brief description of various computer codes used for severe accident progression, source term, and consequence analysis and the rationale for using these code for non-LWR applications. A common set of rationale for selecting the MELCOR, SCALE, and MACCS codes is described below.

NRC Staff Familiarity – These codes have been used for decades by the domestic and international nuclear research community as well as by NRC staff for safety analysis of LWRs. Therefore, staff is familiar with the code input/output requirements and model development history. Extension to non-LWRs involves minimal staff training compared to adoption of a new set of tools. Some of the existing models in the codes do not require any changes for source term analysis of non-LWRs (e.g., MELCOR has extensive capabilities for containment/confinement analysis and aerosol dynamics modeling supported by experimental validation).

Long-Term Code Development and Maintenance – These codes have a long active history of maintenance and development. MELCOR and MACCS have been under development at Sandia National Laboratories (SNL) and SCALE has been under development at Oak Ridge National Laboratory (ORNL) in response to NRC emerging needs for LWRs. There are existing capabilities for transfer of information between the codes (e.g., the MelMACCS program serves as an interface between MELCOR and MACCS for source term and consequence analysis). It is desirable and it would be very cost-effective to have the same code for both LWR and non-LWR applications to reduce the life cycle cost of code maintenance and user training and leverage improvements for common modeling approaches (e.g., dynamics of fission product aerosols inside the containment).

MELCOR Integrated Severe Accident Code

MELCOR is a fully-integrated, system-level computer code developed by SNL for the NRC originally for modeling the progression of severe accidents in LWR nuclear power plants [7] [8]. Since the project began in 1982, MELCOR has undergone continuous development to address emerging issues, process new experimental information, and create a repository of knowledge on severe accident phenomena. The inherent flexibility in the MELCOR code architecture has already allowed the extension of the code beyond its original LWR application space to non-reactor applications such as spent fuel pools and fusion reactors and more recently, as part of NGNP, application to HTGR analysis. MELCOR has been modified to accommodate certain physics and features of other non-LWR designs such as SFRs and MSRs. Modeling capabilities for HTGRs were added in 2008 and modeling capabilities (for analysis of containment issues only) in sodium-cooled reactors began in 2013. Most recently, a molten salt (FLiBe) fluid model was added to enable further MSR analysis.

The objectives for the development of the MELCOR code and its various physical models are to provide a tool capable of performing severe accident progression modeling and source term characterization while allowing the capability for performing uncertainty analyses and permitting extrapolation of the results of small-scale effects and integral effects experiments to full-scale application. Further, the code must be robust, fast-running, and maintainable, and provide a means for NRC staff to readily and inexpensively perform such analyses. The following criteria determine the success for such code development practices.

1. MELCOR predictions of phenomenological events are in qualitative agreement with the current understanding of the physics of such events based either on the results of certain well-defined/controlled experiments or on analytical results derived from first principles.

2. Uncertainties in key parameters describing a phenomenon as calculated by MELCOR are in quantitative agreement with the uncertainties in experimentally measured or analytically derived values of these parameters.
3. Where feasible, MELCOR phenomenological models are mechanistic in nature and capture the major physical processes. Alternatively, parametric models are used and uncertainties in the phenomena can be adequately represented through parametric variations and sensitivity analysis.
4. Code user guidance is available to facilitate and standardize plant calculations of targeted applications in seeking consistent and reasonable key figure of merit predictions.
5. All plant input models/applications and code assessments are well-documented, and non-proprietary documents are available to users.
6. MELCOR is portable, robust, and relatively fast-running.
7. The maintenance of the code follows software quality assurance standards for configuration control, testing, and documentation.

Such criteria for success and development objectives are applied within the development plan for non-LWR modeling and simulation capabilities.

The development of MELCOR as an integrated tool was a very significant advancement in the capability for performing severe accident analysis for source term characterization. Prior to the development of MELCOR, separate effects codes within the Source Term Code Package (STCP) were run independently and results were manually transferred between codes leading to a number of challenges for transferring data, ensuring consistency in data and properties, and in capturing the coupling of physics. There are numerous feedback mechanisms associated with the myriad of phenomena that are relevant in a severe accident. As fuel fails, it releases radionuclides which can be swept away from the fuel and later deposited downstream through chemisorption or released to the containment through relief valves. The decay heat associated with those released fission products transfers that heat load to the vessel, piping, or the containment. Removal of radionuclides from fuel reduces the thermal energy generated in the fuel materials, affecting temperatures of core components. The heat transferred to pipes can lead to stress or failure of pipes. Heat transfer to the containment affects the containment which provides boundary conditions for the RCS which then impacts the rate of core degradation and release of radionuclides.

Depending on the design, such complicated feedback may not be possible to capture even when the separate effects codes are coupled. For example, a code that calculates degradation of fuel but does not also model the release of radionuclides to the coolant will not adequately capture the heat load and thermal response of the coolant system. Having a single, integrated code that calculates the system response to the degrading fuel as well as aerosol/vapor transport accounts for the temperature response and boundary conditions for aerosol physics. It is not possible to calculate the aerosol/vapor physics separately from the fuel performance because the fuel performance calculation provides the detailed boundary conditions throughout the system that is necessary for the balance of the calculation.

The advantages of using a fully-integrated tool for performing source term analysis are significant and are summarized here. Though other advantages exist, several important ones for consideration are as follows:

1. Integrated accident analysis is necessary to capture the complex coupling between a myriad of interactive phenomena involving movement of fission products, core materials, and safety systems. Integration of models within a single integrated code represents the ultimate in code/modeling coupling, which is the only means of capturing all relevant feedback effects.

2. A calculation performed with a single, integrated code as opposed to a distributed system of codes reduces errors associated with transferring data downstream from one calculational tool to the next. This was also a key conclusion in a recent study by Argonne National Laboratories to scope out remaining issues for calculating a mechanistic source term for sodium fast reactors [9]:

   "First, the analysis of radionuclide behavior within the fuel pin, and subsequent release to the sodium pool and cover gas region, utilized several computer codes (HSC, IFR bubble code, and ORIGEN) and other side calculations, which taken together, involved many data communication steps. Each transfer of information between codes presented an opportunity for error introduction as data was converted. Properly separating and combining data from the multiple analysis tools was not trivial, even for the simplified analysis of only three fuel batches. An attempt to perform a more precise source term assessment, with many different fuel groups within the core, would be a significant effort utilizing this framework."

3. Performing an analysis with a single integrated code assures that the results are generally repeatable. Calculations that are performed using a specific code version using a specific input model version can be rerun with the expectation that identical results will be obtained when run on the same computing system. Furthermore, the MELCOR development team has carefully chosen code optimization strategies that will lead to identical results for many test calculations when run on either Windows or Linux OS. This is much more difficult to guarantee with distributed tools using different versions of code, optimized for different systems, particularly if user intervention is required to transfer data from one calculation to the next.

4. There will always be uncertainty in the results obtained by any modeling and simulation system. Uncertainties exist in the models that are incorporated, uncertainties in the model parameters, and uncertainties in the boundary conditions imposed by the modeler. Consequently, uncertainty analysis is essential for any modeling and simulation tool. Methods for performing uncertainty analysis with an integrated tool such as MELCOR are well established. Several large uncertainty studies have been performed (Grand Gulf Hydrogen UA, Surry UA, Sequoyah UA, Peach Bottom UA, and Fukushima UA) using MELCOR (and some also using MACCS) and are documented. Challenges exist in

performing such analysis using distributed tools or even coupling codes together. A high success rate of completion is essential and guaranteeing such success is difficult when using multiple computational tools supported and developed by many organizations.

5. Time step issues are internally resolved within the integral code. Coupling codes together can lead to solution convergence issues related to time step resolution.

In addition to broad domestic use, MELCOR and MACCS are used by a number of international organizations (about 30) under the Cooperative Severe Accident Research Program (CSARP). CSARP is an international program on severe accident phenomenological research and code development activities organized by NRC. Through CSARP, NRC has access to large number of international severe accident research programs (especially those from Europe and Asia). MELCOR Code Assessment Program (MCAP) is an annual technical review meeting that focuses on the MELCOR code development and assessment. The European MELCOR/MACCS User Group (EMUG) and the Asian MELCOR/MACCS User Group (AMUG) are annual meetings focused on exchange of information among the participating organizations regarding the use of MELCOR and MACCS, and to improve the feedback among the code users and the code developers. Many code users are already using MELCOR models developed for non-LWR applications, and in the most recent MELCOR workshop there were sessions on HTGR and SFR modeling. Appendix F of this report contains a presentation from the 2018 EMUG meeting that showed successful application of the code for HTGRs.

Examples of other integrated severe accident progression codes include MAAP (mainly used by the nuclear power industry) and ASTEC (developed by IRSN in France). These codes have somewhat similar capabilities for modeling of LWR accident scenarios and there has been cross-walk benchmarking of these codes against MELCOR. NRC staff participate in these activities through various international activities and CSARP. MAAP currently has no capabilities for modeling of non-LWR designs and there is currently no plan to include the required modeling in the MAAP code. While ASTEC has some capabilities for simulating sodium reactors, there does not seem to be any capabilities for other designs such as HTGRs, whereas MELCOR has extensive modeling enhancements. In addition, MELCOR is developed at SNL for NRC, so there is access to the source code, and SQA is in place. Other tools such as the Department of Energy (DOE) Nuclear Energy Advanced Modeling and Simulation (NEAMS) do not have the necessary capabilities for performing an integrated source term analysis (see the discussion above for the need for an integrated severe accident code).

<u>SCALE Reactor Physics Code</u>

SCALE is a multi-disciplinary tool developed by ORNL for NRC to combine nuclear system simulation tools into one cohesive package. This was intended to mitigate human errors from data transfer and manipulation between code packages, consolidate experience, and speed up analysis times.

SCALE provides a comprehensive, verified and validated, user-friendly tool set for nuclear data, criticality safety, reactor physics, radiation shielding, radioactive source term characterization, activation, depletion and decay, and sensitivity and uncertainty analysis under a software quality assurance program. Since the 1970s, regulators, licensees, and research institutions around the world have used SCALE for safety analysis.

SCALE is used by nearly 100 licensed users across NRC. SCALE is used in 10 CFR Part 100, 71, 72, 68, and 50 reviews. It is also used by downstream codes such as FAST (fuel performance), PARCS (core simulator), TRACE (design basis analysis), MELCOR (severe accident progression analysis) and MACCS (consequence analysis).

An extensive modernization effort was undertaken for the 2016 release of SCALE version 6.2 to provide an integrated framework with dozens of computational modules, including three deterministic and three Monte Carlo radiation transport solvers selected based on the user's desired solution strategy. SCALE includes nuclear data processing tools and current nuclear data libraries for continuous energy and multigroup neutronics and coupled neutron-gamma calculations, as well as activation, depletion, and decay calculations. SCALE includes unique capabilities for automated variance reduction for shielding calculations, as well as sensitivity and uncertainty analysis. SCALE's graphical user interface assists with accurate system modeling and convenient access to desired results. The NRC is the primary sponsor of SCALE for its application in licensing current and advanced reactors, fuel cycle facilities, and radioactive material transportation and storage.

SCALE has been used extensively in conjunction with MELCOR and MACCS for LWR severe accident analysis, recently with the new spent fuel isotopics generation application, ORIGAMI, which enables rapid analysis and has been applied to probabilistic risk assessments involving ~3000 fuel assemblies, each with unique operating histories. The rapid isotopics calculation scheme is a hallmark of SCALE. Additional minor developments and assessments in SCALE are necessary to provide the same robustness and flexibility for non-LWRs as are available for LWRs (e.g., in fast spectrum systems, where the assumption of reflective assembly boundary conditions must be revisited, or for moving fuel forms, where user input describing the irradiation history in terms of this motion should be added).

The development and assessment of SCALE for non-LWR applications has additional benefits. For example, developing a high-level, intuitive user interface, and quick running tool will allow staff to quickly and easily develop criticality and shielding analyses from the inventory and decay heat data generated using this methodology. Additionally, because the Fulcrum interface has been developed to also support the NRC's SNAP interface, the data can be quickly used by other NRC codes such as PARCS and TRACE through templates.

MACCS Consequence Analysis Code

The MELCOR Accident Consequence Code System (MACCS) suite is used to model atmospheric releases of radioactive materials into the environment and the subsequent consequences of such releases. MACCS is the only tool for modeling within a probabilistic framework all the technical areas in the ASME/ANS RA-S-1.3-2017 Standard for Radiological Accident Offsite Consequence Analysis (Level 3 PRA) to Support Nuclear Installation Applications [10]. These include (1) radionuclide release, (2) atmospheric transport and dispersion, (3) meteorological data, (4) protective actions and site data, (5) dosimetry, (6) health effects, (7) economic factors, and (8) conditional consequence quantification and reporting.

The MACCS code suite [11, 12] has been under active use and development over several decades. The suite of codes includes the user interface, WinMACCS, and various pre- and post-processor codes including MelMACCS [13], SecPop [14], COMIDA2 [15], and an animations tool AniMACCS. MelMACCS is a pre-processor code that converts source term data from MELCOR into MACCS format. SecPop is another pre-processor code that facilitates use of site-specific population, land use, and economic data. The COMIDA2 pre-processor is used to provide food chain input parameters for MACCS ingestion dose calculations. The MACCS animations tool, AniMACCS, enables visualization of atmospheric dispersion and resulting air and ground concentrations around a site for a given weather trial.

MACCS has a wide user base beyond NRC including nuclear power licensees and applicants, DOE, research organizations, and academia. The MACCS code suite is shared internationally through the Cooperative Severe Accident Research Program (CSARP) [16] with many organizations from 25+ member countries.

At NRC, the MACCS code suite supports a variety of regulatory applications. MACCS is used in regulatory cost-benefit analyses to estimate the potential benefits of safety improvements in terms of the averted accident consequences and supports 10 CFR 50.109, "Backfitting." MACCS is used in the new reactor licensing process for analyses of Severe Accident Mitigation Design Alternatives (SAMDAs) as per 10 CFR 51.30, "Environmental Assessment" which are needed to comply with the National Environmental Policy Act (NEPA). Similarly, MACCS is used in analyses of Severe Accident Mitigation Alternatives (SAMAs) as per 10 CFR 51.53, "Postconstruction Environmental Reports," in the license renewal process to comply with NEPA if SAMDA analyses were not previously conducted during the design application phase.

MACCS is also used in several areas to support emergency planning and preparedness for nuclear power plants. MACCS, which enables modeling of emergency-phase protective actions including evacuation, is closely tied to evacuation time estimate (ETE) studies which are required by licensees in 10 CFR 50 Appendix E, "Emergency Planning and Preparedness for Production and Utilization Facilities." Pending the outcome of the ongoing rulemaking process on Emergency Preparedness for Small Modular Reactors and Other New Technologies, MACCS may be used for probabilistic dose exceedance vs. distance-type calculations to inform emergency planning zone (EPZ) size needed for a given site. If codified in NRC regulations, this would be discussed in 10 CFR 50.160 as shown in Figure 1-3 above.

Additionally, as the only U.S. probabilistic consequence code, MACCS is used in Level 3 PRA studies including NRC's ongoing full-scope Level 3 PRA project. This project helps support extracting new risk insights to enhance regulatory decisionmaking and helps focus agency resources on issues most important to risk. MACCS is used in research studies of accident consequences including the State-of-the-Art Reactor Consequence Analyses (SOARCA) to update our understanding of realistic accident consequences and shed light on margins to NRC's quantitative health objectives.

MACCS has primarily been used for analysis of consequences of atmospheric releases from accidents at conventional large LWRs. MACCS is a very flexible code and its input decks can generally be made plant-specific, site-specific, and accident-specific by modifying a subset of the hundreds of input parameters and the handful of input files. MACCS can also be used for analyzing atmospheric releases from spent fuel pool accidents and dry cask accidents, as is being done in the full-scope Level 3 PRA project [17]. MACCS modeling best practices have evolved significantly over the past decade as staff has completed several major consequence analyses. These include the State-of-the-Art Reactor Consequence Analyses (SOARCA) of selected scenarios at Peach Bottom [18], Surry [19], and Sequoyah [20]. These also include post-Fukushima analyses of the potential benefits of containment vents and external filters [21] and expedited transfer of spent fool from pools to dry casks [22]. MACCS modeling best practices as applied in SOARCA were published [23] while staff continues to complete an updated MACCS input parameter guidance report [24].

MACCS is uniquely suited for consequence analysis of non-LWRs because of its flexibility and broad range of models and phenomena considered. Other computer codes are available to compute offsite doses and they have some overlap in modeling areas with MACCS. However none consider such a wide spectrum of modeling areas and types of consequence outputs. For example, many models are available which treat atmospheric dispersion and calculate doses at different locations. The MACCS code suite is the only modeling tool which considers the full range of protective actions (evacuation, sheltering, relocation, ingestion of potassium iodide, decontamination, etc.), the full range of weather variability, and the full range of consequence measures (including doses, fatality risks, economic costs, land contamination, and societal consequences). MACCS also has a built-in capability for uncertainty analysis which makes it unique relative to other codes. The RADTRAD code has some overlap with MACCS in that it may be used to calculate a site boundary dose without protective actions. RASCAL is another code which can calculate offsite doses and it is used in incident response situations by NRC's Operations Center during drills and emergencies. RADTRAD and RASCAL are actively developed and used for various regulatory applications. Their application to non-LWR analysis and associated code development needs will be discussed in a separate report, Volume 4. RADTRAD and RASCAL are not as well suited for consequence analysis because both are much more constrained in their capabilities for radionuclide release in that much of their source term information is hard-coded and not easily adapted by users. MACCS is much more flexible in its ability for users to modify source term information.

<u>**Summary of Non-LWR Design Types and Applicable Code Development Tasks**</u>

Table 1-1 lists the designs currently under consideration grouped into ten generic design types. The model development for MELCOR will be designed with extensive flexibility to be applicable to all these designs based on information (in some cases limited) available today. The last column in the table maps the development items discussed in MELCOR and SCALE plans for each generic design type.

Table 1-1. Generic Listing of Non-LWR Designs.

Plant Type No.	Description	Example(s)	Fuel	Development Item		
				MELCOR	**SCALE**	**MACCS**
1	HTGR; prismatic core, thermal spectrum	Framatome	TRISO (rods or plates)	M2.1, M2.2	A1-A10, D1-D6	CA1-3, CA5-6
2	PBMR; pebble bed core, thermal spectrum	X-energy Starcore	TRISO (pebbles)	M2.1, M2.2	A1-A10, D1-D6	CA1-3, CA5-6
3	GCFR; prismatic core, fast spectrum	GA	SIC clad UC (plates)	M2.1, M2.2	A1-A10, D1-D6	CA1-3, CA5-6
4	SFR; sodium cooled, fast spectrum	PRISM ARC	Metallic (U-10Zr)	M1.2-M1.7, M1.9-M1.11	A1-A3, D1-D3	CA1-3, CA5-6
5	LMR; lead cooled, fast spectrum	Westinghouse Columbia Basin Hydromine	Not available	M1.2-M1.4, M1.7, M1.9-M1.11	TBD	CA1-3, CA5-6
6	HPR; heat pipe cooled, fast spectrum	Oklo Westinghouse	Metallic (U-10Zr)	M1.1-M1.11	A1-A3, D1-D3	CA1-3, CA5-6
7	MSR; prismatic core, thermal spectrum	AHTR	TRISO (plates)	M3.5	A1-A4, D1, D2, D5	CA1-6
8	MSPR; pebble bed, thermal spectrum	Kairos	TRISO (pebbles)	M3.5	A1-A4, D1, D2, D5	CA1-6
9	MFSR; fluoride fuel salt, thermal/epithermal spectrum	Terrestrial Thorcon FliBe	Fuel salt	M3.1-M3.4	A1, A2, D3-D5	CA1-6
10	MCSR; chloride fuel salt, fast spectrum	TerraPower Elysium	Fuel salt	M3.1-M3.4	A1, A2, D3-D5	CA1-6

2. MELCOR DEVELOPMENT PLANS FOR NON-LWRS

Much of the physics already captured in MELCOR is agnostic to reactor technology. Physics such as thermal conduction, radiant heat transfer, energy and mass balance, fluid flow, and aerosol transport are applicable in the context of non-LWRs. The NRC has leveraged this versatility for purposes other than LWR analysis. MELCOR has been used to track fuel damage in both reactor core and Spent Fuel Pool (SFP) scenarios, to calculate mechanistic source terms with respect to both the initial release and subsequent transport of radionuclides in the reactor coolant system, and to model the behavior of radionuclides, aerosols, and vapors in a containment structure or building. Furthermore, the Department of Energy has included MELCOR in its Safety Software Central Registry ("toolbox" codes) to model the progression of hazardous material source term through DOE facilities and buildings with complicated internal structures. Because it is an integral code, MELCOR offers great flexibility to users in generating source term calculations that are self-consistent across a broad range of phenomena, that are highly repeatable, and that easily lend themselves to performing uncertainty analyses. This self-consistency eliminates errors associated with explicit coupling of independent codes.

New models capturing missing physics for High Temperature Gas-Cooled Reactors (HTGR) and Sodium Fast Reactor (SFR) containment have already been added to MELCOR either through new model development (HTGR and SFR) or migration of existing models from the CONTAIN-LMR code into MELCOR for SFR analysis. A timeline showing this development is provided in Figure 2-1. Development of non-LWR capabilities has been an ongoing effort (alongside LWR model development and MELCOR code modernization efforts) for more than a decade though the dedicated funding levels have not always been substantial. The development plan for non-LWRs is expected to allow completion of essential HTGR, SFR, and MSR models within three years development time.

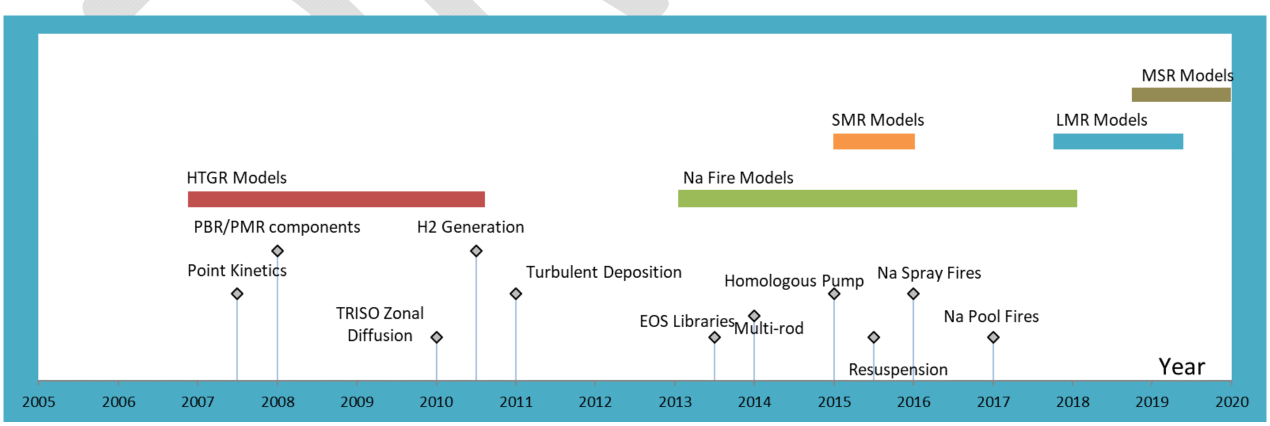

Figure 2-1. Timeline of MELCOR Advanced Reactor Model Development.

Note that as models are added for any of the specific advanced reactor types, such development often facilitates modeling of other advanced reactor types. For example, when sodium was added as a working fluid (for SFR analysis), it was introduced in the context of a general framework that enables similar incorporation of other working fluids (such as FliBe or Lead) through library files. As a further example, a multi-rod model was added in support of spent fuel pool analysis. This model may be leveraged to predict the propagation of core degradation from localized failure of heat pipes or for modeling multiple HTGR pebbles within a single COR cell. Similarly, addition and modification of vaporization/dissolution models in a sodium pool would advance MELCOR SFR modeling capability, but would also advance MSR modeling capability. Finally, development of fuel components for heat pipe should also aid in the development of fuel components for SFRs. There are several such examples in MELCOR development where the careful addition of a new model enables other seemingly unrelated capabilities.

A method for assessing the maturity level of computational modeling and simulation was developed at Sandia National Laboratories and has been applied to MELCOR in estimating the level of readiness of the code for application to non-LWRs. The Predictive Capability Maturity Model (PCMM) provides a means of addressing six important elements of modeling and simulation (1) representation and geometric fidelity, (2) physics and material model fidelity, (3) code verification, (4) solution verification, (5) model validation, and (6) uncertain quantification and sensitivity analysis. The PCMM is a structured albeit somewhat subjective method of determining the maturity of the analysis tool.

Code validation is an important element of a software quality assurance (SQA) program. Proper validation of physical models encoded into analytical tools is essential to provide developers the necessary guidance in developing and improving algorithms and numerical methods for describing physical processes. Moreover, validation results are essential for code users in order to gain confidence in applying the code to real-world applications. It is important that such validation exercises be performed objectively by both developers, who may better understand the nuances of particular models, as well as users, who may have a more distant knowledge of the internal models but may have a greater knowledge of real-world applications.

Many validation studies have been performed for MELCOR and are well documented. Volume 3 of the MELCOR documentation [25] is the code assessment report which discusses analysis of MELCOR's models in simulating experimental assessment cases. Validation cases have been selected from a variety of separate effects tests, integral tests, International Standard Problems (ISPs) and actual reactor severe accidents (TMI-2 and Fukushima). Recognizing that validation should be performed for each physical model under the domain of state conditions expected for a particular accident, it is understood that validation of new and even existing models should be performed for each new reactor type. Even so, it is also recognized that validation of many models represented in MELCOR are agnostic to the particular reactor technology and therefore existing validation cases can in some cases support the modeling for advanced reactor concepts.

Figure 2-2 depicts the current LWR validation base as well as validation cases that have been proposed for non-LWR application. Several validation tests for sodium spray fires and sodium pool fires have already been added to the MELCOR validation base (see Appendix B) and additional validation cases are proposed in the body of the report which follows. Together this validation basis can provide confidence in accuracy of the proposed modeling efforts.

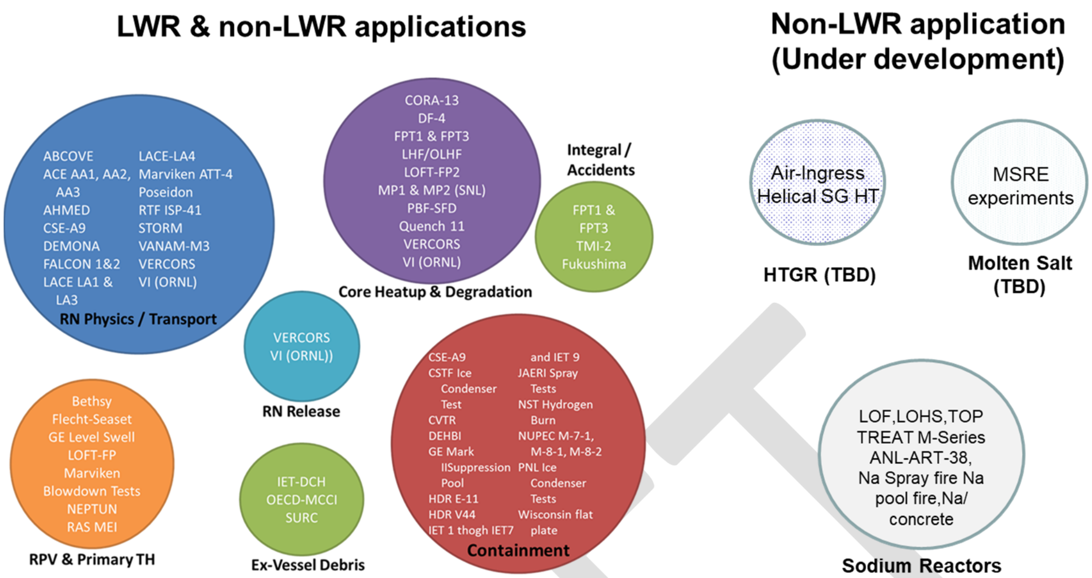

Figure 2-2. MELCOR 2.2 Validation Cases.

Table 2-1 has been developed to address model improvements, enhancements, and development of new models that are proposed to extend the MELCOR modeling capabilities in preparation to perform source term and severe accident licensing calculations. The development items addressed in this plan provide those capabilities necessary to demonstrate licensing readiness. This plan currently spans three years' development time and was organized to address more immediate needs early on and provide practical code capabilities along the development path with specific deliverables (see Table 2-2) for successive fiscal years. Beyond FY20, code development activities will focus on specific advanced reactor technologies and design specific modifications and code assessments as those details and funding become available.

Development of input models to test new code features is implicit in the tasks described in Table 2-1. At the completion of all the tasks listed below, reference input models will be available to test the functionality of all of the code packages in an integral fashion. More detailed plant models will be developed as information becomes available.

The sections that follow will discuss each reactor type, the key phenomena as determined by PIRTs, and specific recommended modeling improvements. Those recommended modeling improvements discussed in those sections are referenced to the development items listed in this table.

Table 2-1. MELCOR Non-LWR Development Plan Start Dates.

Reactor Type/ Development Item (DI)	Phenomenological Area (MELCOR)	Description of Tasks (needs)	FY18	FY19	FY20
SFR (M1.1)	Development of core components	3 new components (fuel region, fuel cell duct, heat pipe walls) need to be added to COR package. Radiation use existing models. (Applies to HPR designs)	✓		
SFR (M1.2)	Core modeling	Fuel degradation model. Fuel thermal-mechanical properties, models for fuel expansion, foaming and melting. Intermetallic reactions at elevated temperatures. (Applies to SFR, LMR, and HPR designs)		✓	
SFR (M1.3)	FP modeling	FP speciation & chemistry and bubble transport through sodium pool. Vaporization of FPs from sodium pool surface. (Applies to SFR, LMR, and HPR designs)		✓	
SFR (M1.4)	FP modeling	Models for FP release (depends on SFR M1.2 & M1.3). (Applies to SFR, LMR, and HPR designs)		✓	
SFR (M1.5)	Containment Modeling	Complete models for sodium chemistry (fires, atmospheric chemistry, concrete interactions). Include sodium water reactions and aerosol aging. (Applies to SFR and HPR designs)		✓	
SFR (M1.6)	Containment Modeling	Hot gas layer formation during sodium fires. (Applies to SFR and HPR designs)		✓	
SFR (M1.7)	Sodium coolant models	Verify EOS and thermal-mechanical properties for sub-atmospheric conditions. Extend fluid model to more than one working fluid. (Applies to SFR, LMR, and HPR designs)	✓		
SFR (M1.8)	Primary heat removal system	High-level model needed for calculating fluid flow and wicking phenomenon within existing CVH/FL package. (Applies to HPR designs)	✓		

Reactor Type/ Development Item (DI)	Phenomenological Area (MELCOR)	Description of Tasks (needs)	FY18	FY19	FY20
SFR (M1.9)	Reactor kinetics	Evaluate neutronic parameters in the existing point kinetics model for reactivity feedback. (Applies to SFR, LMR, and HPR designs)		✓	
SFR (M1.10)	Critical assessment	HEDL SC & SET tests – Sodium/Concrete interactions (depends on SFR M1.5). (Applies to SFR, LMR, and HPR designs)		✓	
SFR (M1.11)	Database	Develop a referenceable compendium of past experiments and analyses that characterize key phenomena of interest, such as fuel-sodium interactions, sodium-water interactions, combustible gas generation, coolability of metallic fuel, etc. (Applies to SFR, LMR, and HPR designs)		✓	
HTGR (M2.1)	Test existing HTGR models	MELCOR has extensive HTGR modeling capabilities. Identify need for specific input models using existing capabilities. FP release models require data on diffusivity (INL experimental program). (Applies to HTGR, PBMR, and GCFR designs)		✓	
HTGR (M2.2)	Critical assessment	Need for air/moisture ingression assessment - scenario specific (depends on HTGR M2.1). (Applies to HTGR, PBMR, and GCFR designs)		✓	
MSR (M3.1)	Molten salt properties	Existing LiF-BeF_2 EOS and thermal-mechanical properties. Develop EOS for other molten salt fluids. Develop test decks to demonstrate molten salt properties. (Applies to MFSR and MCSR designs)			✓
MSR (M3.2)	Fission product modeling	FP interaction with coolant, speciation, vaporization, and chemistry. (Applies to MFSR and MCSR designs)			✓

Reactor Type/ Development Item (DI)	Phenomenological Area (MELCOR)	Description of Tasks (needs)	FY18	FY19	FY20
MSR (M3.3)	Core modeling	For liquid fuel geometry, control volume hydrodynamics and radionuclide packages can model flow of coolant and advection of internal heat source with minimal changes. Models needed for calculation of neutronics kinetics for flowing fuel. (Applies to MFSR and MCSR designs)			✓
MSR (M3.4)	Database	Develop a referenceable compendium of past experiments and analyses that characterize key phenomena of interest, such as FLiBE chemical reactivity with core materials, decay heat removal systems, etc. (Applies to MFSR and MCSR designs)			✓
FHR (M3.5)	Test existing models and evaluate need for any specific models	MELCOR models for MSR and HTGR applications adopted for this specific reactor. (Applies to MSR and MSPR designs)			✓
FHR (M3.6)	Database	Develop a referenceable compendium of past experiments and analyses that characterize key phenomena of interest, such as FLiBE chemical reactivity with core materials, decay heat removal systems, etc. (Applies to MSR, MSPR, MFSR, and MCSR designs)			✓

Table 2-2. Yearly Deliverables – MELCOR Development Plan

Year	Deliverable
FY18	Demonstrate accident analysis for heat pipe design, limited to core damage and thermal hydraulics (fission product and transport model will be developed FY19)
FY19	Demonstrate accident analysis with MELCOR for generic SFR and HTGR designs
FY20	Demonstrate accident analysis with MELCOR for generic MSR and FHR designs

2.1. HTGR

Beginning in 2008, MELCOR code development was focused on modeling both the pebble-bed and prismatic HTGR designs. At this time the NGNP program had not made a final selection of a reactor design, and consequently the modeling capabilities in the current version of MELCOR (v2.2) support modeling of both reactor types with specific attention to severe accident phenomenology. The modified radionuclide transport path shown in Figure 2-3 below identifies key phenomena for source term calculation. Models for reactor components, fission product release from TRISO fuel, point kinetics, dust lift-off, and turbulent deposition were all added to the code. All but the resuspension and turbulent deposition models were results of the NGNP initiative, and these models have been reviewed by the ACRS as part of NGNP. Additionally, some of these models have been validated/ assessed either as part of the MELCOR validation work or by external MELCOR code users performing assessment calculations [26], [27]. Additional details related to the HTGR reactor design and the implementation of related physical models into MELCOR is provided in Appendix A.

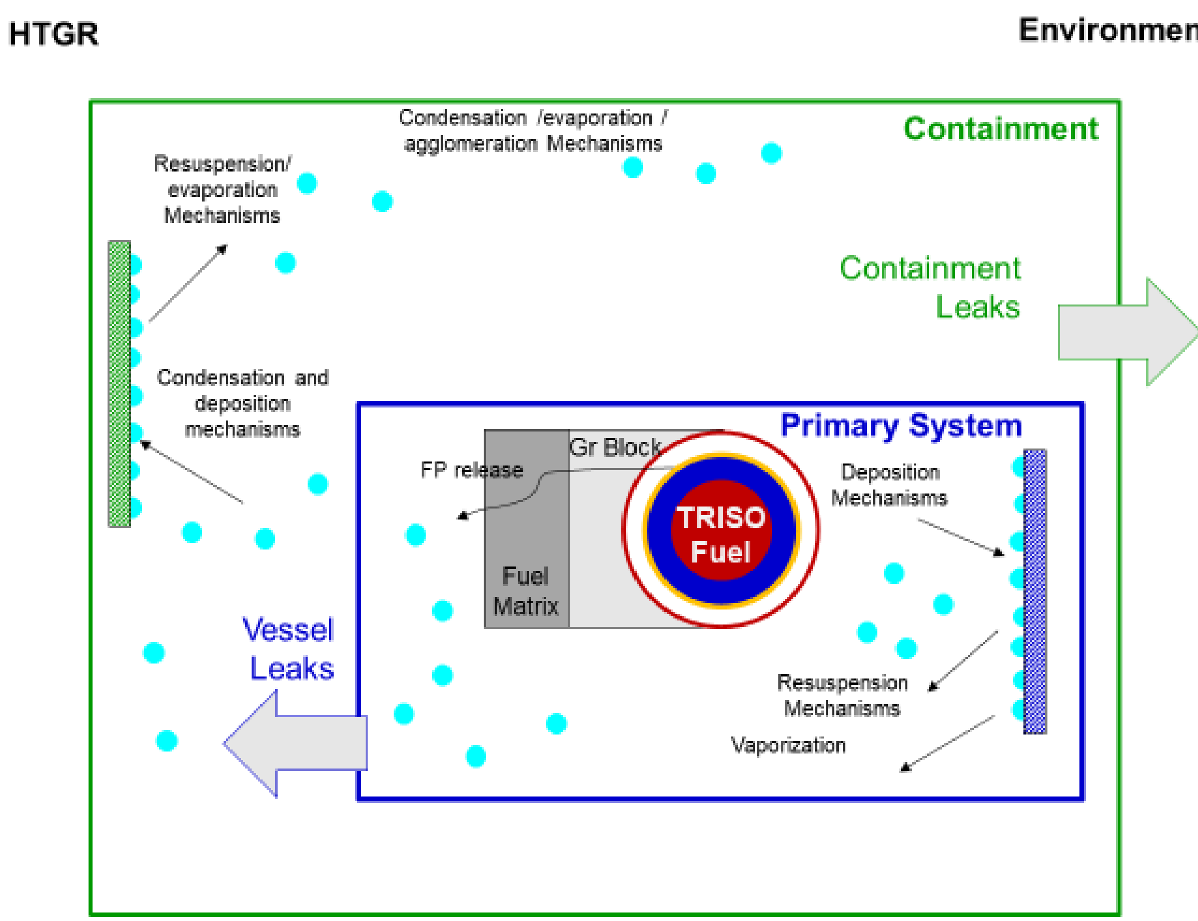

Figure 2-3. Radionuclide transport paths in HTGR designs.

2.1.1. Evaluation Model

The intent in applying the EM calculational framework to a specific LBE is to support licensing review and to provide a technical basis for regulatory decisions. Ultimate licensing and regulatory decisions are based on the application of the framework to an assortment of events deemed relevant to the safety case of a given applicant's proposed design.

An EM calculational framework is a network of computer programs/codes, models, and data as pictured in Figure 2-4 (similar to Figure 1-1 but removing the suite of codes for design basis analysis). In this example, each large light blue box covers an aspect of the confirmatory safety analysis strategy. Each contains or connects to yellow and dark blue boxes. A yellow box indicates either an input to or an output of some model or function indicated by a linked dark blue box. An order of operations is implied by the black arrows both within and between boxes, i.e. certain information is required as model/function input in order for certain outputs to be generated. These outputs, in turn, are either inputs for follow-on models or constitute some desired final outcome. The data/model relationships conveyed by the EM are therefore indicative of inputs/outputs to/from the computational tools used for confirmatory analysis. MELCOR development was based on the concept of this EM.

Table 2-3 lists the inputs/outputs requirements for MELCOR in its role as a confirmatory analysis tool for HTGR applications developed under NGNP. Each input and output can be directly associated with a yellow box. Inputs that inform MELCOR models may come from experiments or other computer codes. The Department of Energy (DOE) Nuclear Energy Advanced Modeling and Simulation (NEAMS) computational suite is one potential tool for providing some of the input requirements, for example, furnish fission product species diffusion coefficients, a temperature and burn-up dependent fuel failure response surface, or information related to graphite dust generation and transport.

The light blue box labeled “Reactor Physics” indicates that nuclear data – Evaluated Nuclear Data Files – can be used to generate nuclear reaction cross-section libraries for use in HTGR fuel and fuel element analyses. More details on the flow of information that provide the input to MELCOR is given in Section 3.

The light blue box labeled “Fission Product Preprocessing” indicates that – given the results of several external operations – an initial fission product, radionuclide, and aerosol/dust spatial distribution in the core (fuel) and primary circuit may be generated. Because of the unique features of the fuel design in HTGRs, this preprocessing is necessary to establish the initial and boundary conditions for the transient analysis. Appendix A gives further information on the subjects of fuel fission product diffusional transport modeling, steady-state initialization of the core/primary thermal-fluid state, graphite dust modeling, and fuel failure and release modeling.

The light blue box labeled “Normal Operation” provides useful information on power distributions, nuclear kinetics parameters and reactivity feedback coefficients, and bypass flow. The specific codes listed in this box are from the 2011 EM and may be replaced by other tools; however, this does not affect MELCOR development.

The light blue box labeled “LBE transient analysis” indicates that MELCOR must be capable of modeling transient, off-normal conditions associated with a given LBE provided certain inputs such as power profile, kinetics parameters, and initial fission product and radionuclide spatial distribution to provide necessary source term for off-site consequence analysis.

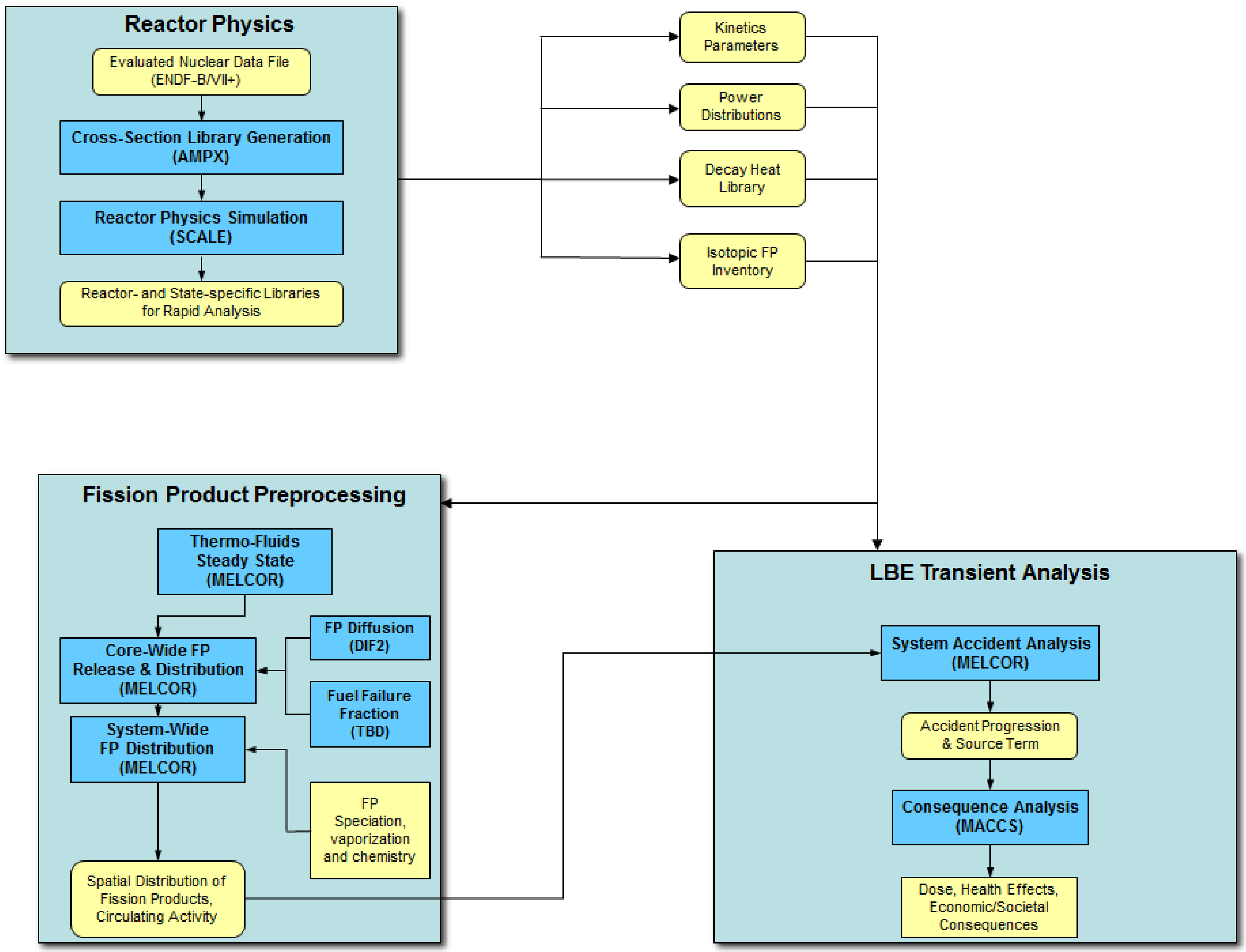

Figure 2-4. Proposed NRC Evaluation Model for HTGRs

Table 2-3. Input/Output for MELCOR in the HTGR EM

Input	Source	Output
FP inventory	SCALE	(1) Thermal hydraulic response of the primary system (core components and fluid temperatures) (2) Thermal hydraulic response of the confinement (temperature, pressures, release paths, etc.) (3) FP and dust distribution during normal operation (4) Source term during accidents (input to DBA source term analysis and for consequence analysis)
FP diffusion coefficients	Experiments (e.g., AGR) and analysis (e.g., DOE tools)	
Core power shape	Radial/Axial profiles (e.g., SCALE or vendor data)	
Fuel particle failure rate response surface (function of temperature and burnup)	Experiments/other codes (e.g., DOE tools)	
Dust generation, lift-off, and FP adsorption on dust (impact of aerosol growth, shape factor, etc.)	Experiments/Historical data and other codes (MELCOR has models for aerosol dynamics, FP condensation/evaporation from aerosols/structures – develop specific HTGR models (e.g., DOE tools))	
FP release under accident conditions including air/water ingress	Experiments	
FP speciation and interaction with graphite and other structures	Experiments (MELCOR has models for FP chemistry including adsorption, chemisorption)	

2.1.2. Development Plan

Review of PIRT Phenomena

Physical models added to the MELCOR code are based on the findings of a Phenomena Identification and Ranking Table (PIRT) study conducted as part of NGNP in 2008 [28]. Models for release of fission products from TRISO fuels, heat transfer models from reactor components, fluid flow modeling for HTGR geometries, transport of radionuclides and graphite dust throughout a system, reactivity modeling and feedback, graphite oxidation and properties, and the ability to perform air-ingress calculations where counter-current flow is important. These phenomena are addressed further in Table 2-4 along with a description of the current modeling capability or plans for MELCOR model development.

Table 2-4. Key Accident Progression Phenomena for HTGRs.

Key Phenomenon	Importance	Existing Capabilities	Modeling Gaps
Modeling of TRISO fuels	Determining release of fission products from fuel and fuel material properties	• Analytic release model • Multi-zone diffusion model • Account for FP recoil, matrix contamination, and initial TRISO defects	• Current modeling uses UO2 material properties, needs to be extended to UCO (Development Items M2.1 and M2.2)
Heat Transfer in Graphite block (PMR)	Thermal response of fuel components and failure of TRISO fuel particles	• Tanaka-Chisaka effective radial conductivity	
Heat Transfer in fuel pebbles (PBR)	Thermal response of fuel components and failure of TRISO fuel particles	• Zehner-Schlunder-Bauer effective thermal conduction	
Reactivity temperature feedback coefficients.	Neutronics power feedback	• Point kinetics model • Reactivity coefficients specific to an application can be implemented via control functions	
Ability to model two-sided reflector component	Heat transfer from overheated core	• Two-sided reflector component	
Modeling graphite dust transport	Pathway for fission product transport and release	• All relevant mechanisms for graphite dust transport, deposition, and resuspension	
Graphite oxidation	Heat generation and release of combustible gases	• Graphite oxidation model and oxidation products	
Air/moisture Ingress modeling	Air/moisture ingress can lead to oxidation of the graphite structures and release of radionuclides	• Momentum exchange model	

Code Assessment

As conveyed by Table 2-5, an important area of validation needs is associated with the characterization of fission product released from TRISO fuels. Some tests, such as AGR, are ongoing and the data is not yet available. An IAEA code-to-code benchmark [29] comparing models developed for a number of codes is an important first step in assessing the MELCOR models.

There is a significant repository of data that has been accumulated from operating reactors that can be used for validation of the thermal response of the reactor to power transients, some of which has already been exercised by MELCOR users [27].

Finally, data is required for assessing code models for simulation of deposition and liftoff of graphite dust. A number of tests from LWR application space (LACE, STORM, DEMONA, etc.) are already part of the MELCOR validation database and can be reviewed for application to HTGR reactors.

Table 2-5. Proposed MELCOR Assessment Matrix for HTGRs

Experiment/ Assessment	Brief Description	Phenomena Tested	Code Packages Tested
AGR	Fuel irradiation tests performed mostly on UCO TRISO	Modeling of TRISO fuels, air & moisture ingress	COR, RN
HTR-10	Pebble bed test reactor as specified in the International Handbook of Reactor Physics Experiments [30]. Data from Tsinghua University is readily available	Modeling of TRISO fuels Heat transfer in fuel pebbles (PBR) Modeling graphite dust transport	COR, CVH, EOS, RN
HTTF	High Temperature Test Facility at Oregon State University, designed to generate high quality data on thermal fluid behavior in HTGRs. DCC and PCC transients are planned for this facility (Test data not yet available)	Heat transfer in graphite block (PMR) Ability to model two-sided reflector	COR, CVH
HTR-PM	250 MWth PBR twin unit, useful for code-to-code	Thermal hydraulic modeling	COR, CVH, FL, HS

Experiment/ Assessment	Brief Description	Phenomena Tested	Code Packages Tested
	comparison with other analysis codes		
NSTF	Tests performed at the Natural Convection Shutdown Heat Removal Test Facility for characterizing the thermal response of the reactor cavity cooling system (RCCS)	Buoyancy driven convective heat removal and radiation enclosure model	CVH, FL, HS
HTTR	PMR operated by the Japan Atomic Energy Agency, rated at 30 MWth, LOFC tests performed in 2010 [31]	Modeling of TRISO fuels Heat transfer in graphite block (PMR)	COR, CVH, FL, HS
IAEA Benchmark exercise	Code-to-experiment benchmark data for fission product release from TRISO fuel	Modeling of TRISO fuels	COR, RN
COMEDIE BD-1	Integral test conducted by the Commissariat a l'Energie Atomique to generate data for validation of models for simulating fission product release along with deposition/lift-off during depressurization	Modeling of TRISO fuels Modeling graphite dust transport	COR, CVH, FL, RN
AVR	Arbeitsgemeinschaft Versuchsreaktor was a 46 MWth PBR, tests to characterize effects of dust on FP transport in the primary circuit	Modeling of TRISO fuels Heat transfer in fuel pebbles (PBR) Modeling graphite dust transport	COR, CVH, FL, RN

PCMM Characterization

The PCMM process was applied to the HTGR modeling capability, and the results are summarized in Table 2-6. Note that this evaluation applies to all HTGR types listed in Table 1-1 (PBR, PMR, and GCFR). The HTGR models are relatively mature and most modeling capability is already in place. Validation of these models is perhaps the greatest need at this time.

Table 2-6. MELCOR Maturity for HTGR Analysis

Element	Maturity Level[1]	Comments
Representation and Geometric Fidelity	3	• Components representing the reactor fuel, the graphite matrix, and reflector have all been added providing adequate representation. • Reviewed by ACRS as part of NGNP
Physics and Model Fidelity	2	• Physics-based models for all important processes. • Need for more complete test data on TRISO fuel failure. • Need to add properties for UCO fuel • Reviewed by ACRS as part of NGNP
Code Verification	2	• Extensive SQE, many capabilities have been benchmarked and some peer review.
Solution Verification	2	• Some informal assessments both internally as well as assessment by code users.
Model Validation	2	• Extensive validation of most physics models though not all within the domain of HTGRs. • External assessment
Uncertainty Quantification and Sensitivity Analysis	2	• Uncertainties and numerical propagation of errors has been examined extensively for LWR applications though not for HTGR application.

[1]Maturity Levels

- level 0, little or no assessment of accuracy and completeness and highly reliant on personal judgment and experience;
- level 1, some informal assessment of accuracy and completeness, and some assessment has been made by an internal peer review group;
- level 2, some formal assessment of accuracy and completeness, and some assessments have been made by an external peer review group; and
- level 3, formal assessment of accuracy and completeness, and essentially all assessments have been made by an independent, external peer review group.

2.2. SFR

The SFR is among the most well-developed of the generation IV, non-LWR concepts due to its advanced technology base and accumulated world-wide operating experience. France, Japan, Russia, the United Kingdom, Germany, the U.S. and a few other countries have some operating experience with SFR installations. In the U.S., EBR-II, FERMI-I, and the FFTF are some past and present SFR installations. There are a few relatively mature SFR design proposals in existence e.g. SAFR, PRISM, and the Integral Fast Reactor (IFR) - formerly known as the Advanced Liquid Metal Reactor (ALMR). SFR design philosophy in the U.S. tends toward metal alloy fuel (as opposed to oxide fuel) and liquid sodium pools for cooling (as opposed to loop cooling).

The diagram in Figure 2-5 below depicts the transport of radionuclides released from fuel to the environment. The sodium pool design suggests a covered core even in the event of core melt and degradation. Transport of radionuclides through the sodium as well as transport of radionuclides due to bubbles rising to the pool surface become important. In addition, release of aerosols from sodium fires as well as atmospheric chemistry of sodium species are important considerations.

Several recent reactor design concepts have been proposed that utilize heat pipes for the removal of generated heat. Such designs are intended for operation in remote locations and are designed with small power levels and are transportable. Examples include the Oklo reactor and the Westinghouse eVinci reactors. Though sodium is used in the cooling of these reactors, the design is a significant departure from traditional pumped circulating sodium designs. Though Figure 2-5 applies to pool-type SFRs, some phenomenological aspects in containment still apply to heat pipe reactors. Details of this reactor type are described more fully in Appendix B.

Other proposed liquid metal fast reactor designs might include lead or lead-bismuth coolant. It is important to recognize that development of modeling capabilities for sodium fast reactors will benefit other liquid metal fast reactor designs.

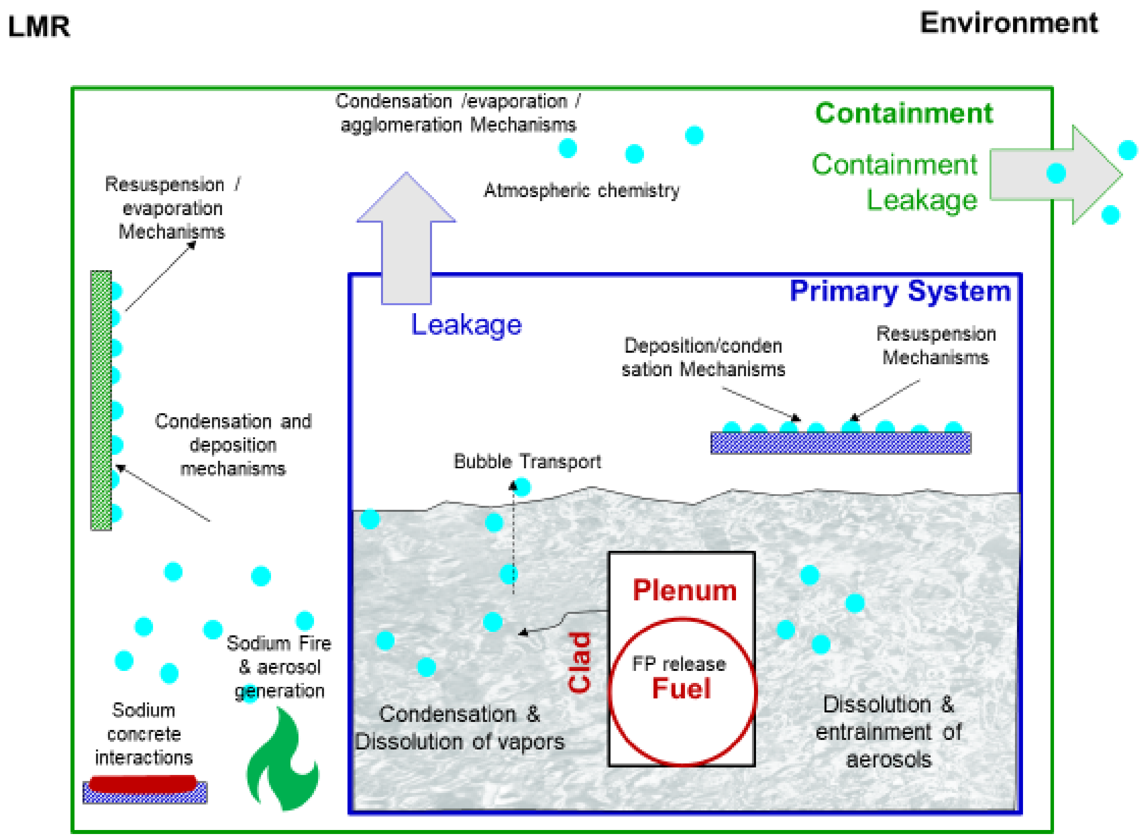

Figure 2-5. Radionuclide release paths for pool-type SFR designs.

2.2.1. Evaluation Model

Figure 2-6 illustrates the proposed EM for SFRs. This follows the EM approach for HTGRs and is simplified to focus only on MELCOR and its input requirements. Input and output requirements are also described in Table 2-7.

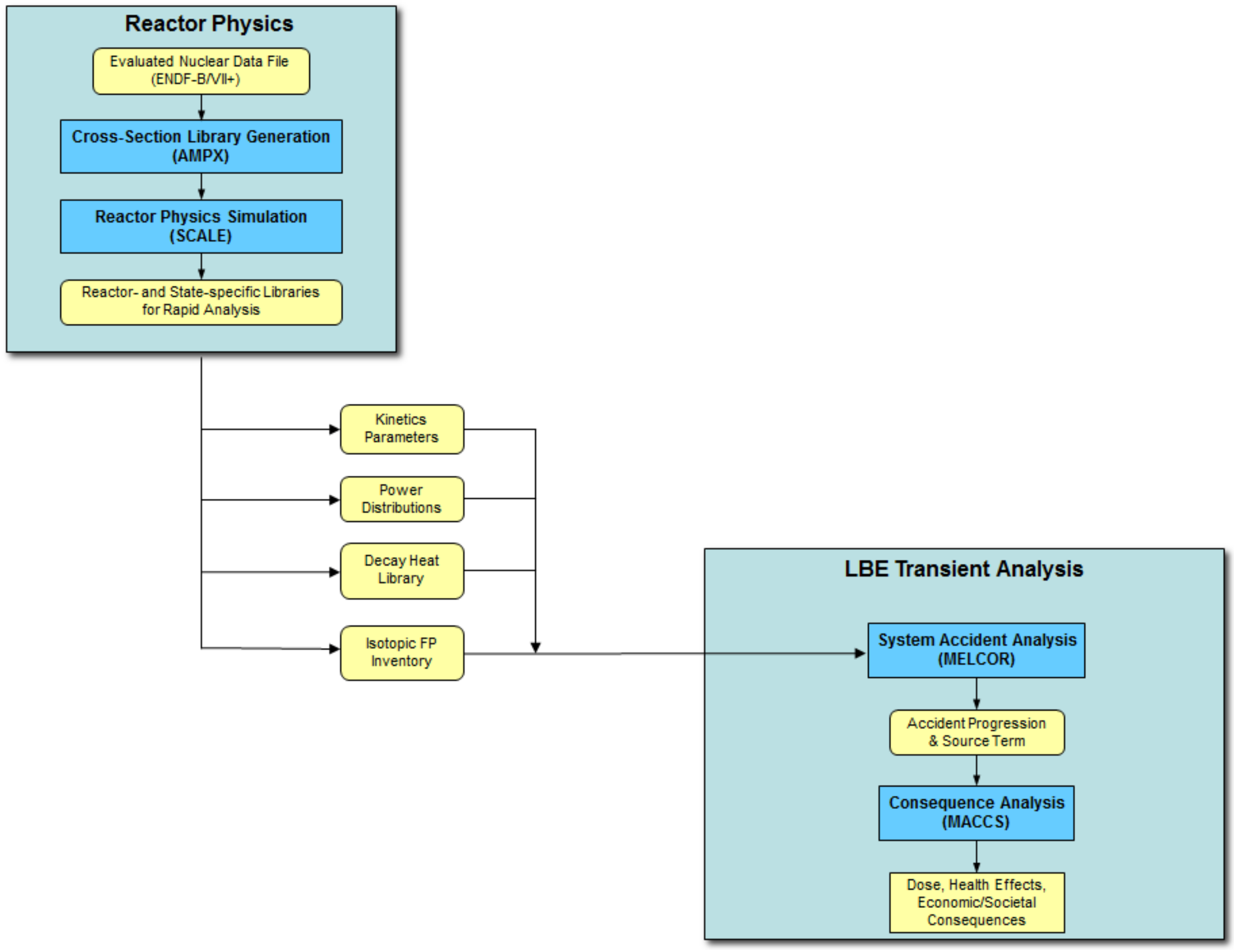

Figure 2-6. Proposed NRC Evaluation Model for Sodium Fast Reactors

Table 2-7. Proposed Input/Output for MELCOR in the SFR EM

Input	Source	Output
FP inventory	SCALE	(1) Thermal hydraulic response of the primary system (core components and fluid temperatures) (2) Thermal hydraulic response of the confinement (temperature, pressures, release paths, etc.) (3) Source term during accidents (input to DBA source term analysis and for consequence analysis)
FP release from damaged fuel	Experiments	
Core power shape	Radial/Axial profiles (e.g., SCALE or vendor data)	
Fuel failure (function of temperature, burnup, etc.)	Experiments/other codes (e.g., DOE tools)	
Kinetics parameters and reactivity feedback coefficients	Experiments/other codes (e.g., SCALE)	
Equilibrium Constants for release from sodium pool	Experiments/other codes (e.g., DOE tools)	

2.2.2. Development Plan

<u>Review of PIRT Phenomena</u>

Several SFR studies have been conducted in the way of PIRT-like analyses, mechanistic source term development, and safety/licensing support (e.g. preliminary safety information/evaluation documents/reports). Thus, the most immediate SFR modeling needs are reasonably well-defined [32] [33] [34].

As shown in Figure 2-5, mechanisms for radionuclide deposition (and condensation), dissolution, resuspension (and evaporation) have been included as they are necessary in quantifying source term. Such mechanisms are similar to those that are found for other reactor types though they would need to be validated for this application. Modeling fuel release and transport of radionuclides through the coolant, and atmospheric chemistry may be significantly different than those models that exist for LWR design.

A number of additional phenomena are important in modeling potential sodium fire and chemistry interactions in the containment in the event of sodium leakage during an accident. Such phenomena include the modeling of sodium spray fires, sodium pool fires, stratification due to a hot gas layer, atmospheric chemistry, and sodium concrete interactions. Many of these models have already been added to the MELCOR code.

For a heat pipe reactor design, the modeling of the heat pipe is important in predicting the extent of core degradation and the corresponding release of fission products from the fuel. Currently there is a lack of information regarding the reactor design, so modeling needs are based on expert judgement. Even so, it is clearly important to be able to model propagation of failure from a local failure. Failure of one or two heat pipes may be tolerable but propagation of failure to adjacent fuel cells must be calculated to adequately calculate source term. Explicit modeling of these new heat pipe components is also a departure from the existing LWR framework requiring model development such as described in references [35] and [36]. Implementation of a heat pipe model and MELCOR components requires major changes in the COR package as described in Table 2-8. At present, significant progress has been made in implementing the heat pipe models, as described further in Appendix B.

Finally, modeling of electromagnetic pumps, supercritical CO2 power cycle, heat exchangers, and additional miscellaneous systems may be needed to simulate particular accident scenarios. It is anticipated that such systems can be modeled already with MELCOR control functions as well as existing pump modeling or heat exchanger capabilities or the need for such system modeling has not been demonstrated. Consequently, there are no current plans to implement such capabilities.

These phenomena are addressed further in Table 2-8 along with a description of the current modeling capability or plans for MELCOR model development along with a reference to the development plan. Additional details regarding current MELCOR modeling capability and proposed modeling needs are provided in Appendix B.

Table 2-8. Key Accident Progression Phenomena for SFRs.

Key Phenomenon	Importance	Existing Capabilities	Modeling Gaps
Liquid Metal to be used as a working fluid	Modeling the liquid metal coolant heat transfer properties is essential in simulating the reactor response to accident conditions	Na equation of state libraries already available to MELCOR.	• Ability to model sodium as the working fluid in some control volumes and water in others will be added (development Item M1.7) • Addition of Pb and Pb/Bi EOS/Properties (infrastructure developed under development item M1.7)
Fission Product Speciation	Affects the release, vapor pressure, and chemical interactions of fission products.	MELCOR utilizes radionuclide classes organized by chemical similarities that can be easily adapted for reactor application	• Determination of MELCOR class structures (development Item M1.3)
Fission Product Release Model	Determines distribution of fission products between the fuel and fission gas plenum.	MELCOR has a generic release model easily adapted for metallic fuel.	• Extension of existing modeling for FP release for metallic fuel (development Item M1.4)
Fuel degradation model.	Degraded fuel components lead to release of fission products from the fission gas plenum as well as some fuel/clad material.	MELCOR has models for fuel components that can be extended to SFP application	• Extend MELCOR fuel component to capture melting fuel in fuel matrix • Model for cladding failure from eutectic penetration or molten fuel contact • Ejection of fuel/sodium from failed rod. (development Item M1.2)
Sodium fire modeling	Sodium fires provide a source of heat to the containment and also provide a path for transport of sodium and fission products to the atmosphere.	Sodium pool fire and spray fire models, as well as atmospheric chemistry models have already been added to the code.	• Addition of a hot gas layer model during sodium fires (development Item M1.6)
Sodium concrete interactions	Important source of aerosols and possible combustible gases		• Add sodium concrete interactions (development Item M1.5)

Key Phenomenon	Importance	Existing Capabilities	Modeling Gaps
Dissolution of RN and vaporization of dissolved species	Transport of radionuclides to and from the sodium pool and into the cover gas		• Add models for dissolution and vaporization of dissolved species (development Item M1.3)
Bubble Transport/ partitioning between bubble & sodium pool	Transport of radionuclides directly to the atmosphere.	MELCOR's SPARC model might be leveraged, though modified significantly for this application	• Development of bubble transport model (development Item M1.3)
Heat Pipe Thermal Hydraulics	The heat pipe is the primary means of heat removal from fuel.		• MELCOR does not currently have a heat pipe model. Code modifications have been proposed to remove this gap (see Appendix B) (development Item M1.1)
Reactor kinetics	Calculate transient power feedback	Existing point kinetics and reactivity feedback model	• Evaluate neutronics parameters in the existing point kinetics model (development Item M1.9)
Failure of Individual heat pipes and propagation of failure to adjacent fuel elements	Determines the extent of core degradation and source term released from fuel.	Existing multi-rod model can be leveraged in calculating propagation of local heat pipe failure (development Item 1.8)	• Development of heat pipe models Development Item M1.8.

Code Assessment

Code assessments for SFRs can be generally categorized in four different areas: Thermal response of the reactor to design basis accidents, fuel failure and core degradation modeling, fission product transport modeling, and sodium chemistry modeling (fires and sodium concrete interactions). No validation data exists for heat pipe type reactors. Additional discussion on modeling assessments is provided in Table 2-9 and in Appendix B. MELCOR input models will be developed for each of the experiments listed below, and calculation results will be compared to available data.

Table 2-9. Proposed MELCOR Assessment Matrix for SFRs

Experiment	Brief Description	Phenomena Tested	Code Packages Tested
TREAT M5-M7	Transient over-power tests aimed at observing metal fuel performance under unprotected accident conditions	Liquid metal to be used as a working fluid Fission product release model Fuel degradation model Reactor kinetics	COR, CVH, EOS, FL, RN
EBR-II	Unprotected loss of forced cooling tests provide data useful for validating point kinetics models	Liquid metal to be used as a working fluid Fuel degradation model Reactor kinetics	COR, CVH, EOS,FL
FFTF	Fast Flux Test Facility, loss of forced cooling tests	Liquid metal to be used as a working fluid Reactor kinetics	COR, EOS, CVH, FL
HEDL	Small and intermediate scale tests (1978) investigating sodium/concrete interactions, penetration, and off-gassing (described in Appendix E)	Sodium-concrete interactions	CVH, EOS, FL, RN, CAV
ABCOVE (AB1[1], AB5[1], AB6, AB7)	Aerosol Behavior Code Validation and Evaluation, matrix of aerosol experiments performed in the Containment Systems Test Facility by HEDL to examine sodium fires (pool and spray) AB1 and AB5 part of current MELCOR validation matrix (described in Appendix E)	Sodium fire modeling (spray, pool)	CVH, EOS, FL, NAC, RN

[1]MELCOR validation has already been performed for this test and is part of the MELCOR validation suite (see Appendix B)

PCMM Characterization

The PCMM process was applied to SFR modeling capability as shown in Table 2-10. This is a preliminary evaluation of the maturity levels for the MELCOR code. Note that this evaluation applies to all liquid-metal-cooled reactor types listed in Table 1-1 (SFR, LMR, and HPR).

Table 2-10. MELCOR Maturity for SFR Analysis

Element	Maturity Level[1]	Comments
Representation and Geometric Fidelity	1	Missing components for representing heat pipe geometry. Modify fuel component for heat pipe and sodium pool application.
Physics and Model Fidelity	1	EOS for sodium is well established Sodium fire models well established Missing models for aerosol/vapor behavior in sodium. Missing models for heat pipe Missing models for fuel rod failure
Code Verification	2	Extensive code verification for existing MELCOR models Verification of new EOS models Verification of sodium fire models
Solution Verification	0	
Model Validation	1	Extensive validation of aerosol physics models Validation of containment models (sodium fires) No validation of fission product release and transport Need validation of sodium properties and EOS models
Uncertainty Quantification and Sensitivity Analysis	1	Uncertainties and numerical propagation of errors has been examined extensively for LWR applications though not for Na application

[1]Maturity Levels
- level 0, little or no assessment of accuracy and completeness and highly reliant on personal judgment and experience;
- level 1, some informal assessment of accuracy and completeness, and some assessment has been made by an internal peer review group;
- level 2, some formal assessment of accuracy and completeness, and some assessments have been made by an external peer review group; and
- level 3, formal assessment of accuracy and completeness, and essentially all assessments have been made by an independent, external peer review group.

2.3. MSR

There are two broad types of molten salt reactor designs to be considered. The first type, Fluoride salt-cooled High temperature Reactors (FHRs), utilize a fixed fuel arrangement (or quasi-fixed arrangement such as a pebble bed) in which a circulating molten salt provides the heat removal mechanism from the fuel. This fixed fuel may exist as rod bundles, pebbles, or plate geometry. The radionuclide transfer path showing the release of fission products from the fixed fuel to the coolant as well as mechanisms for deposition/resuspension, condensation/evaporation, bubble transport and vaporization from the molten salt is depicted in Figure 2-7. For the second type - salt-fueled reactors – a fuel salt circulates with the coolant salt. Such a design is a paradigm shift from conventional reactor designs for which the fuel is fixed and a circulating coolant removes thermal energy. The radionuclide transfer path for salt-fueled reactors is similar to that of salt-cooled reactors (Figure 2-8) except the fuel exists within the molten coolant. Details of this reactor design are described more fully in Appendix C.

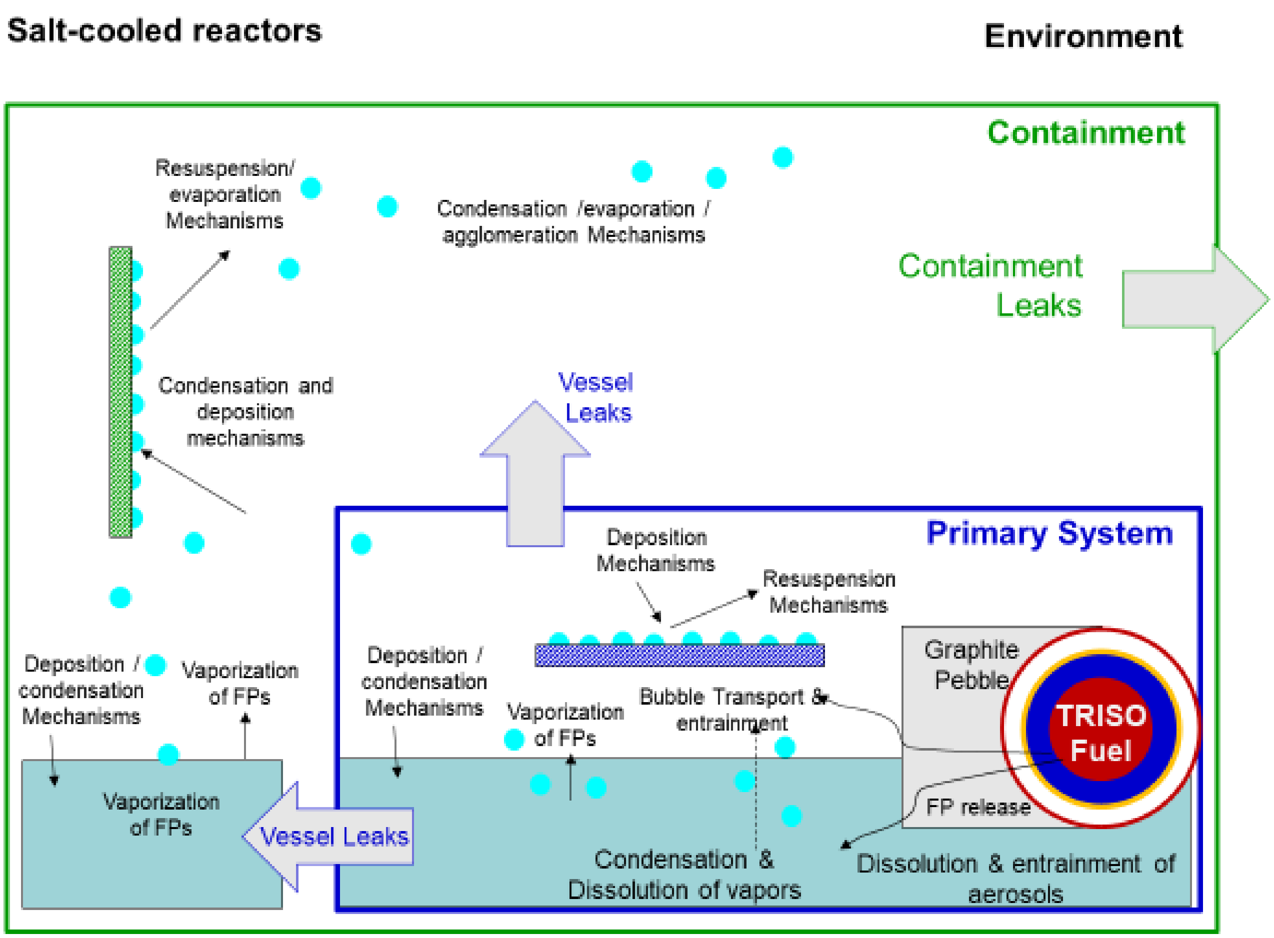

Figure 2-7. Radionuclide release paths for salt-cooled designs.

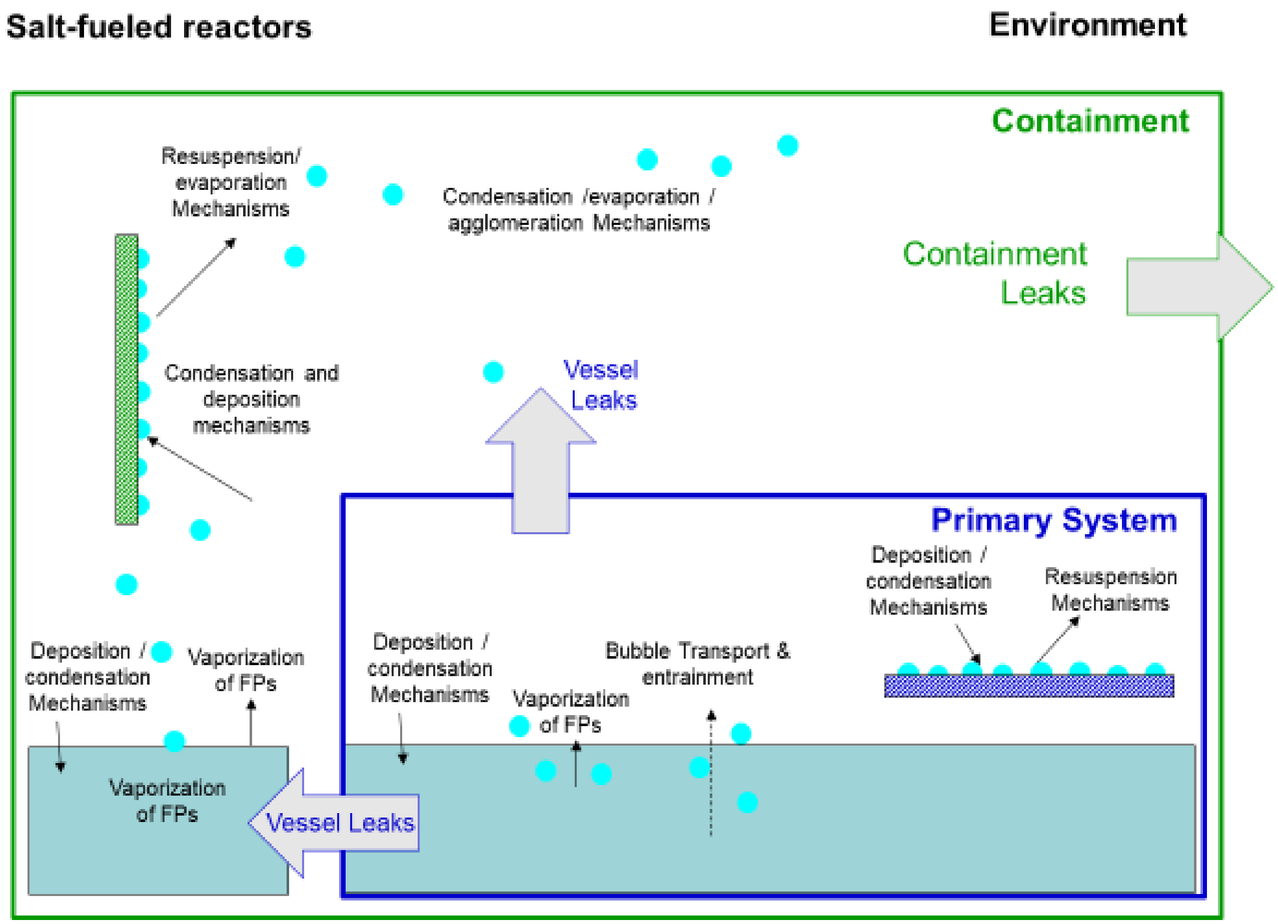

Figure 2-8. Radionuclide release paths for salt-fueled reactor designs.

2.3.1. Evaluation Model

Figure 2-9 and Figure 2-10 illustrate the proposed EMs for various MSR designs. This follows the EM approach for HTGRs and SFRs and is simplified to focus only on MELCOR and its input requirements. Input and output requirements are also described in Table 2-11.

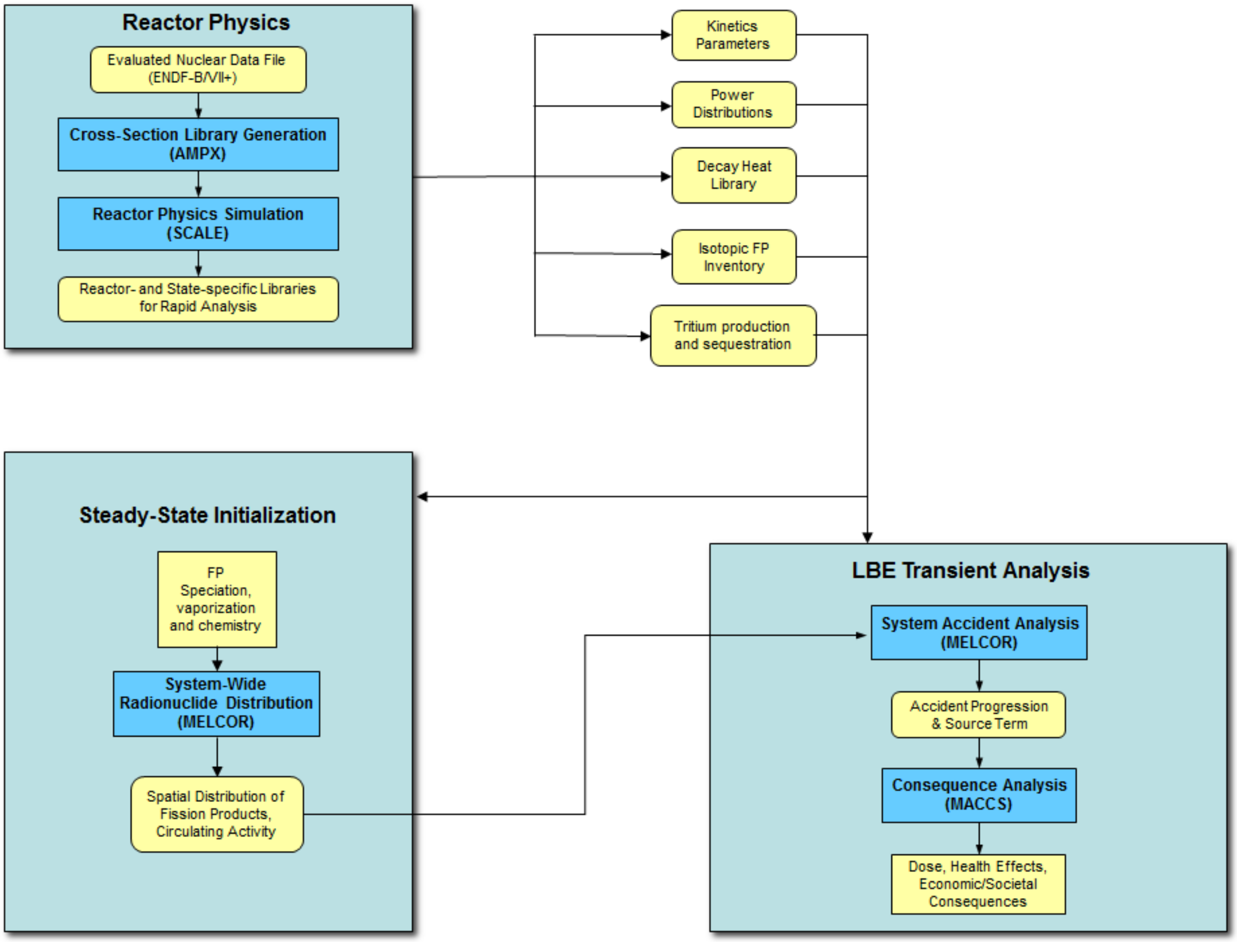

Figure 2-9. Proposed NRC Evaluation Model for Salt Cooled Reactor

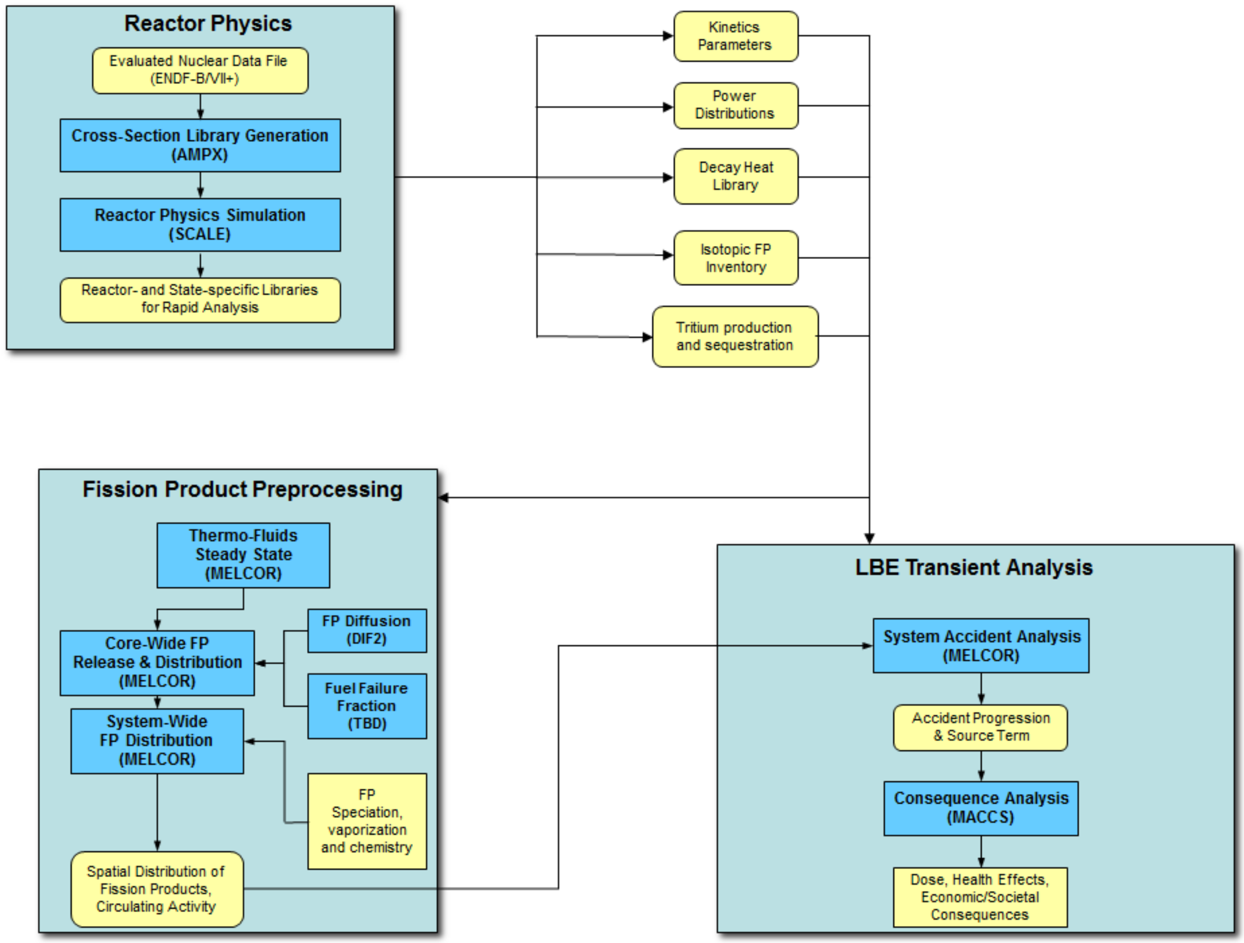

Figure 2-10. Proposed NRC Evaluation Model for Salt Fueled Reactor

Table 2-11. Proposed input/output table for MELCOR in the MSR EM

Input	**Source**	**Output**
FP inventory	SCALE	(1) Thermal hydraulic response of the primary system (core components and fluid temperatures) (2) Thermal hydraulic response of the confinement (temperature, pressures, release paths, etc.) (3) Source term during accidents (input to DBA source term analysis and for consequence analysis)
FP diffusion coefficients (FHR)	Experiments/other codes (e.g., DOE tools) Similar to HTGR (FHR)	
Core power shape	Radial/Axial profiles (e.g. SCALE or vendor data)	
Fuel failure (FHR)	Experiments/other codes (e.g., DOE tools) Similar to HTGR (FHR)	
Kinetics parameters and reactivity feedback coefficients	Experiments/other codes (e.g., SCALE, DOE tools)	
Equilibrium Constants for release from molten pool (salt)	Experiments/other codes (e.g., DOE tools)	

2.3.2. Development Plan

<u>Technical Development Issues</u>

A pre-PIRT analysis (pre-PIRT because a particular design is not assessed) was performed by Brookhaven National Laboratories on the important phenomena needed for simulating molten salt reactors [37]. In addition, a thermal hydraulics PIRT was performed for the AHTR [38]. These PIRTs examine the phenomena necessary for thermal hydraulics and neutronics but little guidance is provided for radionuclide transport.

For fixed fuel designs, most of the development issues are associated with the coolant and modeling the transport of fission product gases through the coolant. Release of fission products from fuels would be similar to existing fuels or TRISO fuels such as have been proposed for HTGR modeling.

Modeling the transport of fission products in molten salts requires additional model development. Fission products released from fuel will be trapped, at least temporarily, in the molten salt. To contribute to an accident source term from the nuclear plant, the radionuclides will have to escape from the molten salt to the cover gas that will vent along some leak path to the containment and into the environment. Escape of the noble gases from the molten salt is immediately plausible and at least two primary mechanisms for the escape of other fission products from the molten salt to the gas phase are expected, entrainment of contaminated molten salt droplets in the gas flow and vaporization of fission products from the molten salt.

Additional details regarding current MELCOR modeling capability and proposed modeling needs are provided in Table 2-12 and in Appendix C.

Table 2-12. Key Accident Progression Development Issues for MSRs

Key Phenomenon	Importance	Existing Capabilities	Modeling Gaps
Physical Properties	Fundamental to simulation of steady state temperature and flow distributions.	FLiBe EOS and properties already implemented in MELCOR.	Validation of properties (development items M3.1, M3.4 and M3.6)
Heat Transfer Coefficients	Transfer of heat to calculate heat loads to structural materials	Existing generic correlation forms	Implement and validation of heat transfer coefficients (development items M3.4 and M3.6)
Track the flow of gas through the molten salt	Important for calculating entrainment of fission products from molten salt (next item)	SPARC model for aerosol scrubbing in liquid pools exists in MELCOR	Extend the SPARC model and bubble rise model (development items M3.2).
Entrainment of contaminated molten salt droplets in the gas flow	The primary mechanism for such entrainment of droplets is of course the rupture of gas bubbles at the molten salt surface.	Similar capability exists for molten corium pool	Use of correlations derived from data for droplet formation during bubble bursting in aqueous systems. This phenomenon is described further in Appendix C and is part of development Item M3.2 MSR
Vaporization of fission products from the molten salt.	Release of volatile fission products to cover gas.	Similar capability exists for molten corium pool	This phenomenon is described further in Appendix C and is part of Development Items M3.2 and M3.3 MSR

<u>Code Assessment</u>

Data from the experimental programs outlined in Table 2-13 can be used to assess the thermal-hydraulic response of an MSR. MELCOR input models will be developed for each of the available experiments, and calculation results will be compared to the experimental data.

Table 2-13. Proposed MELCOR Assessment Matrix for MSRs

Experiment	Brief Description	Phenomena Tested	Code Packages Tested
MSRE	Molten Salt Reactor Experiments. Both steady state and transient tests investigating fuel pump start-up and coast-down are available [39, 40, 41].	Thermal hydraulics, fission product transport, fission product chemistry	CVH, EOS, FL, RN
Other Experiments	Experiments for TRISO fuels from HTGR are applicable to FHR		COR, RN

PCMM Characterization

The PCMM process was applied to MSR modeling capability as shown in Table 2-14. This is a preliminary evaluation of the maturity levels for the MELCOR code. Note that this evaluation applies to all molten salt reactor types listed in Table 1-1 (MSR, MSPR, MFSR, and MCSR).

Table 2-14. MELCOR Maturity for MSR Analysis

Element	Maturity Level[1]	Comments
Representation and Geometric Fidelity	2	• High level of maturity for FHR design • Flexibility in MELCOR representation of thermal hydraulics and major components
Physics and Model Fidelity	1	Molten salt properties have been implemented, mature aerosol physics models, modeling of TRISO fuels, adaption of existing capabilities for modelling flow of RN and decay heat.
Code Verification	1	Extensive assessment of existing modeling capabilities for non MSR reactor designs (see Physics and Model Fidelity)
Solution Verification	1	Extensive assessment of existing modeling capabilities for non MSR reactor designs (see Physics and Model Fidelity)
Model Validation	1	Extensive assessment of existing modeling capabilities for non MSR reactor designs (see Physics and Model Fidelity)
Uncertainty Quantification and Sensitivity Analysis	1	Extensive assessment of existing modeling capabilities for non MSR reactor designs (see Physics and Model Fidelity)

[1]Maturity Levels

- level 0, little or no assessment of accuracy and completeness and highly reliant on personal judgment and experience;
- level 1, some informal assessment of accuracy and completeness, and some assessment has been made by an internal peer review group;
- level 2, some formal assessment of accuracy and completeness, and some assessments have been made by an external peer review group; and
- level 3, formal assessment of accuracy and completeness, and essentially all assessments have been made by an independent, external peer review group.

3. SCALE DEVELOPMENT PLANS FOR NON-LWRS

Since the early 1990s SCALE has been used to provide necessary data to MELCOR for severe accident analysis including fission product and radionuclide inventories, decay heat, reactor kinetics parameters, and power distributions. Active development projects are underway to facilitate transfer of data from SCALE to MELCOR and MACCS.

The overarching strategy described in this section is to provide near-term readiness for initial assessments that enable NRC staff to identify key phenomena of interest for further investigation. This needs-driven approach will evolve in an adaptive manner in partnership with NRC's licensing technical review staff and the SCALE development team as more is revealed about the specific designs of technologies being brought forward by the reactor developers.

The SCALE code system is a widely used (by 60 countries, approximately 9,000 users and 33 regulatory bodies) modeling and simulation suite for nuclear safety analysis and design that is developed, maintained, tested, and managed by the Reactor and Nuclear Systems Division (RNSD) of the Oak Ridge National Laboratory (ORNL) [42]. SCALE provides a comprehensive, verified and validated, user-friendly tool set for criticality safety, reactor physics, radiation shielding, radioactive source term characterization, and sensitivity and uncertainty analysis. Since 1970's, regulators, licensees, and research institutions around the world have used SCALE for safety analysis and design. An extensive modernization effort was undertaken for the 2016 release of SCALE 6.2 to provide an integrated framework with dozens of computational modules, including three deterministic and three Monte Carlo radiation transport solvers selected based on the user's desired solution strategy. SCALE includes current nuclear data libraries and problem-dependent processing tools for continuous energy and multigroup neutronics and coupled neutron-gamma calculations, as well as activation, depletion, and decay calculations. SCALE includes unique capabilities for automated variance reduction for shielding calculations, as well as sensitivity and uncertainty analysis. SCALE's graphical user interfaces assist with accurate system modeling and convenient access to desired results. The NRC is the primary sponsor of SCALE for its application in licensing current and advanced reactors, fuel cycle facilities, and radioactive material transportation and storage.

A primary goal of SCALE is to provide robust calculations while reducing requirements for user input. The user does not need to have extensive knowledge of the intricacies of the underlying code and data architecture. SCALE provides standardized sequences to integrate many modern and advanced capabilities into a seamless calculation that the user controls from a single input file. Additional utility modules are provided primarily for post processing data generated from the analysis sequences for advanced studies. The user provides input for SCALE sequences in the form of text files using free-form input, with extensive use of keywords and engineering-type input requirements. SCALE's GUI helps the user create input files, visualize geometry and nuclear data, execute calculations, view output, and visualize results. A diagram showing the key capabilities of SCALE is provided in Figure 3-1 below.

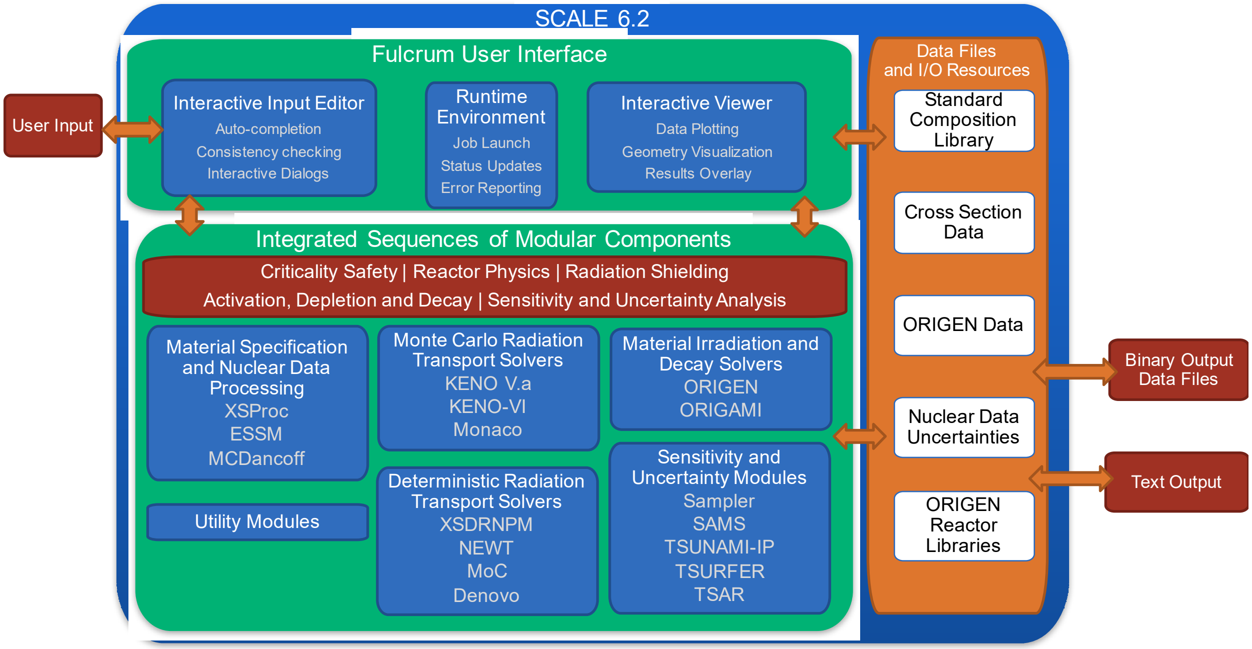

Figure 3-1. Integrated capabilities of modernized SCALE 6.2.

An overview of the major SCALE capabilities and the analysis areas they serve is provided in Table 3-1.

Table 3-1. Summary of major SCALE capabilities

Area	Code	Function
User Interface	Fulcrum	Graphical user interface for SCALE provides syntax highlighting, error checking, job submission, output inspection and visualization. Interfaces with NRC's SNAP GUI
	SCALE Runtime	Command line interface to run SCALE jobs, report errors, initiate parallel computations.
Nuclear Data	AMPX	Process raw nuclear data from sources such as ENDF/B files into data appropriate for use in computer codes. Processed data include continuous energy and multi-group libraries, ORIGEN data and Covariance data necessary for sensitivity/uncertainty analyses.
Criticality Safety	CSAS	3D multigroup and continuous energy eigenvalue Monte Carlo analysis and criticality search capability (with KENO or Shift transport kernels) with supporting capabilities for • burnup credit analysis using 3D Monte Carlo (STARBUCS) • hybrid 3D deterministic/Monte Carlo analysis with optimized fission source distribution (Sourcerer) and • statistical approach for applying validation data in setting upper subcritical safety limits (USLSTATS)
Radiation Shielding	MAVRIC	3D multigroup and continuous energy fixed source neutron transport (with MONACO or Shift transport kernels) with automated variance reduction using a hybrid deterministic importance generation capability (DENOVO) to optimize scoring for a wide

Area	Code	Function
		range of responses. Can import sources from ORIGAMI and ORIGEN.
Reactor Physics	TRITON	Coupled neutronics and depletion with • 1D fast running coupled depletion and neutronics (XSDRNPM) • 2D general purpose lattice physics depletion calculations including generation of few-group cross section data for use in nodal core simulators (NEWT), and generation of ORIGEN reactor libraries • 3D multigroup and continuous energy Monte Carlo depletion analysis with KENO transport • 3D multigroup and continuous energy depletion analysis with Shift transport which includes generation of few group cross section data for use in nodal core simulators • generation of ORIGEN Reactor Libraries
	Polaris	2D streamlined reactor lattice physics depletion calculations and generation of few-group cross section data for use in nodal core simulators
Activation, depletion and decay	ORIGEN	General purpose point depletion and decay code to calculate isotopic concentrations, decay heat, radiation source terms, and curie levels
	ORIGAMI	Rapid characterization of reactor spent fuel isotopics supporting full assembly, axial, radial, and 3D approximate modelling using ORIGEN Reactor Libraries
	ORIGEN Reactor Libraries	Pre-generated burnup libraries for a variety of fuel assemblies for commercial and research reactors
Sensitivity and uncertainty analysis	TSUNAMI	Sensitivity analysis capability embedded in other sequences with • 1D multigroup eigenvalue and reaction rate sensitivity (XSDRNPM), • 2D multigroup eigenvalue and reaction rate sensitivity analysis (NEWT) 3D multigroup and continuous energy eigenvalue and reaction rate sensitivity analysis (KENO or Shift). Post-processing sensitivity data for • determination of experiment applicability and biases for use in code and data validation, • similarity rankings based on sensitivity and uncertainty, and • data adjustment.
	SAMPLER	Stochastic uncertainty quantification in results based on uncertainties in nuclear data and input data as well as parametric analysis to identify trends
Material Specification and Cross section Processing	XSProc	Temperature correction, resonance self-shielding, and flux weighting to provide problem-dependent microscopic and macroscopic multigroup cross section data integrated with computational sequences, but also available for stand-alone analysis. Includes capabilities for multi-region geometry, arrays of repeating structures, and double-heterogeneity such as TRISO fuel.

Area	Code	Function
	Standard composition library	Library used throughout SCALE that provides individual nuclides; elements with tabulated natural abundances; compounds, alloys, mixtures, and fissile solutions commonly encountered in engineering practice
	MCDancoff	3D Monte Carlo calculation of Dancoff factors especially for use in XSProc for irregular arrays
Monte Carlo transport kernels	KENO V.a/ KENO-VI	Eigenvalue Monte Carlo codes applied in many computational sequences for multigroup and continuous energy neutronics analysis
	Monaco	Fixed source Monte Carlo code applied in the MAVRIC sequence for multigroup and continuous energy analysis
	Shift	Monte Carlo transport kernel developed for high performance computing as a replacement for KENO and Monaco.
Deterministic transport kernels	XSDRNPM	1D discrete ordinates transport applied for neutron, gamma, and coupled neutron/gamma analysis
	NEWT	2D extended step characteristic transport with flexible geometry applied to neutronics analysis, especially within the TRITON sequences
	Denovo	3D Cartesian geometry discrete ordinates transport applied for neutron, gamma, and coupled neutron/gamma analysis, especially to generate biasing parameters within the MAVRIC and Sourcerer sequences
Other tools	Various	Utility packages that perform pre- and post-processing data introspection and format conversion

It is also of note that SCALE is a cross-cutting tool within the Agency and is already developed to work with several other Agency tools such as PARCS and TRACE. SCALE is also the tool for NMSS confirmatory calculations for fuel cycle facilities, fresh fuel transportation, and spent fuel transportation and storage. Because of the extensive overlap in capabilities needed for NRO and NMSS, the activities enumerated below will provide validated, near term, capabilities for severe accident analysis and also enable the accelerated reviews for fuel cycle and transportation reviews by NMSS.

Ongoing developments for SCALE 6.3 are enhancing and assessing capabilities for the analysis of non-LWRs including MSRs, HTGRs, FHRs, and SFRs, with key capabilities identified in each technology-specific section below. A cross cutting activity for all non-LWRs is the generation of a very fine group cross section library that has been demonstrated to provide good performance for many technology concepts. An initial very fine group library developed in FY18 will be available in the FY19 beta release of SCALE 6.3, with an optimized version to follow in the final release. SCALE 6.3 will also include new ENDF/B-VIII.0 data libraries, which have new evaluations of particular importance for non-LWRs such as new scattering kernels for reactor grade graphite.

Another important development in SCALE 6.3 is the introduction of the Shift Monte Carlo transport code as a new transport kernel in SCALE's criticality safety (CSAS), radiation shielding (MAVRIC), reactor physics (TRITON), and sensitivity/uncertainty analysis (TSUNAMI) applications. The complete transition to Shift will likely take years but this process has been greatly accelerated by Shift support through the DOE-NE Consortium for the Advanced Simulation of LWRs (CASL) as well as the DOE Office of Science (DOE-SC) Exascale Computing Project

(ECP), which both have funded Shift development. Recent NRC sponsored activities within SCALE have also provided CASL with capabilities such modernized neutron and gamma physics modules, nuclear data, and a particularly strong validation basis.

A further area of collaboration is the potential use of CASL features to support code verification activities. CASL's integrated multiphysics Virtual Environment for Reactor Applications (VERA) core simulator originally developed and assessed for specific LWR application has been extended to provide the VERA-MSR as a reference capability for integrated neutronics, thermal fluidics, mass transport, and depletion with feedback effects from delayed neutrons, Xenon, fuel density and more [43, 44, 45].

Note that within SCALE there is the capability to enable a file-based data transfer to MELCOR/MACCS of the following quantities.

1. Time and space-dependent inventory (mol), $n_i(r,t)$, where i is an isotope index.
2. Fundamental nuclide and decay data.
    a. Nuclide mass (g/mol), M_i.
    b. Decay constants (1/s), λ_i.
    c. Energy release per decay (J/decay), Q_i.
3. Nuclide effective generation and destruction rate data (mol/s), $G_i(r,t)$ and $D_i(r,t)$.

Responses may have any spatial fidelity level from a single fuel grain to an entire core, as the analyst is in complete control of creating this data set from one or more SCALE calculations. The "labelSet" provides additional user-defined data that can help interpret or select specific responses from large data sets. In LWR work, detailed single-assembly isotopics were lumped into reactor radial zones with sensitivity analyses performed on the zoning.

A detailed development plan for SCALE based on the MELCOR and MACCS data needs (decay heat, fission product inventory, activity) is shown in Table 3-2 (details are discussed in the following sections). Further development and assessment needs are found in Section 3. The activities detailed are based on a reference design that is to be developed for each of the areas. Beyond FY20, code development activities will focus on advanced reactor technologies and design specific modifications and code assessments as those details and funding become available.

The SCALE computer code is at the stage where further development and refinement requires assessments.

Table 3-2. SCALE Non-LWR Development Plan Start Dates.

Reactor Type/ Development Item (DI)	Phenomenological Area (SCALE)	Description of Tasks (needs)	FY18	FY19	FY20
SFR (A1-A3)	Reactor physics assessments	Perform assessment calculations for a standard SFR core design, producing power, isotopic, and reactivity distributions for MELCOR severe accident initialization.		✓	
SFR (D1-D2)	Production SFR ORIGEN reactor libraries	Develop SFR ORIGEN library parametrization and create production-quality ORIGEN reactor libraries for two SFR types.		✓	
SFR (D3)	Reactor physics automation, development and training	Extend existing ORIGAMI automator to include irradiation features implemented above and provide training to NRC staff on performing assessments.		✓	✓
HTGR (A1-A10)	Reactor physics assessments	SCALE has extensive HTGR modeling capabilities. In this task, the production release of SCALE 6.2.3 will be applied to provide fission product inventories, decay heat, power distributions, kinetics parameters, as well as reactivity coefficients for thermal feedback. In this task, individual models will be constructed and data sets archived. The impact of modeling assumptions and simplification will be assessed including pebble history effects.		✓	
HTGR (D1,D2)	ORIGAMI pebble depletion capability and production HTGR ORIGEN reactor libraries	ORIGAMI pebble depletion mode including development of new ORIGEN reactor libraries for two HTGRs.		✓	
HTGR (D3-D5)	Include additional data in ORIGEN libraries to support MELCOR initialization	In TRITON, develop automated scheme for calculation of reactivity coefficients and kinetics data, writing that data through the ORIGEN-API to the ORIGEN library. Post-processing of all data to MELCOR formats available through ORIGEN or ORIGAMI interfaces.		✓	

Reactor Type/ Development Item (DI)	Phenomenological Area (SCALE)	Description of Tasks (needs)	FY18	FY19	FY20
HTGR (D6)	Reactor physics automation, development and training	Extend existing ORIGAMI automator to include pebble irradiation features implemented above and provide training to NRC staff on performing assessments.		✓	✓
MSR (A1)	Reactor physics assessments	Calculate MSRE benchmark isotopics, power, kinetics and other MELCOR parameters with the TRITON MSR capability and compare the CASL VERA-MSR simulator.		✓	
MSR (A2)	Calculation of chemical species formation	Use the thermal dynamic equilibrium code Thermochimica to calculate species formed at various locations in the MSR loop		✓	
MSR (D3)	Integration of Thermochimica in ORIGEN	Enables inline calculation of species formation within ORIGEN (depends on MSR/A2).		✓	✓
MSR (D4)	Extension of ORIGEN to model MSR loops, lines, and tanks	Implement new components in the ORIGEN input that allows detailed generation of all MELCOR data within the MSR system.		✓	✓
MSR (D5)	Reactor physics automation, development and training	Extend existing ORIGAMI automator to include irradiation features implemented above and provide training to NRC staff on performing assessments.		✓	✓
FHR (A1-A4)	Reactor physics assessments	Leveraging experience from the HTGR assessment tasks (HTGR/A1-A10), the additional assessment for the FHR is limited to creation of a new FHR core model and estimation of the tritium production in the FLiBe coolant which can be modeled as an independent irradiation calculation in ORIGEN.		✓	
FHR (D1)	Production FHR ORIGEN reactor libraries	Develop two new FHR ORIGEN reactor libraries to allow rapid FHR isotopics calculations (depends on HTGR/D1)		✓	

Reactor Type/ Development Item (DI)	Phenomenological Area (SCALE)	Description of Tasks (needs)	FY18	FY19	FY20
FHR (D2)	Streamlined tritium production assessment in ORIGAMI	Isotope production in the working fluid (e.g. FLiBe salt) will become a standard part of ORIGAMI, applied to tritium production (depends on FHR/D1)		✓	
FHR (MSR/D5)	Reactor physics automation, development and training	Extend existing ORIGAMI automator to include irradiation features implemented above and provide training to NRC staff on performing assessments.		✓	✓

3.1. HTGR/FHR

For HTGRs and FHRs, SCALE provides fission product and radioactive nuclide inventories, decay heat, power distributions, kinetics parameters, as well as reactivity coefficients for thermal feedback. The production release of SCALE 6.2 provides unique capabilities for continuous-energy and multigroup neutronics and source terms analysis of gas-cooled HTGRs and fluoride-salt cooled FHRs. Through the US Department of Energy's Next Generation Nuclear Plant (NGNP) program, the NRC supported enhancements to SCALE for tri-structural isotropic (TRISO) double-heterogeneity fuel modeling, especially for interoperability with the PARCS core simulator for HTGR license reviews [46]. These capabilities were further enhanced through international cooperative research to integrate and extend TRISO features within the modernized SCALE framework and to develop enhanced features for additional fuel forms and molten salt coolants.

Enhanced HTGR/FHR features for SCALE 6.3 include 3D capabilities with the Shift Monte Carlo code for the generation of nodal cross sections for core simulator calculations and modeling random TRISO particle loading. In addition, new multi-group and continuous-energy cross section libraries processed from ENDF/B-VIII.0 include significant improvements in nuclear data for graphite as well as uranium nuclides compared to earlier SCALE libraries [47].

SCALE is applied extensively in international benchmarks for HTGRs, especially for its capabilities to assess the impact of nuclear data uncertainties on neutronics and burnup calculations, with a 3D Monte Carlo model of the HTR-10 benchmark shown in Figure 3-2 [45, 48]. Additionally, the thermochemical equilibrium state of the irradiated FHR salt coolant will be generated with ORNL's Thermochimica code with information provided to MELCOR [49]. Thermochimica receives ongoing support from the NEAMS program for its interoperability with ORIGEN isotopic data in other tools, so no NRC resources are required except to integrate it into severe accident workflow.

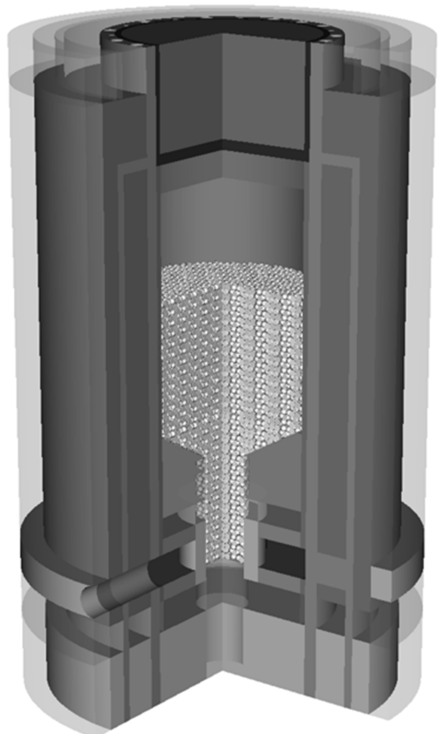

Figure 3-2. SCALE Monte Carlo Model of HTR-10 Benchmark.

3.1.1. HTGR Reactor Physics Considerations

The pebble bed HTGR is a thermal spectrum reactor which utilizes circulating fuel pebbles (~200,000 in a core) composed of TRISO fuel particles (~8000 per pebble) in a graphite matrix with helium coolant. Fixed fuel prismatic reactors utilized TRISO fuel particles in graphite blocks with helium coolant channels. SCALE/CSAS MG calculations have been made in the past to generate core-wide flux and power distributions for pebble bed and prismatic HTGRs as part of the NGNP project, with a unique double-heterogeneity treatment developed during this project [50]. For SCALE 6.3, a continuous-energy Monte Carlo capability to model randomized TRISO particles in a pebble will be available as a reference capability, especially to verify assumptions for criticality and depletion calculations. SCALE/ORIGAMI (and predecessor capability) has also been used successfully for many years to generate data for LWR accident analysis with MELCOR via ORIGEN reactor libraries and the ORIGAMI sequence in SCALE. Limited enhancements are needed to leverage these existing capabilities into a new, streamlined capability for severe accident analysis of HTGRs with MELCOR.

HTGR reactor physics data from SCALE

SCALE reactor physics calculations can be used to provide the following tabulated data for severe accident analysis of HTGRs with MELCOR. Note that SCALE may provide approximate spatially-dependent (r) quantities allowing for modeling of simple operating histories leading up to the severe accident scenario, as indicated by the dependence on initial time t_0.

1. Fission product mass inventory, $m_i(r, t_0)$, where i is an isotope index.
2. Fission product decay heat, $H_i(r, t_0)$.

3. System power distribution, $P(r, t_0)$.
4. Kinetics data.
    a. Six-group delayed neutron precursor kinetics data, $\beta_j(r, t_0)$ and $\lambda_j(r, t_0)$.
    b. Temperature reactivity coefficients, $\alpha_{T_{fuel}}(r, t_0)$.

The system power and kinetics data transfer require new development.

These nuclear data quantities provided through SCALE enable a more fundamental connection of MELCOR and MACCS to current nuclear data, as well as the ability to reconstruct the quantities of interest from fundamental components. Consider the following examples.

1. Time, space, and isotope-dependent activity, $A_i(r, t) = \lambda_i n_i(r, t)$.
2. Time, space, and isotope-dependent decay heat, $H_i(r, t) = Q_i A_i(r, t)$.
3. Time, space, and isotope-dependent mass inventory, $m_i(r, t) = M_i n_i(r, t)$.

SCALE analysis/development tasks

The overarching strategy is a more detailed version of the introduction provided in Table 3-2, and is designed to enable incremental delivery of capability with initial data to MELCOR. We will also focus on the user of this tool performing various pebble irradiation scenarios and constructing hypothetical HTGR cores from this “bank” of available pebbles.

<u>**Analysis Tasks**</u>

The following analysis tasks can be completed with the current SCALE 6.2.3 available from RSICC with no additional development. In the course of executing the tasks, the process would be documented and repeatable by other analysts for additional HTGR scenarios.

Calculate the equilibrium HTGR core spatial flux spectrum and power distribution. [SCALE/HTGR/A1]
(No task dependencies.)
Calculate the scalar flux and power throughout the core for an assumed pebble and temperature distribution (vendor information and/or DOE tools may be used for initial conditions) using SCALE/CSAS for the HTR-10 neutronics benchmark [IAEA Tech Doc 1694]. These SCALE models already exist but the detailed, spatially dependent information has not been investigated. Compare to benchmark power distributions. The power distribution calculated in this task is one of the fundamental inputs to MELCOR. Implicit with this effort is a review of the nuclear data.

Perform single-pebble irradiations with fixed constant power. [SCALE/HTGR/A2]
(No task dependencies.)
Deplete a single fuel pebble in TRITON. Assess the burnup gradient within a pebble under idealized conditions. Assess both isotopics and ORIGEN reactor library data.

Perform single-pebble irradiations with time-dependent power. [SCALE/HTGR/A3]
(Depends on SCALE/HTGR/A1.)
Assuming a pebble travels in a streamlined path through the core, deplete a single fuel pebble in TRITON with that variable power, including multiple passes to obtain discharge burnup. Compare the burnup gradient within a pebble to SCALE/HTGR/A2. Assess both isotopics and ORIGEN reactor library data.

Perform single-pebble irradiations using buffer zones to simulate the spectrum change as pebbles pass through the core. [SCALE/HTGR/A4]
(Depends on SCALE/HTGR/A1.)
Based on a single-pebble depletion model in TRITON, develop a buffer zone methodology that can add or remove absorbing and reflecting material to drive changes in the flux spectrum and simulate in an approximate sense movement of pebbles through different regions of the core, e.g. near the core barrel with a control rod inserted. As part of this task, we can assess how important modeling variation of the flux spectrum is compared to simply assuming reflective boundaries and depleting according to the power history from task SCALE/HTGR/D1. We will also be able to assess the burnup gradient within a pebble under idealized conditions. Assess both isotopics and ORIGEN reactor library data and compare to SCALE/HTGR/A2 and SCALE/HTGR/A3.

Create assessment single-pebble ORIGEN reactor library. [SCALE/HTGR/A5]
(Depends on SCALE/HTGR/A2, SCALE/HTGR/A3, SCALE/HTGR/4.)
Create single-pebble ORIGEN reactor libraries using TRITON and knowledge gained from previous tasks in SCALE/HTGR/A2, SCALE/HTGR/A3, and SCALE/HTGR/A4. This library will allow rapid isotopics calculations given a power history enabling the spectral parameter feature from the LWR moderator density parameter in order to account for time-dependent spectral changes in the pebble as it moves through the system. Also, compare to TRITON calculations in SCALE/HTGR/A2, SCALE/HTGR/A3, SCALE/HTGR/A4. Comparisons to vendor or DOE tools would be useful to verify spectral changes applied this rapid method.

Construct core distribution of isotopics for MELCOR. [SCALE/HTGR/A6]
(Depends on SCALE/HTGR/A5.)
Using the ORIGEN reactor library in SCALE/HTGR/A5, this task exercises the capability to reconstruct isotopics in a pebble, given any assumed time-dependent irradiation history for each pebble in terms of streamlines through the core. In all likelihood, pebbles will be grouped to reduce computational burden. The end-result is the reconstruction of the isotopic distribution throughout a given MELCOR nodalization based on the pebble content of each MELCOR node. For example, MELCOR radial node 3, axial node 7 contains 50% of pebble type 1 with one pass through the core and 50% of pebble type 2 with three passes through the core. The isotopics distribution calculated in this task is one of the fundamental inputs to MELCOR. Comparisons to vendor or DOE tools would be useful as a code-to-code verification of pebble group burnup history.

Construct core distribution of delayed neutron kinetics parameters for MELCOR. [SCALE/HTGR/A7]
(Depends on SCALE/HTGR/A5.)
Delayed neutron kinetics parameters are calculated as part of the task SCALE/HTGR/A5 TRITON calculation. A script will reformat data for delivery to MELCOR. The delayed neutron kinetics parameters distribution calculated in this task is one of the fundamental inputs to MELCOR. Comparisons to vendor or DOE tools would be useful as a code-to-code verification.

Construct core temperature reactivity coefficients for MELCOR. [SCALE/HTGR/A8]
(Depends on SCALE/HTGR/A5.)
An additional calculation at the TRITON stage (SCALE/HTGR/A5) is required to determine the temperature reactivity coefficient. A script will reformat data for delivery to MELCOR. The reactivity coefficient distribution calculated in this task is one of the fundamental inputs to MELCOR. Comparisons to vendor or DOE tools would be useful as a code-to-code verification.

Assess sensitivity to assumed core pebble distribution. [SCALE/HTGR/A9]
(Depends on SCALE/HTGR/A6.)

Task SCALE/HTGR/A1 assumed a pebble and temperature distribution in order to calculate the core power and neutron spectrum distribution. This task will assess alternate pebble distributions, such as the pebble distribution for a first core. It may be important to assess not only the sensitivity to core isotopics distributions but final MELCOR analyses, e.g. two scenarios with half of the core graphite blanks and half 15 wt% pebbles could be analyzed. Comparisons to vendor or DOE tools would be useful as a code-to-code verification.

Assess sensitivity to HTGR core design. [SCALE/HTGR/A10]
(Depends on SCALE/HTGR/A6.)
Perform calculations of the power and flux spectrum distribution in other HTGR (e.g. PBMR, AVR, IAEA benchmarks) and compare to benchmark results. The amount of work in this task is variable: at minimum, we repeat task SCALE/HTGR/A1 for a different core. At maximum, we would proceed through the entire list of other tasks from SCALE/HTGR/A2-A8. Comparisons to vendor or DOE tools would be useful as a code-to-code verification.

Development Tasks

The following development tasks if pursued if FY19 would be released with SCALE 6.3 at the end of FY19. Although no development is necessary to perform the calculations, the efficiency would be greatly improved if the features described below were added to SCALE, mainly in the ORIGAMI isotopics generator.

Develop streamline history capability in ORIGAMI. [SCALE/HTGR/D1]
(Depends on SCALE/HTGR/A5.)
In ORIGAMI, allow the user to provide a time-dependent 3D power and spectral parameter from task SCALE/HTGR/A5 within the core. The user then provides data for a single pebble/pebble group position vs. time. ORIGAMI then has enough information to produce isotopics as a function of lifetime for any pebble.

Included in this task is an update of the ORIGEN library format for non-LWR spectral parameters. For LWRs, the ORIGEN reactor library has enabled a state-of-the-art rapid, high-fidelity isotopics calculation used for spent fuel and source terms throughout NRC. Effectively deploying ORIGEN reactor libraries for a new reactor type requires an assessment of the specific system's most important parameters (task SCALE/HTGR/A5), as well as an incorporation of those parameters into the data structures and code input/output.

Deliver production-quality ORIGEN reactor libraries for HTGR pebbles. [SCALE/HTGR/D2]
(Depends on SCALE/HTGR/D1.)
Deliver tested and quality-assured ORIGEN reactor libraries for HTGR pebbles in the final SCALE 6.3 release. This requires the nomenclature and parametrization for HTGR pebble depletion from task SCALE/HTGR/D1. This task involves creating the template files, production library generation, manual updates, independent testing, and distribution (now and future releases) with SCALE. The existence of these libraries in a SCALE release enables analysts to skip directly to task SCALE/HTGR/A6.

Included delayed neutron kinetics data on ORIGEN reactor library. [SCALE/HTGR/D3]
(Depends on SCALE/HTGR/A7, SCALE/HTGR/D2)
In TRITON, include delayed neutron kinetics data calculated in ORIGEN reactor libraries and available as an additional result alongside isotopics when performing ORIGAMI calculations. This development eliminates the need for the SCALE/HTGR/A7 task as part of the MELCOR data preparation.

Automate temperature reactivity coefficient and include on ORIGEN reactor library. [SCALE/HTGR/D4]
(Depends on SCALE/HTGR/A8, SCALE/HTGR/D2)
In TRITON, automate temperature reactivity coefficient construction from uniform pebble temperature increases. Add to ORIGEN reactor libraries as an additional parameter for interpolation.

Automate construction of core distributions for MELCOR. [SCALE/HTGR/D5]
(Depends on SCALE/HTGR/A6, SCALE/HTGR/D1, SCALE/HTGR/D2, SCALE/HTGR/D3, SCALE/HTGR/D4.)
In ORIGAMI, users will be able to directly generate the necessary MELCOR core distributions given pebble distribution in the core and operating history for each pebble (with options for simple number of passes or burnup for each pebble) from SCALE/HTGR/D1, ORIGEN reactor libraries from SCALE/HTGR/D2, and additional information added to the ORIGEN library in SCALE/HTGR/D3 and SCALE/HTGR/D4 to interpolate and deplete to determine isotopics (SCALE/HTGR/A5 or SCALE/HTGR/D3), kinetics data (SCALE/HTGR/D4), and temperature reactivity coefficients (SCALE/HTGR/D5). With the completion of this task, an analyst using ORIGAMI in SCALE 6.3 will be able to determine MELCOR input isotopic, kinetic, and reactivity distributions in hours, assuming known pebble distribution and operating history. Otherwise, analysts would need to manually perform this task, which is time-intensive and prone to user error. The 3D power distribution cannot be calculated by ORIGAMI and is provided from an external (e.g. SCALE/CSAS) 3D core calculation.

Calculation of core distributions for MELCOR from large-scale pebble distributions. [SCALE/HTGR/D6]
(Depends on SCALE/HTGR/D5.)
The ORIGAMI Automator has been used to generate MELCOR data for site level 3 PRA based on actual assembly shuffling and spent fuel pool movements. This task would implement an extension for inventory analysis with pebble movements to facilitate confirmatory calculations by NRC staff.

<u>PCMM Characterization</u>

The PCMM process was applied to the HTGR modeling capability, and the results are summarized in Table 3-3.. Note that this evaluation applies to all HTGR types listed in Table 1-1 (PBR, PMR, and GCFR). The HTGR models are relatively mature and most modeling capability is already in place. Validation of these models is perhaps the greatest need at this time.

Table 3-3. SCALE Maturity for HTGR Analysis

Element	Maturity Level[1]	Comments
Representation and Geometric Fidelity	3	• Under NGNP effort a double-heterogeneous treatment has been developed to support the two levels of heterogeneity (i.e. TRISO micro-spheres dispersed in the graphite matrix, and the rod-to-rod or sphere-to-sphere neutron interactions). • SCALE has been used to model various aspects of HTGRs • Reviewed by ACRS as part of NGNP
Physics and Model Fidelity	2	• Need for more complete test data to support depletion validation. • SCALE has been used to model various aspects of HTGRs • Reviewed by ACRS as part of NGNP
Code Verification	2	• Extensive SQE, many capabilities have been benchmarked and some peer review.
Solution Verification	2	• Some informal assessments both internally as well as assessment by code users.
Model Validation	2	• Extensive validation of most physics models though not all within the domain of HTGRs. • External assessment
Uncertainty Quantification and Sensitivity Analysis	2	• Uncertainties and numerical propagation of errors has been examined extensively for LWR applications though not for HTGR application

[1]Maturity Levels
- level 0, little or no assessment of accuracy and completeness and highly reliant on personal judgment and experience;
- level 1, some informal assessment of accuracy and completeness, and some assessment has been made by an internal peer review group;
- level 2, some formal assessment of accuracy and completeness, and some assessments have been made by an external peer review group; and
- level 3, formal assessment of accuracy and completeness, and essentially all assessments have been made by an independent, external peer review group.

3.1.2. *FHR Reactor Physics Considerations*

The following is a more detailed plan from the introductory material in Table 3-2. The FHR is similar to the HTGR with circulating fuel pebbles composed of TRISO fuel particles. However, the working fluid for the FHR is liquid salt, typically FLiBe, instead of helium for the HTGR. The strategy for calculating FHR reactor physics data with SCALE to initiate MELCOR severe accident analyses is similar to HTGR but with the additional need to model tritium production in the FLiBe.

FHR reactor physics data from SCALE

SCALE reactor physics calculations can be used to provide the following tabulated data for severe accident analysis of HTGRs with MELCOR. Note that SCALE may provide approximate spatially-dependent (r) quantities allowing for modeling of simple operating histories leading up to the severe accident scenario, as indicated by the dependence on initial time t_0.

1. Fission product mass inventory, $m_i(r, t_0)$, where i is an isotope index.
2. Fission product decay heat, $H_i(r, t_0)$.
3. System power distribution, $P(r, t_0)$.

4. Kinetics data.
    a. Six-group delayed neutron precursor kinetics data, $\beta_j(r, t_0)$ and $\lambda_j(r, t_0)$.
    b. Temperature reactivity coefficients, $\alpha_{T_{fuel}}(r, t_0)$.
5. Tritium mass inventory, generation rate, and destruction rate in FLiBe, $m_{tritium}(r, t_0)$, $G_{tritium}(r, t)$ and $D_{tritium}(r, t)$.

Note that compared to the HTGR, only the additional tritium mass inventory in the FLiBe is required.

SCALE/FHR analysis/development tasks

The overarching strategy is to leverage HTGR developments to minimize cost for FHR extensions.

Analysis Tasks

The following analysis tasks can be completed with the current SCALE 6.2.3 available from RSICC with no additional development. In the course of executing the tasks, the process would be documented and repeated by other analysts for additional FHR scenarios.

Calculate the assumed FHR core spatial flux spectrum and power distribution.
[SCALE/FHR/A1]
(No task dependencies.)
Calculate the scalar flux and power throughout the core for an assumed pebble and temperature distribution using SCALE/CSAS for the TMSR design from the Chinese Academy of Sciences. The SCALE models for these systems do not yet exist, but preliminary core design data is readily available in open literature and conference presentations. The power distribution calculated in this task is one of the fundamental inputs to MELCOR. Vendor information or DOE tools to establish initial assumed pebble and temperature distribution is useful here. Implicit with this effort is a review of the nuclear data.

[Calculate the tritium content/generation rate in FLiBe. SCALE/FHR/A2]
(Depends on SCALE/FHR/A1.)
Using standalone ORIGEN, develop an input for the activation of FLiBe using the flux calculated in SCALE/FHR/A1 including a user-specified tritium filtration and flow of FLiBe through the core. Perform an assessment calculation of the MSRE tritium inventory with comparison to measurement using the same methodology [51]. The tritium inventory, generation rate, and destruction rate is one of the fundamental inputs to MELCOR. Comparisons to vendor or DOE tools would be useful as a code-to-code verification.

Create assessment single-pebble ORIGEN reactor library. [SCALE/FHR/A3]
(Depends on SCALE/HTGR/A5.)
Create single-pebble ORIGEN reactor libraries using TRITON and knowledge gained from SCALE/HTGR/A5. This library will allow rapid isotopics calculations given a power history and a spectral parameter feature that leverages the LWR parameter moderator density in order to account for time-dependent spectral changes in the pebble as it moves through the FHR system. Assess performance of the ORIGEN reactor library by comparison to TRITON calculations. Comparisons to vendor or DOE tools would be useful as a code-to-code verification.

Construct core distribution of isotopics, delayed neutron kinetics parameters, temperature reactivity coefficients for MELCOR. [SCALE/FHR/A4]
(Depends on SCALE/FHR/A3 and SCALE/HTGR/A7, SCALE/HTGR/A8.)
Using the ORIGEN reactor library developed in SCALE/FHR/A3, this task exercises the capability to reconstruct isotopics, delayed neutron kinetics parameters, and temperature reactivity coefficients as performed for the HTGR in SCALE/HTGR/A6, A7, and A8 tasks. Comparisons to vendor or DOE tools would be useful as a code-to-code verification.

Development Tasks

Deliver production-quality ORIGEN reactor libraries for FHR pebbles. [SCALE/FHR/D1]
(Depends on SCALE/HTGR/D1.)
Deliver tested and quality-assured ORIGEN reactor libraries for FHR pebbles in the final SCALE 6.3 release. This requires the nomenclature and parametrization for HTGR pebble depletion from task D1. This task involves creating the template files, production library generation, manual updates, independent testing, and distribution (now and future releases) with SCALE. The existence of these libraries in a SCALE release enables analysts to skip task A3.

Model tritium production in ORIGAMI. [SCALE/FHR/D2]
(Depends on SCALE/FHR/D1.)
In ORIGAMI, users will be able to directly input tritium filtration rates to generate a separate output for tritium inventory and production in FLiBe for MELCOR. By default, it will be assumed that FLiBe experiences the same flux spectrum as the fuel. A comparison to results from A2 will assess the accuracy of this assumption.

Calculation of core distributions for MELCOR from large-scale pebble distributions with FLiBe coolant. [SCALE/FHR/D3]
(Depends on SCALE/HTGR/D6.)
The ORIGAMI Automator has been used to generate MELCOR data for site level 3 PRA based on actual assembly shuffling and spent fuel pool movements. This task would extend the approached for HTGRs created in SCALE/HTGR/D6 inventory analysis with pebble movements and tritium production in FLiBe to facilitate confirmatory calculations by NRC staff.

PCMM Characterization

The PCMM process was applied to the FHR modeling capability, and the results are summarized in Table 3-4. The FHR capabilities are relatively mature and most modeling capability is already in place. Validation of these models is perhaps the greatest need at this time.

Table 3-4. SCALE Maturity for FHR Analysis

Element	Maturity Level[1]	Comments
Representation and Geometric Fidelity	2	• The 3D continuous energy Monte Carlo neutronics + depletion capabilities essentially allow the maximum fidelity of representation within nuclear engineering for predicting neutron and nuclide distributions throughout the system, but with an associated high cost of calculation. Depending on the system, only the formality of assessment varies. • The 1D/2D multi-group energy deterministic capabilities allow a much faster running capability ideal for design and safety analysis, where many perturbations/variations are needed. Depending on the system, the modeling strategy may need refinement, e.g. the double-het treatment to support multi-group, deterministic TRISO calculations.
Physics and Model Fidelity	2	• Need for more complete test data to support depletion validation. • Validation data for the working fluid to support model approximations would be needed, and support nuclear data refinement
Code Verification	2	• Extensive SQE, many capabilities have been benchmarked and some peer review.
Solution Verification	2	• Some informal assessments both internally as well as assessment by code users.
Model Validation	2	• Extensive validation of most physics models though not all within the domain of HTGRs. • Aspects of FHRs which are markedly different from NGNP designs require additional verification of modeling fidelity.
Uncertainty Quantification and Sensitivity Analysis	1	• Uncertainties and numerical propagation of errors has been examined extensively for LWR applications though not for FHR application

[1]Maturity Levels

- level 0, little or no assessment of accuracy and completeness and highly reliant on personal judgment and experience;
- level 1, some informal assessment of accuracy and completeness, and some assessment has been made by an internal peer review group;
- level 2, some formal assessment of accuracy and completeness, and some assessments have been made by an external peer review group; and
- level 3, formal assessment of accuracy and completeness, and essentially all assessments have been made by an independent, external peer review group

3.2. SFR

For SFRs, SCALE will provide fission product inventories, decay heat, power distributions, kinetics parameters, as well as reactivity coefficients for thermal feedback and core expansion. SCALE 6.2 has been applied in the study of SFRs, especially through the OECD/NEA Benchmark for Uncertainty Analysis in Modelling (UAM) for Design, Operation, and Safety Analysis of SFRs [52]. The analysis of models ranging from a pin cell up to a full core is to be performed to systematically assess the influence of nuclear data uncertainties on fast reactor simulations including eigenvalues, reactivity feedback, and the generation of few-group cross sections. Recent activities relating to advanced reactor systems involve the generation of multigroup cross section and covariance libraries for the analysis of SFR systems for SCALE 6.2 [53, 54]. SCALE is also being coupled with the FAST fuel performance code to provide accurate power distributions and isotopic inventories. Additionally, the thermochemical equilibrium state of the irradiated coolant will be generated with ORNL's Thermochimica code with information provided to MELCOR.

SFR Reactor Physics Considerations

The SFR is a solid-fueled reactor and does not require fuel movement modeling like the HTGR or FHR. A special consideration with the SFR is the need to model reactivity effects due to thermal expansion. The strategies outlined here apply broadly to the metallic fuel heat pipe microreactors as well. The strategy for calculating SFR reactor physics data with SCALE to initiate MELCOR severe accident analyses is similar to what has been done for LWR severe accident analysis, but with additional considerations for fast neutron leakage effects due to the location of the region of interest within the core. Because MELCOR will calculate the core temperatures during the evolution of the accident, a series of 3D core calculations can be computed *a priori* with the Shift Monte Carlo code at various states to provide MELCOR with rapid property lookups during the evolution of the accident, enabling NRC analysts with convenient means of assessing safety. The thermal expansion for the fuel elongation and radial core expansion can be computed using the in-progress coupling of Shift with the FAST fuel performance code, which is suitable use with traditional sodium-cooled fast reactors as well a heat pipe reactors. An example SCALE model of the EBR-II reactor is shown in Figure 3-3.

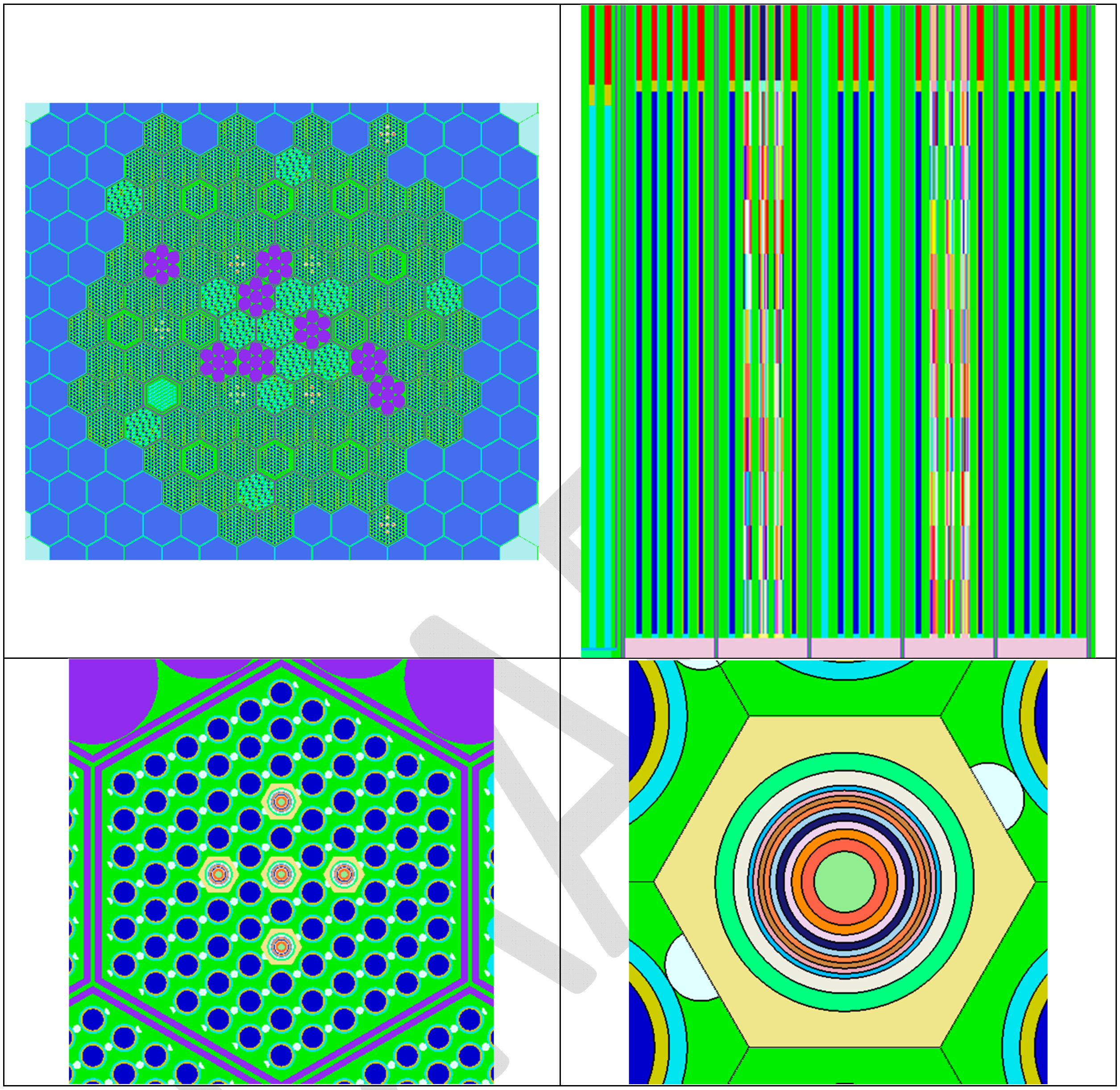

Figure 3-3. SCALE/Shift model of EBR-II SFR (top left: radial view of core, top right: axial view of core, lower left: radial detail of fuel assembly, lower right: radial view of fuel pin).

SFR Reactor Physics Data from SCALE

SCALE reactor physics calculations can be used to provide the following tabulated data for severe accident analysis of SFR with MELCOR. Note that SCALE may provide approximate spatially-dependent (*r*) quantities allowing for modeling of simple operating histories leading up to the severe accident scenario, as indicated by the dependence on initial time t_0.

1. Fission product mass inventory, $m_i(r, t_0)$, where i is an isotope index.
2. Fission product decay heat, $H_i(r, t_0)$.
3. System power distribution, $P(r, t_0)$.
4. Kinetics data.
    a. Six-group delayed neutron precursor kinetics data, $\beta_j(t_0)$ and $\lambda_j(t_0)$.

b. Temperature reactivity coefficients, $\alpha_{T_{fuel}}(r, t_0)$.
c. Void reactivity coefficients, $\alpha_V(r, t_0)$.

Note that compared to previous analyses on thermal systems, spatial delayed neutron precursor kinetics data cannot be provided currently without additional development. However, MELCOR does not currently have spatial kinetics capability so there is no loss of capability in the MELCOR model.

SFR Analysis/Development Tasks

The overarching strategy is to leverage existing capability and extend for SFR and heat pipe reactors.

Analysis Tasks

The most recent SCALE 6.3 beta 1 development version of SCALE is required to model all relevant aspects of the SFR for MELCOR accident scenario initialization (for HTGR and FHR, SCALE 6.2.3 available currently from RSICC is sufficient). In the course of executing the tasks, the process would be documented and repeatable by other analysts for additional SFR scenarios. The following is more detailed plan from that presented in Table 3-2.

Calculate power, isotopics, and delayed neutron data with full-core Monte Carlo with depletion. [SCALE/SFR/A1]
(No task dependencies.)
Calculate the scalar flux, power, and isotopics distribution as a function of core operation using SCALE/TRITON with 3D Monte Carlo continuous energy and multi-group physics. Assembly design, materials, temperature, and density distribution should be specified. The SCALE models for EBR-II and other standard SFRs exist and are readily available. Assembly-level homogenization with some axial mesh will be used for the depletion, which can be used in development task SCALE/SFR/D1. The isotopics distribution, power distribution, and core-average kinetics parameters calculated in this task are fundamental inputs to MELCOR. Comparisons to vendor or DOE tools would be useful as a code-to-code verification.

Calculate void coefficient of reactivity. [SCALE/SFR/A2]
(Depends on SCALE/SFR/A1.)
Using the core model developed in *SCALE/SFR/*A1, the sodium void in each node will be introduced, one at a time, in order to estimate the void coefficient of reactivity. The void reactivity does not require a geometry change. A script will be created to translate void reactivity coefficient data on the assembly-wise and axial mesh to the MELCOR nodalization. The void coefficient of reactivity is one of the fundamental inputs to MELCOR. Comparisons to vendor or DOE tools would be useful as a code-to-code verification.

Calculate temperature coefficient of reactivity. [SCALE/SFR/A3]
(Depends on SCALE/SFR/A1.)
Using the core model developed in *SCALE/SFR/*A1, the temperature coefficient of reactivity will be calculated by increasing power and temperature together at various depletion statepoints, modeling a simple thermal expansion of components, and recalculating the core neutronics for the expanded geometry. This process may be verifiable by FAST. This yields the global temperature coefficient of reactivity. In order to calculate the distribution, density and temperature change at each node will be calculated from the global calculation and then each node will be

increased in temperature and decreased in density one at a time and reactivity change calculated node-by-node. Finally, the node-by-node results will be normalized to have the correct global result. Comparisons to vendor or DOE tools would be useful as a code-to-code verification.

A script will be created to translate temperature reactivity coefficient data on the assembly-wise and axial mesh to the MELCOR nodalization. The temperature coefficient of reactivity is one of the fundamental inputs to MELCOR.

Development Tasks

Develop ORIGEN library parametrization for SFR assemblies. [SCALE/SFR/D1]
(Depends on SCALE/SFR/A1.)
The SFR core depletion in task *SCALE/SFR/*A1 will produce as a byproduct a set of nodal SFR ORIGEN libraries. This development task will determine a reasonable parametrization to collapse all data for the same assembly type into a single ORIGEN reactor library capable of reconstructing the core isotopic distribution.

Deliver production-quality ORIGEN reactor libraries for SFR assemblies. [SCALE/SFR/D2]
(Depends on SCALE/SFR/D1.)
Based on the development in *SCALE/SFR/*D1, deliver tested and quality-assured ORIGEN reactor libraries for SFR in the final SCALE 6.3 release. This requires the nomenclature and parametrization for SFR pebble depletion from task *SCALE/SFR/*D1. This task involves creating the template files, production library generation, manual updates, independent testing, and distribution (now and future releases) with SCALE. The existence of these libraries in a SCALE release enables analysts to skip the costly depletion calculations associated with full-core Monte Carlo depletion modeling in *SCALE/SFR/*A1 and generate isotopics from assumed assembly operational histories.

Calculation of core distributions for MELCOR from large-scale core calculations. [SCALE/SFR/D3]
(Depends on SCALE/SFR/D1.)
The ORIGAMI Automator has been used to generate MELCOR data for site level 3 PRA based on actual assembly shuffling and spent fuel pool movements. This task would implement an extension for inventory analysis with fuel movement and core expansion to facilitate confirmatory calculations by NRC staff.

PCMM Characterization

The PCMM process was applied to SFR modeling capability as shown in Table 3-5. This is a preliminary evaluation of the maturity levels for the SCALE code. Note that this evaluation applies to all liquid-metal-cooled reactor types listed in Table 1-1 (SFR, LMR, and HPR). Major need, consistent with the other designs, is the need to validate capability.

Table 3-5. SCALE Maturity for SFR Analysis

Element	Maturity Level[1]	Comments
Representation and Geometric Fidelity	3	Capability to model reactor designs for the needs of MELCOR/MACCS is available. However there needs to be further assessment work performed
Physics and Model Fidelity	3	Capability exists to model SFR designs to support MELCOR calculations. However there needs to be further assessment work performed
Code Verification	2	Internal SQA program provides coverage for code verification
Solution Verification	2	SCALE has been used for the SFR UAM and been provided with some formal review. Assessments continue.
Model Validation	1	Assessments continue with EBR2
Uncertainty Quantification and Sensitivity Analysis	2	Uncertainties and numerical propagation of errors have been examined extensively for LWR applications though not for Na application

[1]Maturity Levels

- level 0, little or no assessment of accuracy and completeness and highly reliant on personal judgment and experience;
- level 1, some informal assessment of accuracy and completeness, and some assessment has been made by an internal peer review group;
- level 2, some formal assessment of accuracy and completeness, and some assessments have been made by an external peer review group; and
- level 3, formal assessment of accuracy and completeness, and essentially all assessments have been made by an independent, external peer review group.

3.3. MSR

For MSRs, SCALE will provide fission product inventories, decay heat, tritium produced in salts that contain lithium, power distributions, kinetics parameters, as well as reactivity coefficients for temperature and density feedback. New features for SCALE 6.3 include time-dependent chemical processing model and delayed neutron precursor drift models to allow time-dependent modeling of the molten salt fuel [55]. Improved capabilities include a generic geometry capable of modeling multi-zone and multi-fluid systems, enhanced time-dependent feed and separations, and a critical concentration search. An example of the delayed neutron concentration distribution for fuel flowing through the core and the primary loop is shown in Figure 3-4. Additionally, the thermochemical equilibrium state of the irradiated fuel salt will be generated with ORNL's Thermochimica code with information provided to MELCOR.

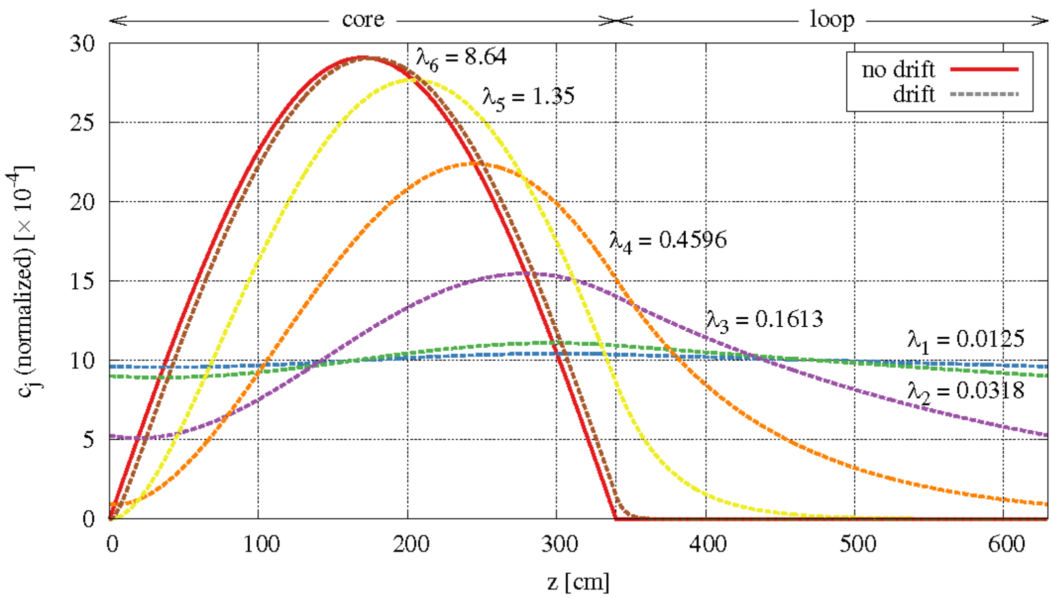

Figure 3-4. SCALE MSR Delayed Neutron Precursor Drift Modeling.

<u>MSR Reactor Physics Considerations</u>

The MSR has a liquid fuel salt circulating through the primary loop. MSR plants also include a significant amount of chemical processes and filtration and feed systems. At this point, the severe accident scenarios for MSRs are not widely understood or agreed upon and thus the reactor physics strategy minimizes development that may or may not be applicable. The streamline history modeling approach developed for the HTGR is also applicable to the MSR, albeit with much faster fuel flow rates, and mass transport of the fuel under irradiation, decay, separation, feed, and temperature effects must be taken into account. The initiating events that are ultimately determined can be verified by comparison to the VERA-MSR integrated multiphysics tool, where convenient tabulated data are provided to MELCOR through SCALE calculations.

MSR reactor physics data from SCALE

SCALE reactor physics calculations can be used to provide the following tabulated data for severe accident analysis of MSR with MELCOR. Note that SCALE may provide approximate spatially-dependent (*r*) quantities allowing for modeling of simple operating histories leading up to the severe accident scenario, as indicated by the dependence on initial time t_0.

1. Isotopics data.
    a. Fission product mass inventory, $m_i(r, t_0)$, where i is an isotope index.
    b. Fission product decay heat, $H_i(r, t_0)$.
2. System power distribution, $P(r, t_0)$.
3. Kinetics data.
    a. Six-group delayed neutron precursor kinetics data, $\beta_j(z, t_0)$ and $\lambda_j(z, t_0)$ including precursor drift where z is the axial location.
    b. Temperature reactivity coefficients, $\alpha_{T_{fuel}}(t_0)$.
    c. Void reactivity coefficients, $\alpha_V(t_0)$.
4. Chemical species data using Thermochimica.

MSR analysis/development tasks

The overarching strategy is to leverage HTGR analysis and development and emerging features in SCALE 6.3 beta 1 to minimize MSR modeling cost.

__Analysis Tasks__

The most recent SCALE 6.3 beta 1 development version includes an MSR modeling capability with multi-compartment material tracking, feed, removal, and neutron pre-cursor drift.

Calculate power, isotopics, and delayed neutron data with TRITON MSR. [SCALE/MSR/A1]
(No task dependencies.)
Calculate the scalar flux, power, and isotopics distribution as a function of core operation using SCALE/TRITON with the new MSR capability in SCALE 6.3 beta 1. Material feed and removal schemes should be provided as input based on assumed chemical processes. The isotopic distribution, power distribution, and properly drifted core-average kinetics parameters calculated in this task are fundamental inputs to MELCOR. Simple core-average temperature and void reactivity coefficients will be calculated. Comparison to vendor, the higher fidelity CASL VERA-MSR core simulator, or other DOE tools would be useful as a code-to-code verification.

Use Thermochimica to calculate species formation in the MSR loop. [SCALE/MSR/A2]
(No task dependencies.)
Use the thermal equilibrium code Thermochimica to calculate the formation of different chemical species in the MSR loop. Provide data to MELCOR regarding the species which exist in the molten salt fuel. Comparisons to vendor or DOE tools would be useful as a code-to-code verification.

__Development Tasks__

Develop ORIGEN library parametrization for MSR. [SCALE/MSR/D1]
(Depends on SCALE/MSR/A1.)
The MSR core depletion in task *SCALE/MSR/*A1 will produce as a byproduct a set of MSR ORIGEN libraries. This development task will determine a reasonable parametrization to collapse all data into a single ORIGEN reactor library capable of reconstructing the core isotopic distribution.

Deliver production-quality ORIGEN reactor libraries for MSR assemblies. [SCALE/MSR/D2]
(Depends on SCALE/MSR/D1.)
Based on the development in *SCALE/MSR/*D1, deliver tested and quality-assured ORIGEN reactor libraries for MSR in the final SCALE 6.3 release. This requires the nomenclature and parametrization for SFR pebble depletion from task *SCALE/MSR/*D1. This task involves creating the template files, production library generation, manual updates, independent testing, and distribution (now and future releases) with SCALE. The existence of these libraries in a SCALE release enables analysts to skip the coupled TRITON depletion modeling in *SCALE/MSR/*A1 and generate isotopics from assumed MSR operational histories.

Thermochimica integration into ORIGEN and ability to filter on species. [SCALE/MSR/D3]
(Depends on SCALE/MSR/A2.)

By integrating the Thermochimica equilibrium chemistry solver into the ORIGEN-API, one can predict the formation of chemical species under different salt conditions. The ORIGEN input will need to accept temperature information for materials as well as extend the elemental filter mechanism to operate on species. Automatically generate the species information MELCOR needs.

Ability for ORIGEN to handle length/time/velocity conversions and "stage" modeling. [SCALE/MSR/D4]

(Depends on SCALE/MSR/A1.)

Simple flowing system models could be constructed in ORIGEN with two minor additions. The first is the calculation of time variables from velocity and length variables, e.g. where one could define a length scale for a given stage and a velocity through that stage in order to calculate the residence time. The stages would be linked together to form loops or lines to tanks. Slugs of fuel can be initialized at the "inlet" of any stage. Directly generate all data MELCOR needs from this representation of the MSR problem.

Calculation of core distributions for MELCOR from large-scale core calculations. [SCALE/MSR/D5]

(Depends on SCALE/SFR/D4.)

The ORIGAMI Automator has been used to generate MELCOR data for site level 3 PRA based on actual assembly shuffling and spent fuel pool movements. This task would implement an extension for inventory analysis under various operating conditions and histories (e.g. material removal and feed) to facilitate confirmatory calculations by NRC staff.

<u>PCMM Characterization</u>

The PCMM process was applied to MSR modeling capability as shown in Table 3-6. This is a preliminary evaluation of the maturity levels for the SCALE code. Note that this evaluation applies to all molten salt reactor types listed in Table 1-1 (MSR, MSPR, MFSR, and MCSR).

Table 3-6. SCALE Maturity for MSR Analysis

Element	Maturity Level[1]	Comments
Representation and Geometric Fidelity	2	SCALE 6.3 includes a translation of the ChemTRITON capability into TRITON-MSR, described in a peer-reviewed journal article, which allows initial characterization of MSR designs to support MELCOR data needs. However, further assessment/validation work is required to assess accuracy limits of the geometric representation.
Physics and Model Fidelity	1	Higher-fidelity solutions are possible through VERA-MSR. Neutronics and depletion physics are the same as in the rest of SCALE, which should receive 2 or 3, however the fluid flow model is highly simplified, and designed to be applicable for estimating fuel cycle parameters (e.g. thorium feed required for a particular design). Assessment of the accuracy compared to higher-fidelity solutions are possible through VERA-MSR.
Code Verification	2	SCALE SQA requires review of implementations by an external party not involved in the development of that particular capability (hence external). However, this does not approach the rigor for LWRs of implicit external verifications by one of the thousands of code users who have received and used SCALE for LWR analyses.
Solution Verification	2	SCALE SQA requires review of capabilities by an external party not involved in the development of that particular capability (hence external). However, this does not approach the rigor for LWRs of explicit external verifications as part of a document such as an NRC NUREG.
Model Validation	1	Some comparisons of ChemTRITON to MSRE were made. The methodology in TRITRON-MSR is essentially the same with some improvements but re-evaluation has not yet been formally performed.
Uncertainty Quantification and Sensitivity Analysis	1	Uncertainty and sensitivity capabilities for any model in SCALE are available through SCALE/Sampler, however specific sensitivity and uncertainty analyses for the MSR have not been performed yet.

[1]Maturity Levels

- level 0, little or no assessment of accuracy and completeness and highly reliant on personal judgment and experience;
- level 1, some informal assessment of accuracy and completeness, and some assessment has been made by an internal peer review group;
- level 2, some formal assessment of accuracy and completeness, and some assessments have been made by an external peer review group; and
- level 3, formal assessment of accuracy and completeness, and essentially all assessments have been made by an independent, external peer review group.

4. MACCS DEVELOPMENT PLANS FOR NON-LWRS

The MELCOR Accident Consequence Code System (MACCS) suite is used to model atmospheric releases of radioactive materials into the environment and the subsequent consequences of such releases. MACCS is the only tool for modeling within a probabilistic framework for all the technical areas in the ASME/ANS RA-S-1.3-2017 Standard for Radiological Accident Offsite Consequence Analysis (Level 3 PRA) to Support Nuclear Installation Applications [10]. These include (1) radionuclide release, (2) atmospheric transport and dispersion, (3) meteorological data, (4) protective actions and site data, (5) dosimetry, (6) health effects, (7) economic factors, and (8) conditional consequence quantification and reporting.

MACCS has primarily been used for analysis of consequences of atmospheric releases from accidents at conventional large LWRs. MACCS is a very flexible code system and its input decks can generally be made plant-specific, site-specific, and accident-specific by modifying a subset of the hundreds of input parameters and the handful of input files. MACCS can also be used for analyzing atmospheric releases from spent fuel pool accidents, dry cask storage accidents, and accidents involving multiple release sources, each with their own accident timeline. For consequence analysis, some of the different characteristics of non-LWRs may be reasonably addressed by modifying selected MACCS input parameters and input files. However other differences may be better addressed with MACCS code changes beyond just changing input parameter values. An evaluation was conducted [56] by the MACCS code developer, Sandia National Labs, of non-LWR-specific modeling challenges for MACCS and based on this in part, several areas of MACCS model development are either underway or planned for the near future. These include the following tasks shown in Table 4-1 which are identified by a task number for cross-referencing in the companion spreadsheet with resource estimates. Several tasks are design-specific and can therefore potentially be prioritized based on when NRC expects to receive an application for a given design type. The list also includes several tasks which are technology-neutral and are applicable to non-LWRs because of their potential site/location-related issues. These tasks are described in more detail in Sections 4.1 and 4.2.

Table 4-1. MACCS Non-LWR Development Plan Start Dates.

Reactor Type/ Development Item (DI)	Phenomenological Area (MACCS)	Description of Tasks (needs)	FY18	FY19	FY20
Technology-Neutral (CA1)	Atmospheric Transport and Dispersion	**Near-Field Transport:** Improve MACCS near-field atmospheric transport and dispersion capability to better treat building wake effects in the near field given the need for probabilistic dose calculations closer to non-LWRs relative to large LWRs.		✓	
SFR (CA2.1)	Radionuclide Release	**Radionuclide Screening:** Perform a screening analysis to identify which subset of radionuclides to include in MACCS calculations for each non-LWR type given the different mix of radionuclides that may be released in accidents from each type.		✓	
HTGR (CA2.2)				✓	
MSR (CA2.3)				✓	
FHR (CA2.4)				✓	
SFR (CA3.1)	Radionuclide Release, Atmospheric Transport, and Dosimetry	**Radionuclide Size, Shape, and Chemical Form and Impact on Atmospheric Transport and Dosimetry:** Evaluate potential differences in radionuclide releases from non-LWRs relative to LWRs including different aerosol size distributions, shape factors, and chemical forms. Based on the evaluation, improve MACCS capabilities for atmospheric transport and dosimetry to appropriately capture these issues for probabilistic consequence analysis. If necessary, consider a state-of-practice resistance model for dry deposition.			✓
HTGR (CA3.2)					✓
MSR (CA3.3)					✓
FHR (CA3.4)					✓

Reactor Type/ Development Item (DI)	Phenomenological Area (MACCS)	Description of Tasks (needs)	FY18	FY19	FY20
MSR (CA4)	Dosimetry and Health Effects	**Tritium Modeling:** Develop MACCS model and/or dosimetry updates to better account for the unique behavior of tritium which is very mobile and can enter biological systems as part of water and organic molecules.		✓	
Technology-Neutral (CA5)	Atmospheric Transport and Dispersion	**Radionuclide Evolution in the Atmosphere:** Identify whether non-LWR accident releases may be more subject to evolution in the atmosphere relative to LWR releases based on differences in hygroscopic properties or potential for chemical reactions during transport.		✓	
Technology-Neutral (CA6)	Decontamination	**Decontamination Modeling:** Based on the potential for non-LWRs to be sited closer to developed/urban lands, develop updated decontamination costs, durations, and dose reduction factors to account for the differences in decontaminating more urban areas relative to the generally rural areas where most large LWRs are sited.			✓
Technology-Neutral (CA7)	Chemical Hazards	**Chemical Hazards:** Identify whether non-LWRs themselves, or because of their potential collocation with industrial processing plants, create greater likelihood of chemical releases to the environment. If appropriate, update MACCS to integrate CHEM_MACCS for probabilistic calculations of offsite consequences of chemical releases.			✓

The MACCS code suite [11, 12] has been under active use and development over several decades. The suite of codes includes the user interface, WinMACCS, and various pre- and post-processor codes including MelMACCS [13], SecPop [14], COMIDA2 [15], and an animations tool AniMACCS. MelMACCS is a pre-processor code that converts source term data from MELCOR into MACCS format. SecPop is another pre-processor code that facilitates use of site-specific population, land use, and economic data. The COMIDA2 pre-processor is used to provide food chain input parameters for MACCS ingestion dose calculations. The MACCS animations tool, AniMACCS, enables visualization of atmospheric dispersion and resulting air and ground concentrations around a site for a given weather trial. All of these MACCS pre-processor, post-processor, and utility codes would be used with MACCS for non-LWR consequence analysis.

MACCS is uniquely suited for consequence analysis of non-LWRs because of its flexibility and broad range of models and phenomena considered. Other computer codes are available to compute offsite doses and they have some overlap in modeling areas with MACCS. However none consider such a wide spectrum of modeling areas and types of consequence outputs. For example, many models are available which treat atmospheric dispersion and calculate doses at different locations. However, the MACCS code suite is the only modeling tool which considers the full range of protective actions (evacuation, sheltering, relocation, ingestion of potassium iodide, decontamination, etc.), the full range of weather variability, and the full range of consequence measures (including doses, fatality risks, economic costs, land contamination, and societal consequences). MACCS also has a built-in capability for uncertainty analysis which makes it unique relative to other codes. The RADTRAD code has some overlap with MACCS in that it may be used to calculate a site boundary dose without protective actions. RASCAL is another code which can calculate offsite doses and it is used in incident response situations by NRC's Operations Center during drills and emergencies. RADTRAD and RASCAL are actively developed, have wide user bases, and support various regulatory applications. Their application to non-LWR analysis and associated code development needs will be discussed in a separate report, Volume 4. RADTRAD and RASCAL are not as well suited for probabilistic consequence analysis because both are much more constrained in their capabilities for radionuclide release in that much of their source term information is hard-coded and not easily adapted by users. MACCS is much more flexible in its ability for users to modify source term information. MACCS considers realistic protective actions which aren't modeled in RADTRAD and RASCAL. And finally, MACCS computes the full spectrum of consequence output types which enable specific applications. Only MACCS computes economic costs which are used in regulatory cost-benefit type-applications and only MACCS computes fatality risks for comparing to NRC's quantitative health objectives.

MACCS is subject to software quality assurance practices which include model verification and validation, bug reporting and correction, documentation, user support, and training. Unlike with MELCOR, there is no database of experimental and operation history on non-LWR accidents that can be used to validate the models. The Fukushima accident in 2011, although not at a non-LWR, has been used for benchmarking certain features of MACCS and this process is ongoing separate from the MACCS non-LWR code development process. Several design-neutral components of MACCS have been tested against experimental data or against other codes. The

MACCS Gaussian plume segment atmospheric transport model has been benchmarked against other more complicated ATD models in NUREG/CR-6853 [57] and has performed well for calculations considering a large number of potential weather trials. The typical sets of input parameters which characterize vertical and cross-wind atmospheric dispersion rely on tracer experiments.

Code Maturity

A method for assessing the maturity level of computational modeling and simulation was developed at Sandia National Laboratories and has been applied to MACCS in estimating the level of readiness of the code for application to non-LWRs. The Predictive Capability Maturity Model (PCMM) provides a means of addressing six important elements of modeling and simulation (1) representation and geometric fidelity, (2) physics and material model fidelity, (3) code verification, (4) solution verification, (5) model validation, and (6) uncertain quantification and sensitivity analysis. In general, the MACCS code suite scores well for the various elements.

Table 4-2. MACCS Maturity for Non-LWR Analysis

Element	Maturity Level[1]	Comments
Representation and Geometric Fidelity	2	MACCS uses a polar grid geometry which is generally quite sufficient for modeling offsite releases and consequences.
Physics and Model Fidelity	2	MACCS models are generally physics-based and independent peer review has been conducted for several MACCS applications including SOARCA.
Code Verification	2	MACCS meets software quality assurance standards and undergoes code verification testing as new features are added.
Solution Verification	2	Numerical effects are considered small; simulations can generally be independently reproduced with similar results.
Model Validation	1	Many models within MACCS have been validated but data is limited.
Uncertainty Quantification and Sensitivity Analysis	2	MACCS supports uncertainty and sensitivity analysis.

[1]Maturity Levels

- level 0, little or no assessment of accuracy and completeness and highly reliant on personal judgment and experience;
- level 1, some informal assessment of accuracy and completeness, and some assessment has been made by an internal peer review group;
- level 2, some formal assessment of accuracy and completeness, and some assessments have been made by an external peer review group; and
- level 3, formal assessment of accuracy and completeness, and essentially all assessments have been made by an independent, external peer review group.

4.1. MACCS Development for Non-LWR Site- and Location-Related Issues

Like small modular reactors, many non-LWRs have potential for being located closer to population centers than typical large LWRs. Non-LWRs may be located near or adjacent to industrial facilities which can take advantage of the process heat supplied by a non-LWR such as a HTGR. These factors correspond with non-LWR vendors desiring to have smaller emergency planning zones and raise the importance of considering certain site- and location-related issues for non-LWR consequence analysis.

4.1.1. Near-Field Atmospheric Transport and Dispersion (Task CA1)

Non-LWR (and SMR) applicants generally desire emergency planning zones (EPZs) much smaller than the plume exposure pathway EPZ for large LWRs, ~10 miles. This is proposed based on claims of non-LWR's and SMR's improved safety characteristics relative to large LWRs including smaller, slower, and less likely accidents. Some have proposed EPZs coinciding with the plant's site boundary which could be on the order of several hundred feet from the plant. While the existing MACCS models can be used to probabilistically calculate dose at any distance, the user manual [11, 12] cautions against using the existing MACCS model with typical input parameters at distances closer than 500 m from the plant. Probabilistic calculations of dose at the site boundary for non-LWRs need to adequately address near-field atmospheric dispersion phenomena. These include building wake effects and the potential for recirculation cavity zones that can cause higher air concentrations and doses in such zones compared to the standard area-source treatment currently in MACCS. An NRC team with contractor support is evaluating options to improve MACCS's capabilities for near-field atmospheric dispersion which include integrating other models into MACCS or identifying a more simplistic but conservative approach.

Current MACCS Near-Field Atmospheric Transport Capability

MACCS currently includes a simple model for building wake effects within its Gaussian plume segment atmospheric transport model which scales the initial dimensions of each plume segment based on the dimensions of the building or complex of buildings from which the radionuclides are emitted. The standard guidance is to assume that ground-level concentrations at the edges of the building and the concentration directly above the centerline at the top of the building are 10% of the centerline plume concentration. This guidance translates into assuming the initial crosswind dispersion parameter, σ_{y0} = 0.23 x building width and the initial vertical dispersion parameter, σ_{z0}= 0.47 x building height immediately downstream of the building. The MACCS User Guide suggests this simple building wake model should not be used at distances closer than 500 m with typical sets of input parameters.

Options for Improved Near-Field Atmospheric Transport Capability

Several models are available at differing levels of complexity for calculating air concentrations and deposition in the near-field, close to buildings and structures. These include Lagrangian particle tracking models with 3-dimensional wind fields developed using computational fluid dynamics, Lagrangian particle tracking models with empirically developed 3-dimensional wind fields, and modified Gaussian plume segment models with time-dependent 1-dimensional wind fields. This section describes the different types of models as well as their advantages and disadvantages for potentially integrating into MACCS.

CFD models, whether Reynolds-averaged Navier Stokes (RANS) or large eddy simulation (LES), are considered the most accurate models for calculating complex fluid flows. For application to near-field atmospheric transport, these CFD models would be used to develop 3-dimensional wind fields at the micro-scale, on the order of meters or tens of meters. Then a Lagrangian particle tracking model would be used to calculate resulting air and ground concentrations considering other phenomena including dry and wet deposition. The high accuracy of a CFD-developed 3-dimensional wind field comes at a cost of requiring significant computational resources, user expertise to set up and run problems, and developer expertise to implement the models within MACCS. In addition, CFD models require a detailed grid and set of boundary conditions for each individual facility/site modeled and that level of detail may not be available for a future nuclear site that has not been built yet. The three-dimensional wind field developed using CFD could be highly dependent on the initial and boundary conditions including atmospheric stability, orientation of initial wind direction relative to the building complexes, air temperature, precipitation, etc. These initial and boundary conditions can change significantly over the life of the nuclear plant modeled.

The Quick Urban & Industrial Complex (QUIC) Dispersion Modeling System [58] is an example of a Lagrangian particle tracking model with an empirical model for calculating 3-dimensional wind fields, thus making calculations faster and less computationally intensive relative to CFD calculations of wind fields. Developed by Los Alamos National Laboratory, QUIC is used for modeling chemical, biological, and radiological dispersion on building to neighborhood scales. QUIC accounts for the effects of buildings in an approximate way and provides more realism than non-building-aware dispersion models. Like CFD approaches, QUIC requires a model of each unique site/facility to be developed and it needs a large set of wind data to characterize weather variability. A model like QUIC also has the caveat that calculations may be quite sensitive to the highly variable initial and boundary conditions.

Two modified Gaussian plume models are commonly used for approximating near-field transport of pollutants. The first is the Ramsdell-Fosmire model [59] which modifies the straight-line Gaussian plume model to account for enhanced dispersion near a building at low and high wind speeds. The Ramsdell-Fosmire model is used in the ARCON96 code [60] developed by Pacific Northwest National Laboratory for the NRC for estimating air concentrations at ventilation intakes for control room habitability during a design basis accident. Ramsdell-Fosmire modifications to the Gaussian plume dispersion equation include additional crosswind and vertical dispersion from low wind speed phenomena, primarily plume meander, as well as high wind speed phenomena, particularly, building wake effects.

The other modified Gaussian plume model is the Schulman-Strimaitis-Scire model, PRIME (Plume Rise Model Enhancements) [61], developed for the American Meteorological Society/Environmental Protection Agency Regulatory Model (AERMOD) [62] for estimating environmental pollution levels. The PRIME model for plume meander uses a weighted average of uniform dispersion in all directions and the standard Gaussian dispersion equation. For building downwash and wake effects, PRIME uses a weighted average of a concentration within the building wake and a standard Gaussian plume concentration. The weighting factor depends on several ratios which consider building dimensions and several distances of interest.

Both modified Gaussian plume models are advantageous in that they would be more straightforward for integrating into MACCS and for using by MACCS analysts. In addition, they do not require such detailed geometry for all the different buildings on the site of interest. And while modified Gaussian plume models would not be considered as accurate as the more advanced Lagrangian models, the reduced accuracy is likely less critical given the probabilistic nature of MACCS calculations. Applications that are focused on a specific site and a specific set of weather data may warrant complex models whereas MACCS, which is used for current and future hypothetical sites and for the full range of potential weather conditions, tend not to need quite as much accuracy. Current practice with MACCS is to run on the order of 1,000 weather trials and then to report average consequence measures over the large number of weather simulations.

4.1.2. Evolution of Radionuclide Properties in the Atmosphere (Task CA5)

Current MACCS atmospheric modeling treats particle deposition behavior consistently for a given chemical group and particle size bin as they disperse through the atmosphere and interact with rainfall. However, in reality, particles evolve as they transport through the atmosphere because of either hygroscopic properties or chemical reactions. These processes may impact particle deposition velocity, particularly for an element like iodine. Iodine could be converted from a gaseous form to an aerosol form, or vice versa, following the release. Such changes can result in faster or slower deposition than would be expected if the transformation did not occur. Evolution of deposition behavior, primarily for iodine, is already believed to occur in the case of an LWR release. Deposition behavior for a non-LWR could be influenced by other atmospheric chemical transformations if the released chemical forms were substantially different than for an existing LWR. Therefore, a task is planned to evaluate the different non-LWR technologies to identify the extent to which their released radionuclides could transform in the atmosphere and how significantly deposition behavior could be altered as a result. This task is not proposing an experimental research program; rather it just seeks to evaluate whether this phenomena may be more important for certain non-LWRs relative to large LWRs.

4.1.3. Decontamination Modeling (Task CA6)

MACCS uses a relatively simple approach for modeling the durations, costs, and effectiveness of decontamination efforts in the long-term phase of recovery from a nuclear power accident. MACCS enables different levels of dose reduction and requires a cost and duration for each level for two types of land, farmland and non-farmland. The technical basis for commonly used MACCS decontamination input parameters stems from analysis of mostly rural and suburban land. Non-LWRs have potential for siting much closer to urban land which is full of complex structures and materials. Modeling decontamination for urban land may require unique models or input parameters for existing models to appropriately capture the costs and durations of the process. This task proposes a literature review to identify the state-of-practice for modeling decontamination costs, durations, and effectiveness for urban lands. This task is not specific to non-LWRs by design; rather it applies to non-LWRs by virtue of their potential siting in more urban areas relative to large LWRs.

4.1.4. Chemical Hazards

MACCS models radiological releases to the environment. If non-LWRs themselves, or because of their potential collocation with industrial processing plants, create greater likelihood of chemical releases to the environment, additional codes and models may be needed to also consider non-radiological public health impacts. Back in the 1990s, the CHEM_MACCS tool was developed for probabilistic calculations of offsite consequences from chemical releases [63]. A development team at Sandia National Laboratories modified the existing MACCS code at that time for this purpose by removing subroutines associated with long-term exposures (the CHRONC module) and with radioactive decay, and then added models and equations unique to chemical hazards. This CHEM_MACCS code could be explored for potential use with non-LWRs.

4.2. MACCS Development for Non-LWR Design-Specific Issues

4.2.1. Radionuclide Screening (Task CA2)

The existing MACCS radionuclide library file contains data for 825 radionuclides, and this library should be sufficient for non-LWRs. However, a screening of this large set of radionuclides is needed to identify a subset to include in MACCS calculations. MACCS currently allows up to 150 radionuclides in a calculation, however commonly a smaller number is used. For example, 69 different radionuclides were included in MACCS calculations for the SOARCA project. The selection of radionuclides for consequence analysis should consider several factors including the core inventory, physical and chemical properties including the nature of radioactivity and volatility, atmospheric transport factors including deposition properties, and biological factors including uptake, biological half-life, and specific organ effects. It seems possible or even likely that a different set of radionuclides may be needed for each different non-LWR design. The formation of activation products, especially within the coolant, could be important for consequences and would be unique to the different non-LWR types. More generally, the isotopic inventory, if very different than that of an LWR, may need to be reevaluated to ensure that all important isotopes are included in the analysis. For example, Na-23, the dominant naturally occurring isotope of sodium, can be activated by a single neutron capture to create Na-24, which has a half-life of 15 hours and decays by emitting beta particles to form Mg-24. Na-24 may need to be included in consequence analyses of sodium-cooled reactors. Similarly, K-39 can be activated to K-40 by a single neutron capture; however, K-40 has a half-life that is over a billion years, so it would not contribute significantly to consequences. Several molten salts have been proposed as reactor coolants. These need to be examined to determine whether important activation products might be produced during reactor operation.

4.2.2. *Chemical Form, Particle Size, and Shape Factor of Radionuclides and Impact on Atmospheric Transport and Dosimetry (Task CA 3)*

Radionuclides released into the environment from a non-LWR accident might be in different chemical forms than from LWR accident releases. Differences are possible particularly in SFRs for cesium and iodine, often the two most important radionuclide elements for offsite consequences. As an example, the sodium within the pool of an SFR may interact with iodine such that the dominant chemical form of iodine could be sodium iodide (NaI) rather than cesium iodide (CsI). This could then cause more of the released cesium to be in the form of cesium hydroxide (CsOH) as opposed to CsI or cesium molybdate (Cs_2MoO_4).

Differences in chemical form are also possible when the oxygen potential within the reactor coolant system is substantially different than that of a LWR, where steam is usually the dominant gas-phase component. If, for example, a non-LWR has a highly reducing chemical environment, some of the emitted radionuclides might be in a more reduced rather than an oxide form. This is likely the case for SFRs because of the tendency of sodium to react with available oxygen.

Different chemical forms of radionuclides are potentially important because they affect choices for dose conversion factors and thus affect doses to individuals and resulting consequences. Different chemical forms of radionuclides may change their solubility in the human body which can impact inhalation doses based on the time duration they could be in the lungs or ingestion doses based on how much could be absorbed in the digestive tract. Therefore, a task is planned to explore this further and if needed, develop updated dose conversion factor files. The task could involve use of FGR-13PAK, which is the FORTRAN source code and data files distributed by EPA in the Federal Guidance Report No. 13 CD Supplement.

Current best practice is to model dry deposition using a linear regression equation based on an expert elicitation process [64] that accounts for aerodynamic particle diameter, surface roughness, and wind speed. In this equation, particle diameter typically comes from MELCOR source term results which distribute the released radionuclides into one of ten different particle size bins. MACCS modeling best practice approach is to use the average wind speed over the year of weather data and one surface roughness value based on a weighted average of the different land types within the calculational domain.

Other factors are known to influence dry deposition processes including aerosol shape factor. This may be an issue for non-LWRs, specifically HTGRs. HTGRs use graphite as a structural material and as the neutron moderator. Air ingress accidents for HTGRs expose graphite to an oxygen-containing environment that can produce severe oxidation at high temperatures. This oxidation can produce non-spherical aerosol particles with a shape factor significantly greater than unity. This phenomenon is of potential importance to consequence analysis because it can impact dry deposition. Aerosol dynamic shape factor is a user input for MELCOR and was included as an uncertain parameter in the SOARCA Peach Bottom, Surry, and Sequoyah uncertainty analyses [20]; while these studies shed light on the parameter's importance in LWR severe accidents, dynamic shape factor may be more important for HTGRs and potentially other non-LWRs. Currently the MACCS code suite does not account for dynamic shape factor. The MelMACCS preprocessor code, which converts MELCOR source term output into MACCS-formatted input, calculates particle dry deposition velocities assuming a shape factor of unity (spherical). The impact of particle shape factor depends on particle size since different particle sizes are influenced by the different deposition mechanisms including Brownian diffusion (smallest particles), gravitational settling (largest particles), and impaction and interception.

Another difference for certain non-LWRs relative to large light water reactors is that source terms from non-LWRs may have significantly smaller particle sizes. Large LWR source terms often have aerosol particles in the range of 0.1-40 microns in diameter, however non-LWR releases could have particles closer to the tens of nanometers range. Like in the task above related to the impact of chemical form on dosimetry, this issue of smaller particle sizes may also impact dosimetry. Typical dose conversion factors might assume a median particle diameter of 1 micron so if non-LWRs have the majority of particles released in the tens of nanometers range, the dose conversion factors may need to be regenerated.

A newer approach for dry deposition modeling has been studied in the atmospheric modeling community of practice referred to as a resistance model. Using an electrical analogy, this model assumes that the resistances that affect the particle flux in the quasi-laminar sub-layers of the atmosphere can be combined to consider local features of the mutual influence of inertial impaction processes and of turbulent ones. This type of model has been compared to experimental data from literature and has been considered to capture the main dry deposition phenomena and deposition surfaces with good agreement [65]. The existing MACCS deposition model uses one weighted-average surface roughness value for the entire region of interest whereas the resistance model would be able to consider grid element-specific surface roughness. While this type of model would be equally applicable to any reactor type or size, it may be highly useful for non-LWRs if their dry deposition modeling may be different considering chemical forms and particle sizes.

A task is planned to evaluate the adequacy of the existing MACCS dry deposition model and identify whether the newer resistance model is needed to appropriately address the characteristics of non-LWR radionuclide phenomena. This could result in modifying MACCS or the source term preprocessor code, MelMACCS. Currently, as discussed in NUREG/CR-7161 [66], MelMACCS calculates dry deposition velocities based on a number of parameters including aerodynamic particle diameter, surface roughness, and wind speed; however, the equations could be modified to also account for shape factors.

4.2.3. Tritium Modeling (Task CA4)

Tritium is a radioactive isotope of hydrogen and is formed in nuclear reactors by neutron absorption and ternary fission events. Tritium is particularly important because it can be produced in large quantities during normal operation and because it diffuses rapidly through metals at elevated temperatures. While HTGRs produce more tritium than LWRs, MSRs produce significantly more [67]. Lithium-containing MSRs primarily produce tritium from neutron absorption reactions of ^{6}Li and ^{7}Li.

From a consequence analysis perspective, tritium could be treated as a separate chemical class from the existing set of classes assuming this is consistent with MELCOR accident progression and source term modeling. This would involve some code changes to the MelMACCS preprocessor code which converts MELCOR source term results into MACCS-formatted input files. While tritium can be released to the environment in different forms, it is commonly treated as tritiated water. Dose conversion factors might also need to be modified to account for the unique ways that tritiated water interacts with the human body via inhalation, ingestion, and skin absorption [68].

5. CONCLUDING REMARKS

This report provides the technical approach and computer code development plans applicable to non-LWR technologies for severe accident progression, source term, and consequence analysis. The computer codes include MELCOR (accident progression and source term analysis), MACCS (consequence analysis), and SCALE (reactor physics). This report provides a review of the current extensive modeling and simulation capabilities of these codes and identifies and addresses the modeling gaps to demonstrate functional readiness for confirmatory analysis. The status of code readiness together with validation and data needs supports the delineation of the required detailed development tasks for each computer code. The selection criteria for each code (e.g., staff familiarity, domestic and international use, and life cycle development and maintenance costs) are discussed.

The connection and information flow between the codes is captured in the evaluation models for generic technologies and supports the long-term goal of developing regulatory source term for the various design types. The evaluation model outlines the requisite steps to perform a confirmatory safety analysis for licensing basis events.

This document represents the current and best knowledge of technical needs for development of the MELCOR, MACCS, and SCALE codes for application to advanced, non-light water reactor technologies. This is a living document that will be updated as more experience is gained and as new information regarding specific reactor design needs comes to light.

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APPENDIX A. MELCOR MODELING OF HTGRS

A.1. INTRODUCTION AND BRIEF HISTORY

Gas-Cooled Reactor (GCR) designs have existed in concept for most of the history of commercial nuclear power. There is a considerable amount of accrued operating experience with GCRs both domestically and world-wide. The United Kingdom, France, Germany, Japan, and China have all operated experimental and/or power-producing High-Temperature Gas-Cooled Reactors (HTGRs) and GCRs, while the U.S. has operated two installations (Peach Bottom 1 and Fort St. Vrain). Additionally, there were considerable efforts in the mid-1980's involving the U.S. Department of Energy (DOE) to develop a simpler, safer alternative to LWRs for purposes of commercial power production. The result was the Modular High Temperature Gas Reactor (MHTGR), which could be counted among the earliest HTGR design iterations in the U.S.

HTGRs generally represent evolutions in design from GCR forerunners. The HTGR was selected from among the Very High Temperature Reactor (VHTR) candidate designs to become the Next Generation Nuclear Plant (NGNP) pursuant to the energy policy act of 2005. That initiative was never fully realized, but it did raise the issue of licensing for HTGRs. A South African pebble-bed type HTGR program similarly raised such interest. Beginning in 2008, MELCOR was modified to model both the pebble-bed and prismatic HTGR designs with special attention to severe accident phenomenology and the findings of a Phenomena Identification and Ranking Table (PIRT) study conducted in 2008 [28].

A.2. DESIGN ASPECTS

The original DOE programmatic objectives for the HTGR led to certain high-temperature and safety characteristics that are distinct from earlier but similar thermal-spectrum, graphite-moderated, helium-cooled designs. For purposes of MELCOR modeling and the present discussion, an HTGR is thought of as a tri-isotropic (TRISO) fueled, thermal spectrum, graphite-moderated, helium-cooled system intended to either produce power or generate process heat (or both). The fuel element design is that of either the pebble-type (spherical elements) or the prismatic-type (cylindrical elements). General design features pertaining to HTGRs include:

- Low power density (less power per unit volume of core material)
- Large ceramic (graphite) core inventory (large heat capacity)
- Large, negative Doppler coefficient of reactivity
- Chemically and neutronically inert helium coolant
- Passive decay heat removal (inherent in design)
- Brayton power cycle facilitated by helium turbomachinery

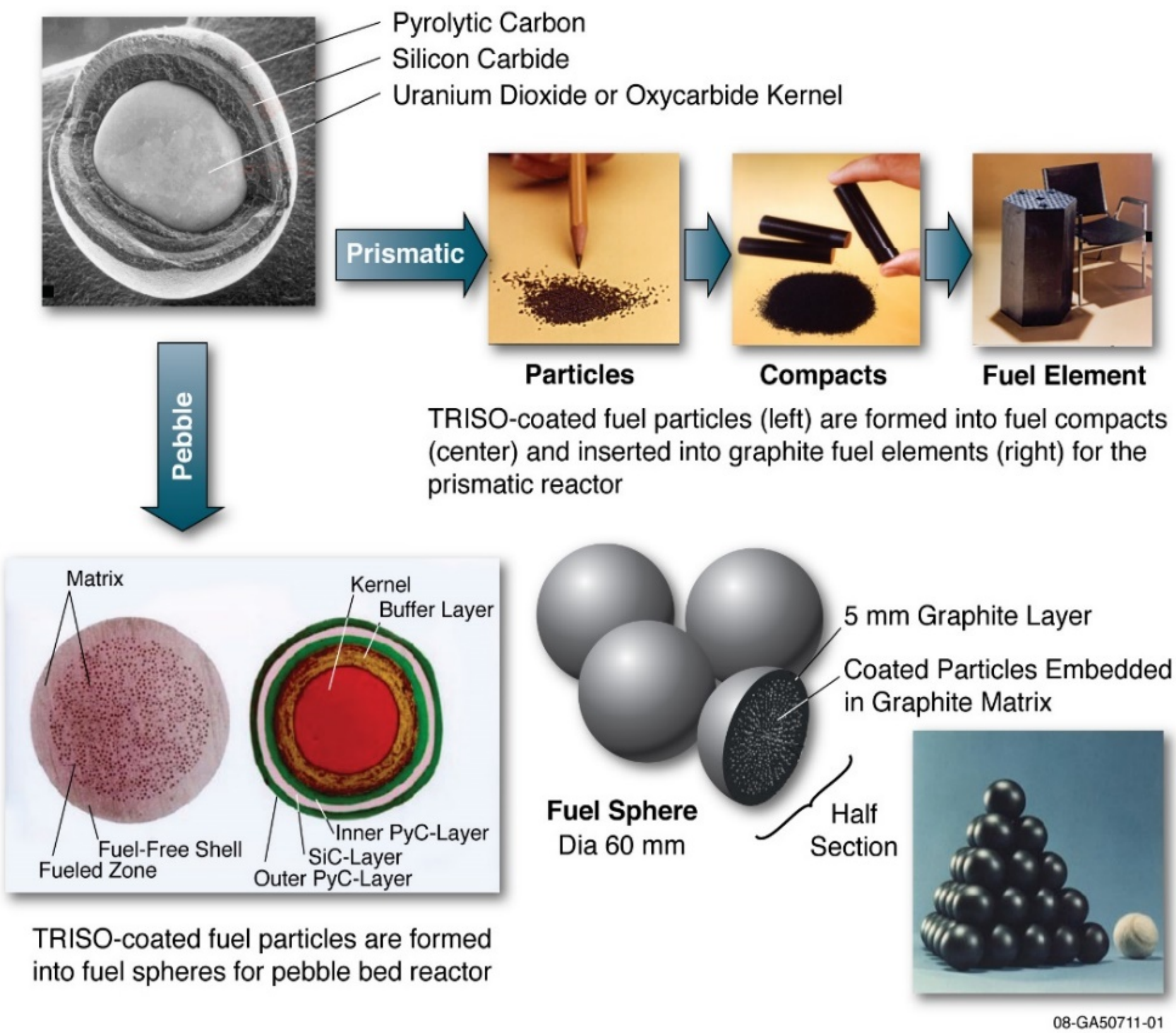

Figure A-1. HTGR fuel element designs [4]

The two types of fuel element design are pictured in Figure A-1. The small fuel kernels (typically UCO or UO_2) are coated in three layers of material (inner porous carbon buffer, middle silicon carbide, outer pyrolytic carbon). The inner layer is designed to trap gaseous fission products and absorb recoil energy. The silicon carbide layer – barring manufacturing defects – provides structural stability against thermal and mechanical stresses. The outer layer is an additional barrier to fission product release. These TRISO particles are packed into a graphite matrix that is spherical for a Pebble Bed Reactor (PBR) or cylindrical for a Prismatic Modular Reactor (PMR). Loose pebbles form a fueled region in the PBR core. Fuel compacts packed into hexagonal graphite blocks for a fueled region in the PMR core.

Both PBR and PMR designs typically have large graphite reflectors at the core interior and the core periphery (to include the top, bottom, and sides). There are typically control rod channels in the central and side reflectors for purposes of reactivity control. The core, reflector, barrel, and pressure vessel design is such that passive conduction/radiation heat removal is possible even under conditions of pressurized/depressurized loss of forced circulation (P/DLOFC). This passive heat transfer pathway is shown in Figure A-2.

Under normal operating conditions, a compressor forces coolant circulation such that helium exiting the active core is channeled via a cross-duct to the Brayton cycle power-production side of the system (a vessel containing gas turbomachinery). The helium is forced to flow from top to bottom across the reactor core such that, in the event of a PLOFC without a breach in the pressure boundary, natural circulation patterns may be established (colder structure at top, hotter at bottom). These circulation patterns ought to redistribute thermal energy in the core (from bottom to top) while the conduction cool-down occurs. The Brayton power cycle utilizes higher working fluid temperatures and has a higher thermal efficiency relative to the typical LWR Rankine power cycle. When the normal means of thermal energy removal fail, decay heat can be ultimately removed from the vessel via the passive reactor cavity cooling system (RCCS) – pictured in Figure A-2 – which operates by radiation and natural circulation of either air or water.

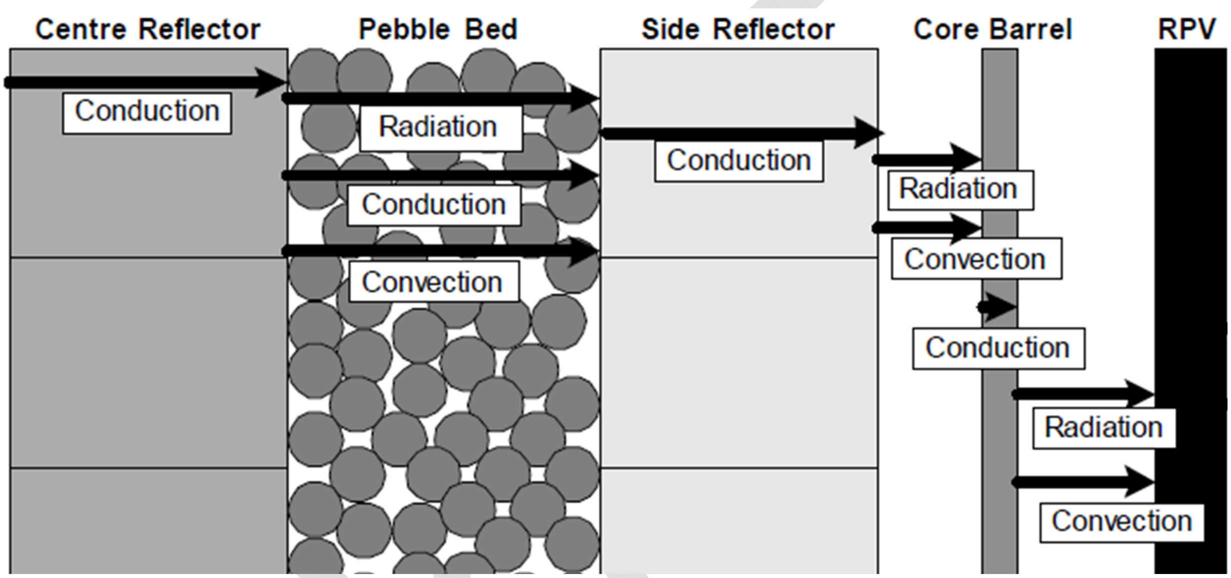

Figure A-2. Passive cooling pathway in HTGRs [69]

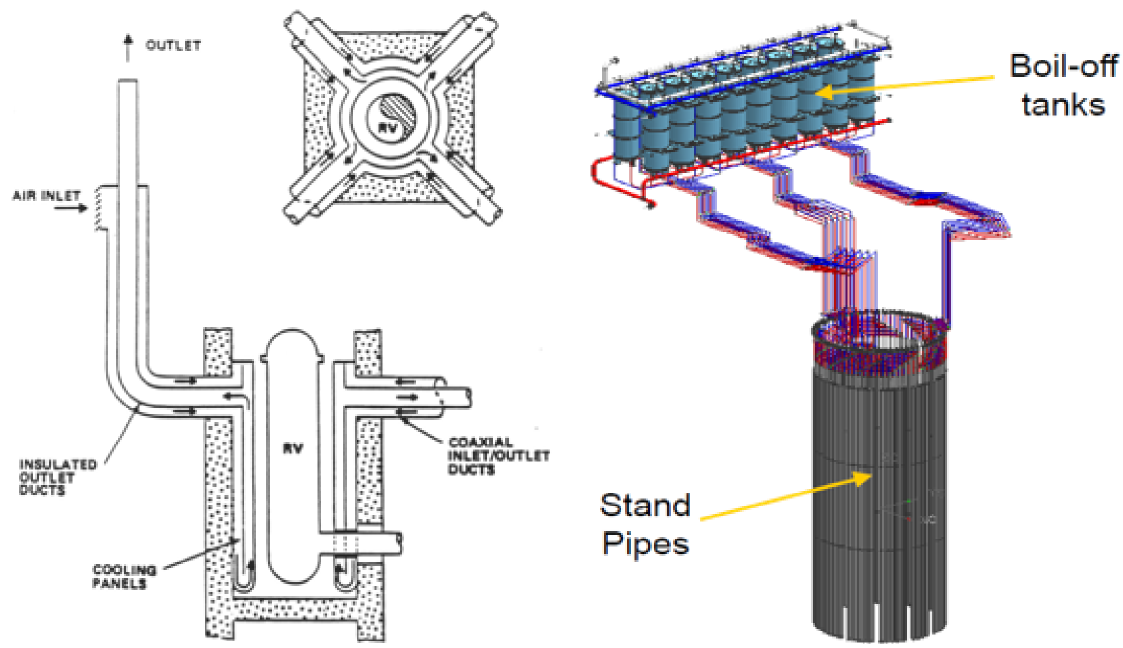

Figure A-3. RCCS strategies in HTGRs

A.3. MELCOR MODELING

Development of the MELCOR models for HTGR application began in 2008 and therefore, at this writing, they have reached a high level of maturity. Models for point reactor kinetics, accelerated steady state initialization, and miscellaneous mechanical models were added to supplement MELCOR's existing capabilities. Core components for both PBR and PMR reactor types have developed as well as models for fission product release from TRISO fuels. Finally, new models for turbulent deposition and particle resuspension were added to complete MELCOR's suite of capabilities for modeling aerosol physics. These HTGR models are documented within the MELCOR Computer code reference manual [8] and user guide. [7] MELCOR is in a 'ready' state and is currently used by researchers around the world in modeling gas reactors [26, 27].

A.3.1. PREVIOUS DEVELOPMENT WORK

Beginning in 2008, active development work began on HTGR modeling in MELCOR. The earliest steps involved a review of gas/graphite properties, models for heat transfer in the core, thermal hydraulics considerations, fuel failure and fission product release, and aerosol physics modeling. Code capabilities and modeling gaps were identified and then addressed in order to obtain a complete working model of an HTGR system.

Core Modeling Capabilities

Subsequently, new reactor types were added to COR including PBR and PMR types which add model components for simulation of either a pebble fuel element or a fuel compact element as and graphite blocks along with a reflector component to represent the central, side, and top/bottom reflectors components in COR.

The PBR reactor type features:

- FU as the fueled part of a pebble fuel element, includes UO_2 as the fuel material and graphite as the "extra fuel material"
- RF (a two-sided component) available for use, graphite is the usual component material
- Imposes a radial fuel temperature profile (notions of peak and surface fuel temperature)
- Enables radial COR cell-to-cell conduction/radiation models (effective bed conductivity)
- Enables packed-bed flow correlations for friction factors, convection heat transfer

The PMR reactor type features:

- FU as the fueled part of a fuel compact element, includes UO_2 as the fuel material and graphite as the "extra fuel material"
- MX (matrix component) representing part of the graphite hex blocks that is "associated" with fuel channels in block
- RF (a two-sided component) available for use, graphite is the usual component material
- Assumed logarithmic radial temperature profile across the MX component.
- Radial COR cell-to-cell conduction/radiation heat transfer, account for hex block gas gap

With respect to oxidation of graphite, air and steam oxidation rate equations were added (subject to rate-limiting by gaseous diffusion as is typical of MELCOR oxidation models). The oxidation characteristics mostly follow from experimental work on the subject. Air oxidation reactions yield carbon monoxide, while steam oxidation reactions may yield carbon monoxide and hydrogen. Note that COR component materials (graphite) may undergo such oxidation.

To model operating transients and certain anticipated transients without scram (ATWS) scenarios, a point kinetics model was added to the COR package. The new capability features:

- Reactivity feedback for fuel (Doppler), and moderator and reflector (temperature, density)
- An ability to spatially-average COR cell temperatures for purposes of feedback
- External reactivity input allowed by control function (CF)
- Kinetics parameters changeable by sensitivity coefficient input

Helium Treatment

With respect to helium equation-of-state and property calculations, an ideal gas approach was chosen as an acceptable approximation (expected < 1% error for anticipated temperature and pressure range of HTGRs). Also, helium property look-up tables are utilized in place of alternative methods.

HTGR Fuel Model

Immediately upon implementing the above improvements (new COR models, oxidation, point kinetics, ideal-gas helium), test input decks were built and run to observe performance. At the same time, further code enhancements and/or modeling strategies were being mapped out. These included:

- TRISO/HTGR fuel element failure
- Fission product release and transport
- Graphite dust generation and transport

The modeling in this area was informed by a couple of key observations pertinent to HTGRs that distinguish them from LWRs in terms of fuel failure and fission product release:

- Failure/release is more spread out in time as there are:
    - Low-level releases during operation due to uranium contamination of fuel matrix and initially defective TRISO particles
    - Releases from fuel occurring more continuously throughout an accident sequence as TRISO particles fail (compare to clad bursts, releases of an LWR)
- Graphite dust particles present in the primary that affect fission product transport

For fission product release in HTGRs, one must consider:

- TRISO particle failure
    - Intact particles: SiC layer acting as a pressure vessel and retaining fission products
    - Failed particles: Initially defective, already-failed or ineffective SiC layer
- Diffusional release from intact and failed TRISO particles
- Graphite dust generation and transport in the primary side
- Uranium contamination of matrix (generation of fission products outside TRISO particles)

Some of the above can only be treated parametrically in the code (i.e. they must be left to the user for specification) or must come from prior analyses with other codes. For example, the fission product inventory typical of HTGRs must come from a burn-up/depletion code such as ORIGEN. Also, core power profiles (radial, axial) and reactivity feedback parameters may need to come from a neutronics code such as PARCS. The initially-failed TRISO particle fraction and the graphite dust generation rate will be required user inputs as no mechanistic models are yet available for implementation. In some cases, certain "initial conditions" of a transient analysis could be ascertained from steady-state MELCOR runs, e.g. fission product distributions in TRISO particles and fission product/graphite dust distribution throughout the primary system.

For TRISO particle failure (failure of an initially-intact SiC-layer of a TRISO particle), a temperature-dependent failure fraction curve that matches key operational/experimental observations was implemented. There are also options for defining a control functions (CF) which allows the user to prescribe a functional dependency derived from available MELCOR state variables. Similarly the user can specify such functional forms using a tabular function (TF) or reading from an external data file (EDF). Note that to obtain steady-state and/or transient fission product distributions, MELCOR uses a general diffusion equation solver (finite difference, temperature-dependent diffusion coefficients) that accepts inputs of fission product yield, core power, fission product decay constants, and diffusion coefficients. The solution accounts for diffusion of fission products from TRISO (intact, initially failed, intact-then-failed, uranium-contaminated) to the carbonaceous matrix, to surrounding graphite, and to coolant. An example output from this model is shown in Figure A-4.

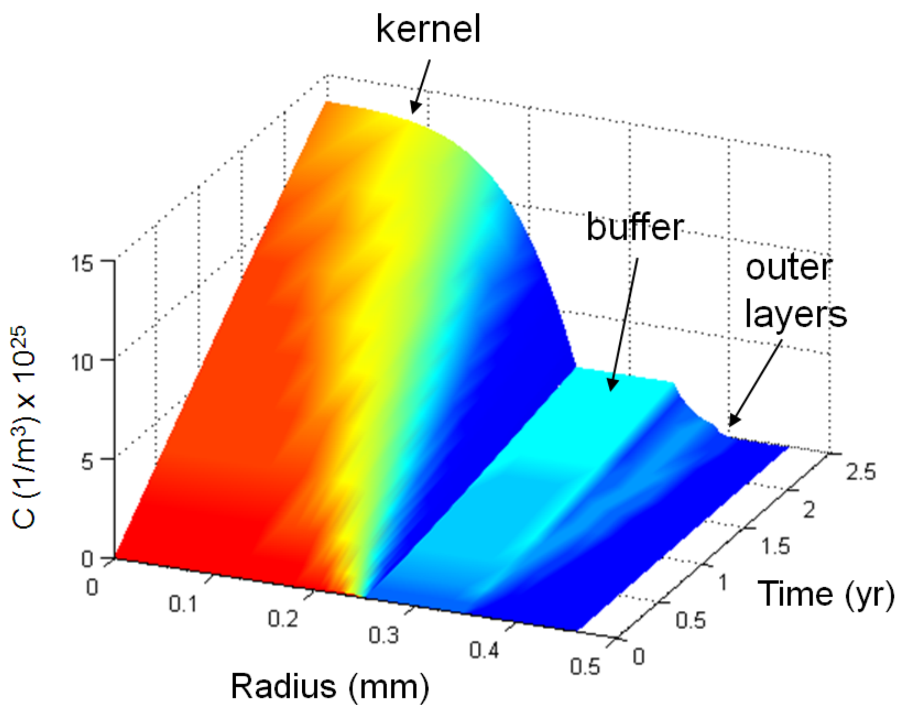

Figure A-4. Example TRISO particle fission product species distribution surface

Total Fission Product Release

Failure of fuel particles will occur at different times in an accident because TRISO particles in the same fuel element may fail at different times (compare to an LWR fuel element that basically releases all its fission product inventory upon clad rupture). The total release fraction in MELCOR is represented as a convolution integral (an integral of the pointwise product of two functions) of 1) the time-derivative of the particle failure fraction, and 2) the release fraction of particles.

Accelerated Steady-State Capability

Since steady-state runs are prerequisite to transient runs, and since HTGRs have a large heat capacity, an accelerated steady-state capability was added to the COR and HS packages in MELCOR. Essentially, the thermal transport properties of COR and HS structures are scaled so as to reach a thermal steady state in less CPU time. More specifically, the volumetric heat capacities of materials in question are reduced for a specified steady-state run time. After the elapsed run-time, material internal energies and heat capacities are restored to their normal values for purposes of a transient run. During a steady-state run (perhaps subsequent to the accelerated steady-state run that establishes a thermal steady-state), the steady-state fission product and graphite dust distributions could also be ascertained using the control volume hydrodynamics (CVH) package and radionuclide (RN) package to track aerosols, radioactivity of fission products, graphite dust, etc.

Miscellaneous Models and Features

There are a few miscellaneous MELCOR features generally applicable to HTGRs that may or may not factor into a given HTGR analysis. These include the turbomachinery model, the integral heat exchanger model, and the counter-current stratified flow model. Of these three, the turbomachinery model is the least developed and the least exercised. It is currently undocumented in the MELCOR reference manual (no description of physics or practical use) but is documented in the MELCOR user guide as recognized Flow Path (FL) package input. The integral heat exchanger and counter-current stratified flow models are well documented both in the reference manual and the user guide.

The turbomachinery model (FL_MCH) – also called the “mechanical model” in the user guide – is meant to allow for a simplified representation of a system component such as a turbine or compressor. It allows the user to define a mechanical model object and to make an association with a flow path. Across the designated flow path, the mechanical model will intervene so as to either provide a pressure boost, modify enthalpies for downstream volumes, or apply forward/reverse flow temperature changes. As it stands presently, the model will apply enthalpy changes based upon the pressure and temperature changes and the isentropic efficiency specified by the user. Work calculations based on pressure difference yield the enthalpy change, and isentropic work is calculated only for a monatomic gas with an assumed specific heat ratio of 5/3. In the phasic velocity equations, the user-supplied pressure change enters in as an explicit source term. Enthalpy changes are affected by altering donor energy density information accordingly. This model, upon further testing and development, could serve to represent certain primary-side and balance-of-plant components in an HTGR system.

The integral heat exchanger model (FL_IHX) simulates the effects of a heat exchanger using two flow path streams and a formulation that implicitly accounts for temperature profiles within the primary and secondary sides of the heat exchanger. The formulation is quasi-steady in nature, and the transformations to hydrodynamic materials occur within the two flow paths in question. Thermal energy removed or added within either flow path is accounted for in the downstream control volume for each flow path. The model is well-documented in the reference manual, and requisite user inputs are described in the user guide. The heat exchanger model could be of use in modeling peripheral systems in an HTGR or in modeling primary-to-secondary heat exchange for systems that use a Rankine power cycle facilitated by a gas-to-water heat exchanger. Parallel and counter-current designs are both available as input choices.

Air ingress scenarios, e.g. due to cross-duct breaks, may be of concern in HTGR accident analyses. To model this situation, one must be able to account for momentum exchange in separated atmosphere flow. This does require two flow paths since the two materials (e.g., air coming in and helium going out) would belong to the same atmosphere phase in a single flow path. The counter-current stratified flow model enables the user to couple two such flow paths and compute momentum exchange of the single-phase, two-component, counter-current flow as consistent with correlations of Epstein and Kenton. The model is well-documented in the reference manual, and requisite user inputs are described in the user guide. Usage of this capability could be key to credibly computing graphite oxidation in HTGR accident scenarios involving a breach of the pressure boundary.

Reactor cavity cooling systems have no specialized code objects and phenomenological models at present. The user can either build such components from control volumes, flow paths, and heat structures, or can impose appropriate boundary conditions that approximate the presence and function of RCCS panels around the reactor pressure vessel (which would presumably be modeled by heat structures itself).

Analysis Strategy

At this point in the code development effort, a solid strategy for HTGR analysis emerged:

- Pre-processing and user input for fission product inventory, neutronics parameters, power profile, TRISO defects/contamination, graphite dust generation, etc.
- Accelerated steady-state analyses to establish a thermal steady state, steady-state fission product and graphite dust distribution in the primary
- Transient analyses
- Consequence analyses if desired

New COR input records were created to facilitate HTGR analytical runs in the order above. These include:

- COR_DIFF handles the steady-state diffusion stage (after a thermal steady-state)
- COR_XPRT handles steady-state transport (fission products, graphite dust in primary)
- COR_DIFT handles transient-mode release

Note that in order to compute steady and/or transient fission product transport and graphite dust transport, models would be required for:

- Turbulent resuspension and deposition
- Size distribution tracking on deposition surfaces
- Fission product and graphite dust interactions

With new records and new models in place, a more detailed outline of an HTGR analysis is:

1. Execute a three-phase steady-state calculation
    a. Establish a thermal steady-state with the accelerated steady-state capability. COR cell and HS structural temperatures reach approximately constant values as a function of steady-state “pseudo-time”
    b. Solve a coupled diffusion problem for fission product distribution and scale the relative amounts of isotopes released
        i. Use temperature-dependent material diffusion coefficients along with COR cell temperatures from (a) above
        ii. Account for intact particle release, initially-failed particle release
        iii. Scale relative results (e.g. based on ORIGEN results)
    c. Solve for fission product and graphite dust distribution in the primary loop
        i. Use results of (b)
        ii. User-input generation rates, models for deposition and resuspension
2. Execute the transient phase of the calculation, stepping off from the steady-state
    a. Fission product release known initially from steady-state
    b. Fission product and graphite dust distribution (COR and HS structures, primary loop) known initially from steady-state
    c. User-input to ascertain TRISO fuel failures during transient phase

Demonstration problems exercising all of the developed HTGR functionalities and physics models were built and validated to the greatest extent possible. This includes input decks that exercise new models individually and several of the new models simultaneously.

Though the current version of the HTGR models in MELCOR assumes a three-phase steady-state initialization as described above for the transient calculation, this process is currently being stream-lined to allow the user the ability to specify all phases in a single input file and then allow the code to automatically progress between phases, eliminating the need to stop/start the code and transfer intermediate files between code execution stages. It is anticipated that the calculation flow will be similar to existing MELCOR runs, where a single calculation is performed to initialize the calculation and a second calculation performs the steady-state initialization and advances the time step.

A.3.2. CURRENT DEVELOPMENT WORK

Current development work has focused on testing models that have been implemented over the past decade in an integrated fashion. Because previous work was stopped due to loss of funding and missing models have been added due to other modeling needs and funding sources, it has not been possible to test all models on a realistic test problem. The following section describes some of the example problems developed for integrated testing of the HTGR models.

Example Problems

To illustrate the process of analyzing an HTGR in MELCOR with new models, a 400 MWth PBR reactor (simplified primary side and secondary side) was created. It includes input options to demonstrate:

- Point kinetics for ATWS-type analyses
- Thermal-hydraulic assessment of a DLOFC (problem time may be several weeks)
- Fission product diffusion/transport/release and graphite dust transport:
  - Accelerated steady-state to calculate a thermal steady-state
  - Steady-state diffusion calculation
  - Steady-state fission product and graphite dust transport calculation
  - Transient calculation

These examples – inputs and outputs - will be outlined in some detail below. All examples start with an accelerated steady-state run period to establish a thermal steady state for structures (COR and HS packages). All examples use a PBR core resembling the nodalization diagram in Figure A-5 below. There is an active core region, inner/outer/bottom reflectors, and a core peripheral region made from heat structures to represent the core barrel, reactor pressure vessel, and RCCS panels. The remainder of the primary loop resembles Figure A-6 below. The secondary side is comprised of time-independent source and sink CVs with one connecting flow path which allows for heat exchange (FL_IHX) with the primary side. The machinery (compressor, FL_MCH) model is employed to force circulation in the primary (triangle marker in Figure A-6).

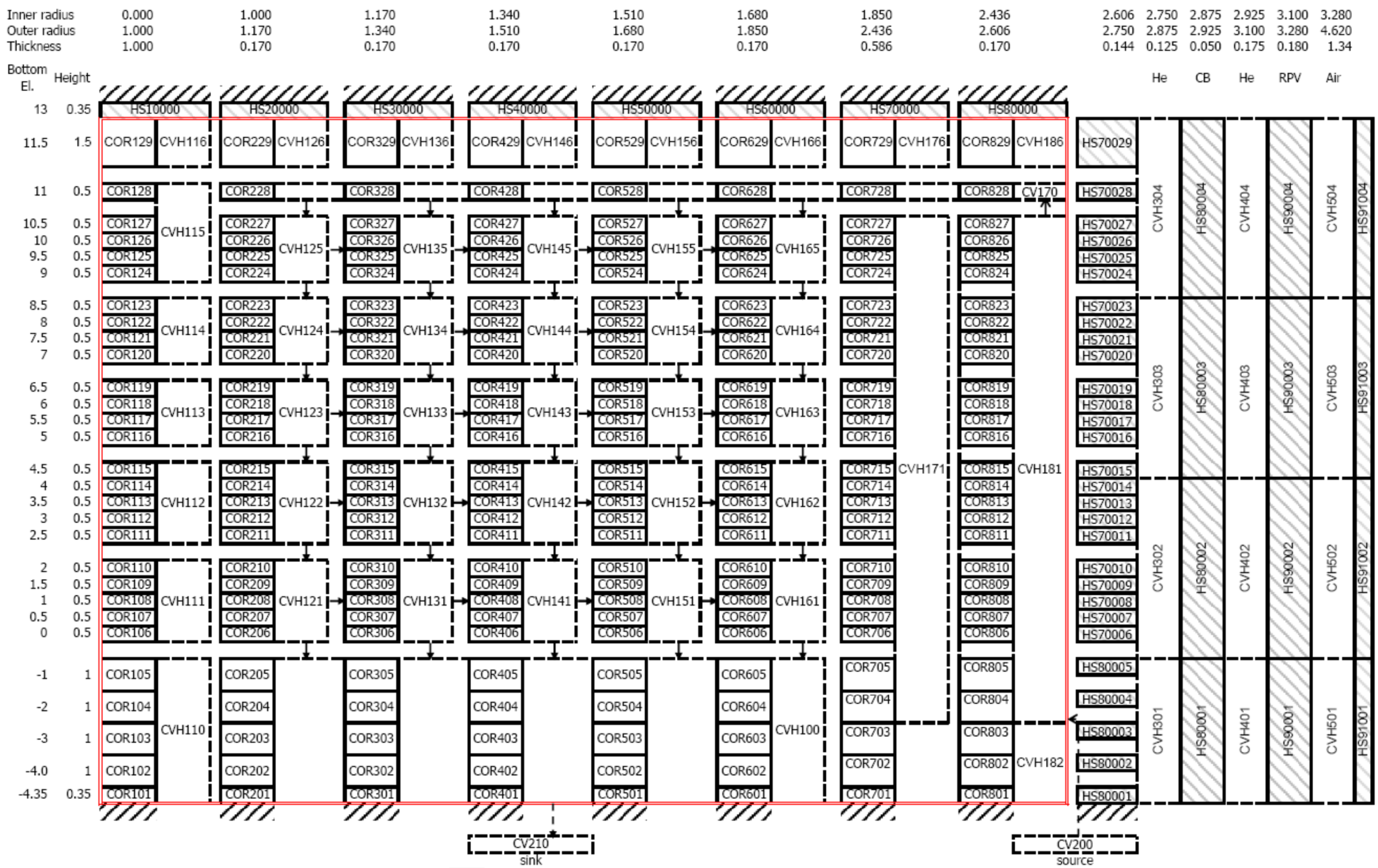

Figure A-5. PBR core nodalization diagram

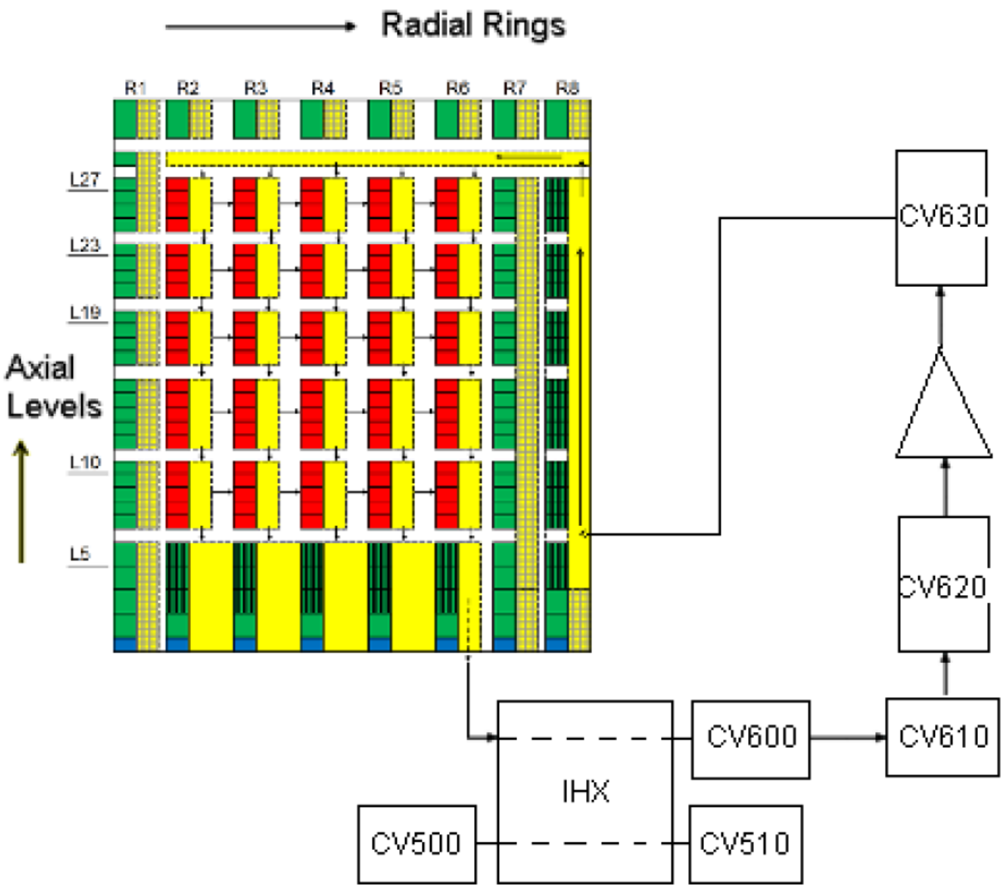

Figure A-6. Entire PBR model with simplified primary and secondary loops

The point kinetics example captures the effects of a $0.5 step reactivity insertion at time zero (accelerated steady-state stage occurs in negative problem time). The response is predicted by MELCOR point kinetics models which account for several components of reactivity feedback including:

- Fuel Doppler effect
- Fuel density change
- Moderator density change

Whole-core temperature averages for “fuel” (TRISO-bearing region of pebble, including UO_2 and graphite) and “clad” (part of the pebble) are used for computing reactivity feedback.

The long-term DLOFC example simulates an incident wherein the helium pressure boundary is compromised, exposing the core to possible air ingress while at the same time diminishing the role of natural circulation as a means of passive residual heat removal. The full effects of possible graphite oxidation were not considered in this particular example. The observed thermal-hydraulic response out to a long time (approximately 300 hours) demonstrates MELCOR capabilities with respect to longer-term transient/accident analyses. This is a distinguishing feature for MELCOR, as other codes have modeling capabilities aimed at shorter-term HTGR accident/transient modeling. The eventual conduction cooldown – occurring in the virtual absence of natural circulation effects – is evident in the results.

The fission product diffusion/transport/release and graphite dust transport example illustrates the sequential calculation of a thermal steady-state, steady-state fission product diffusion, steady-state fission product and graphite dust transport, and transient fission product release/transport and graphite dust transport. The steady-state portions of the calculation occur before fission power is shut off (e.g. by a reactor scram) and decay power is turned on. Then, the transient portion of the calculation proceeds under conditions meant to represent a PLOFC scenario. More details are given in subsequent sections.

Accelerated Steady-State

Results from the initial accelerated steady-state stage are discussed first. Important metrics for judging establishment of a thermal steady-state are:

- COR component structural temperatures (FU, MX, RF)
- HS structural temperatures (core peripheral features)
- CVH and FL temperatures/flows

Assuming boundary conditions imposed on the problem are uniform (source flow, overall core power, RCCS panel sink temperature, etc.), the system ought to reach thermal equilibrium and will do so more quickly in terms of computer time when the accelerated steady-state feature is active in MELCOR.

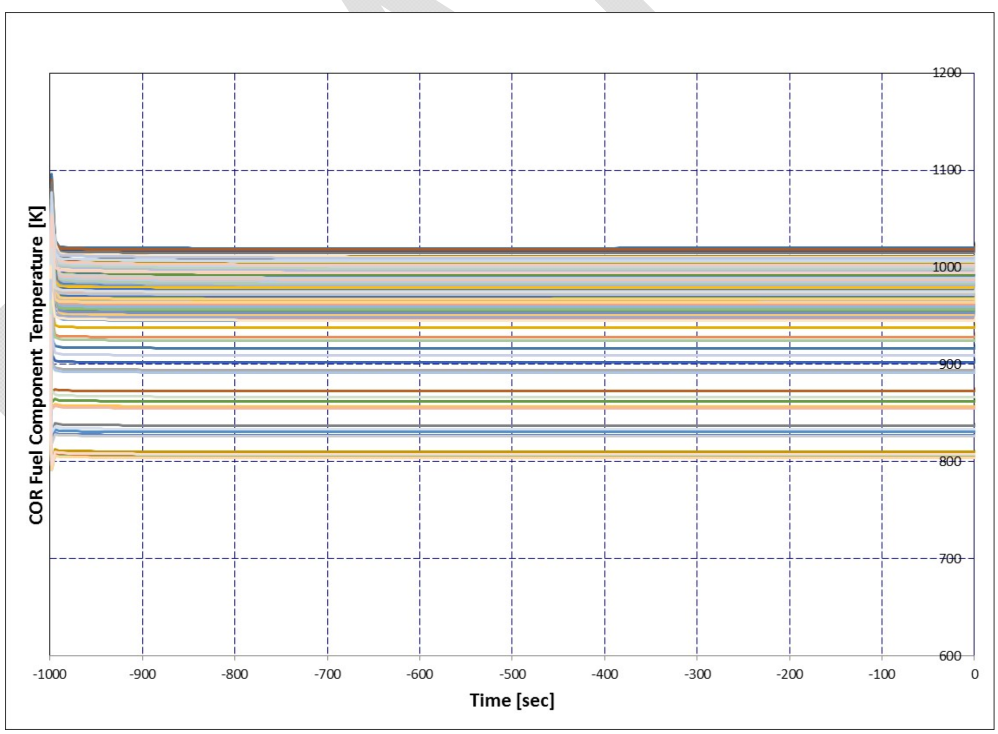

Figure A-7. COR fuel component temperature at steady-state

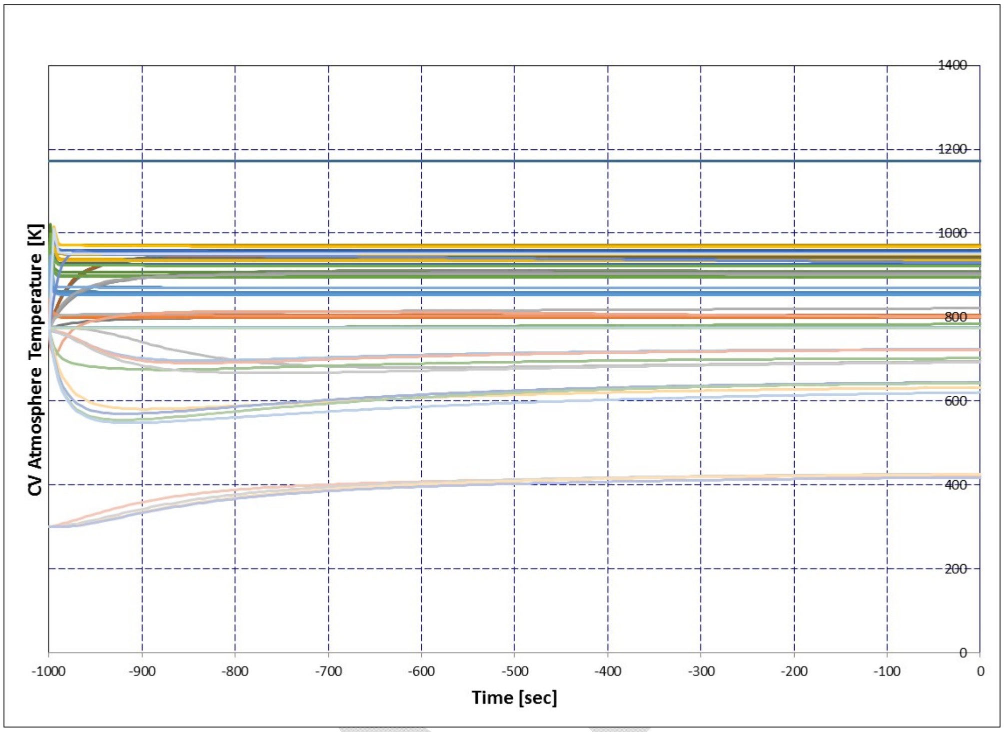

Figure A-8. CV atmosphere temperatures at steady-state

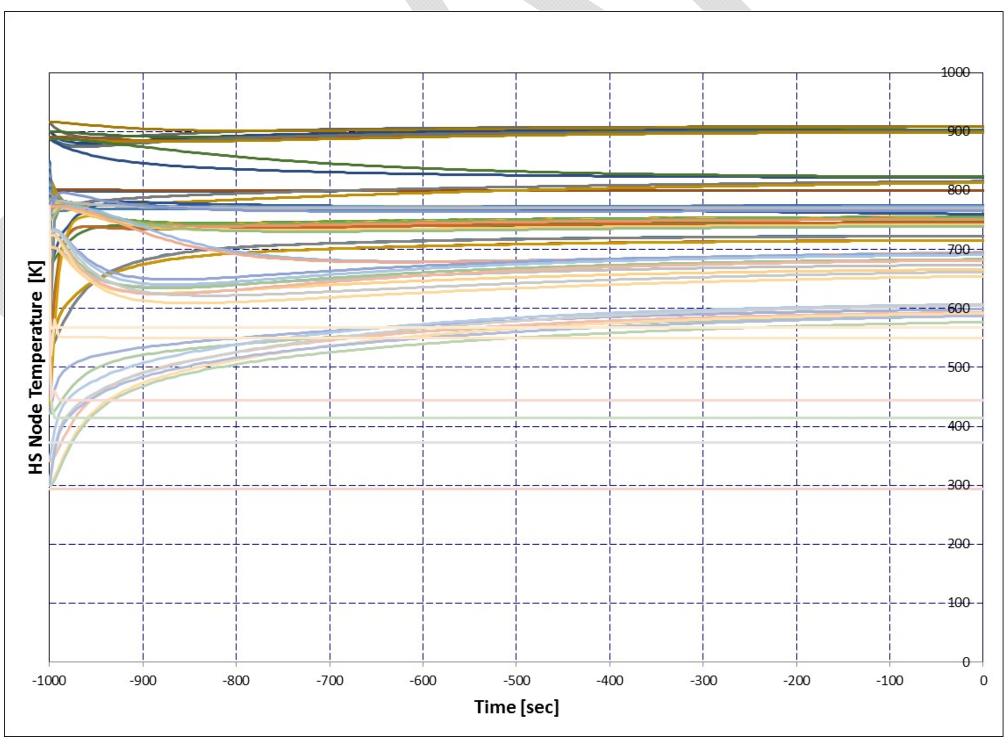

Figure A-9. HS node temperatures at steady-state

Figure A-7, Figure A-8, and Figure A-9 illustrate the steady-state conditions. Clearly, the COR component temperatures reach equilibrium values much sooner than the CV atmospheres reach approximately constant temperatures. The HS temperatures are roughly on par with the CV temperatures in terms of reaching steady values. This is in part a function of the initially-guessed COR, CVH, and HS temperatures as the steady solution is found more quickly when initial guesses are closer to the solution.

Point Kinetics Example

Starting with the PBR core conditions as established by an accelerated steady-state run, a $0.50 reactivity insertion (step increase, held constant thereafter) was programmed at time zero. The subsequent reactor power excursion may be observed by tracking the COR fission thermal power rate. A steady-state will be re-established at some higher power level (above the previously steady-state 400 MW) as governed by the reactivity balance between the inserted reactivity components:

- positive from the step insertion
- negative from the fuel Doppler feedback (higher fuel temperature)
- likely negative from decreased fuel density (less fissile isotopes per unit volume)
- likely negative from decreased moderator density (under-moderated design)

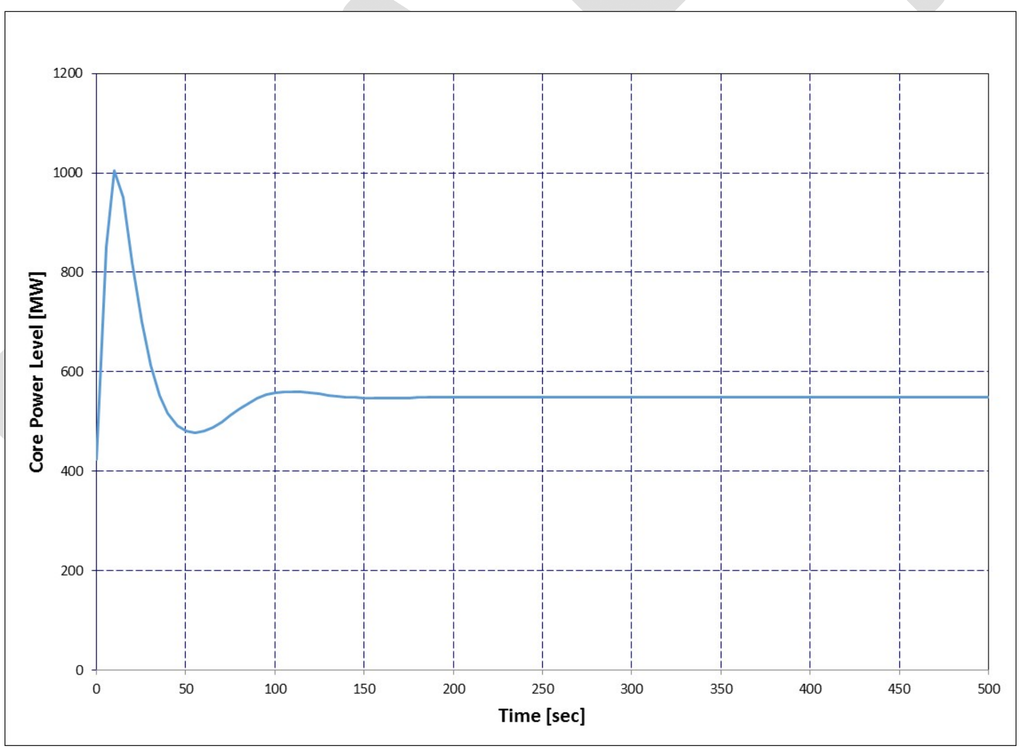

Figure A-10. Core power level, excursion due to a $0.50 insertion

Figure A-10 shows the increase from an initial 400 MW upon external reactivity insertion. The point kinetics model predicts an increase in fission power to nearly 1 GW in dozens of seconds. The inherently negative reactivity feedback mechanisms pull the power level back down and ultimately re-establish a thermal power level of less than 600 MW. The increase in thermal power drives material and coolant temperatures to higher levels as exhibited by fuel component temperatures shown in Figure A-11.

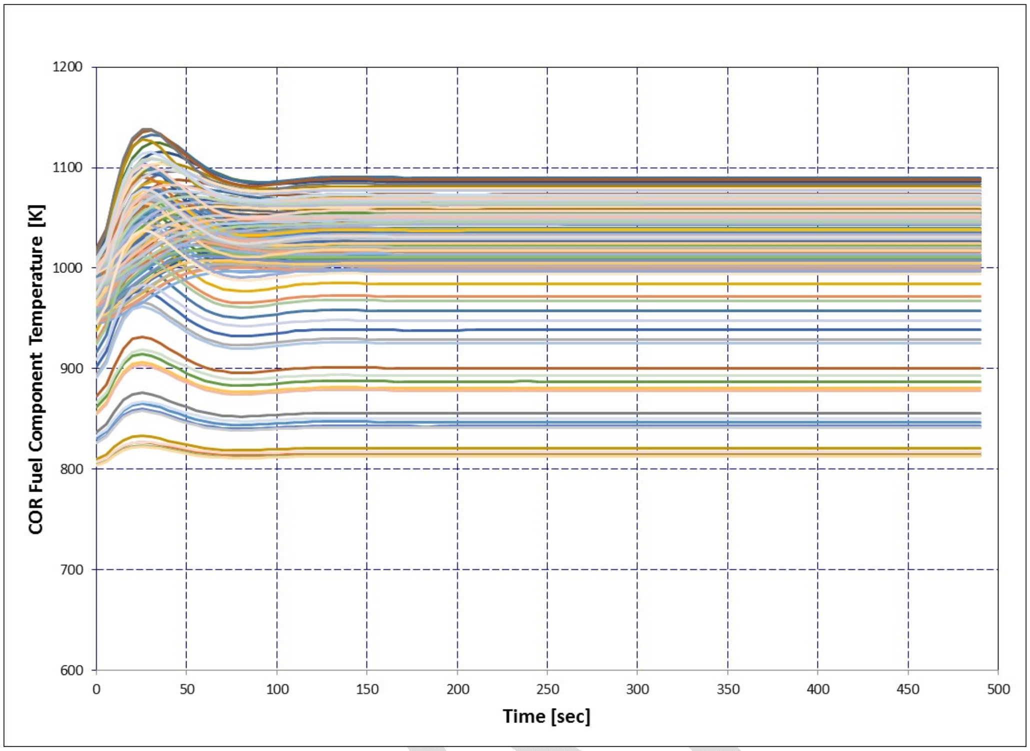

Figure A-11. COR fuel component temperature response due to a $0.50 reactivity insertion

Long-Term DLOFC Example

A 300 hour DLOFC transient was run to completion. The maximum fuel temperature was 1888 K and was found in ring 2 and axial level 21 (the fueled region of the core is modeled in rings 2-6 and axial levels 6-27). The maximum temperature occurred about 25 hours into the transient. Axial fuel temperature variations (Figure A-12) show that in ring 2, the lowest temperature was in level 6, the lowest level of the active core. The maximum temperature difference was 856^{o}C occurring 14 hours into the transient and the temperature difference at the end of the 300 hr transient was 462^{o}C. Radial fuel temperature variation (Figure A-13) shows that structural temperatures decrease in the radial direction, with the lowest temperatures occurring in ring 6. The maximum temperature in each ring also shifts progressively later into the transient as the radius increases. The maximum radial temperature difference (axial level 21) was 487^{o}C occurring 10 hours into the transient, and the temperature difference was 291^{o}C at the transient end [70].

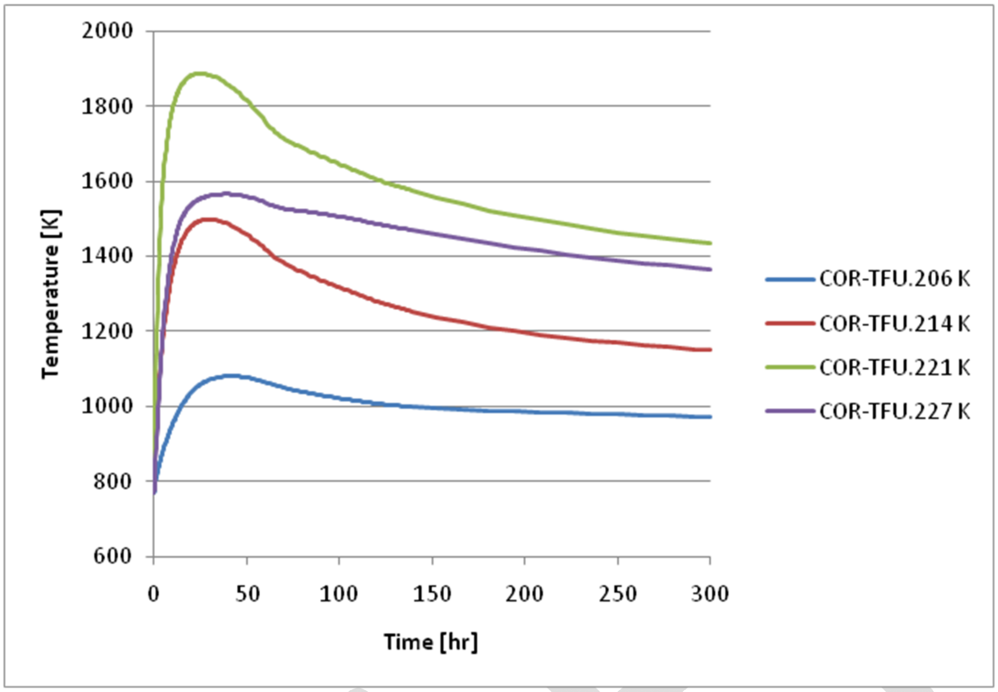

Figure A-12. SNL MELCOR DLOFC: axial fuel temperature variation, ring 2

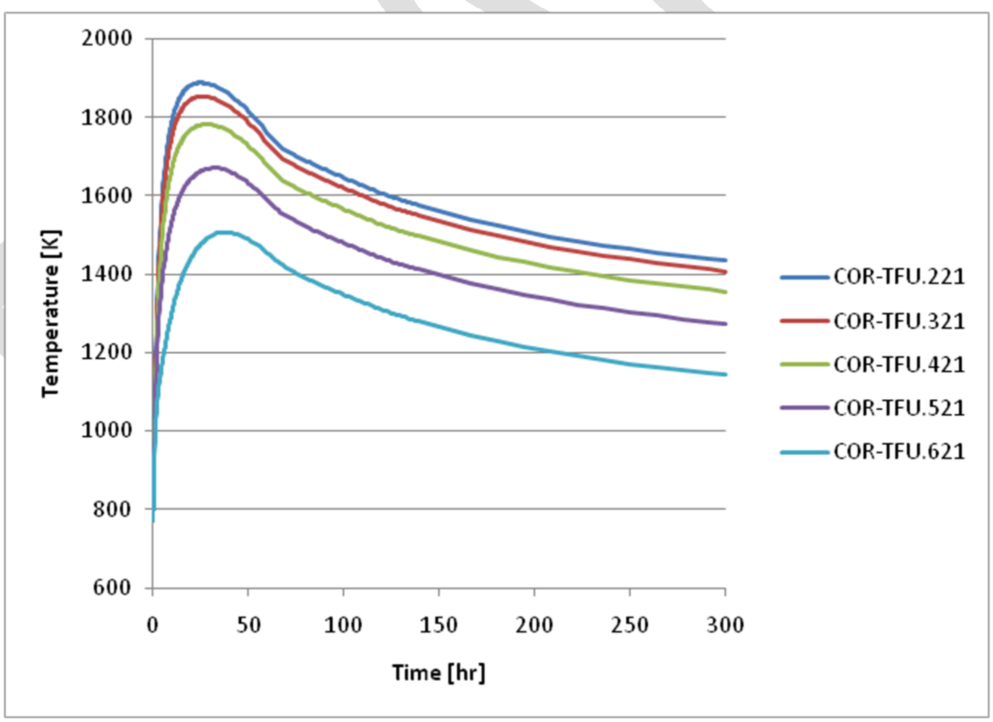

Figure A-13. SNL MELCOR DLOFC: radial fuel temperature variation, level 21

Fission Product and Graphite Dust Example

A sequence of calculations (back-to-back MELGEN/MELCOR executions) were carried out to model graphite dust transport and cesium release from TRISO fuel during a PLOFC transient. An illustration of the steps in this process is included in Figure A-14 which outlines the general process of executing an HTGR transient in MELCOR.

First, a single calculation was run to both establish a thermal steady state and do a steady-state diffusion calculation (for cesium distribution/release in/from TRISO fuel). This step uses a diffusion calculation input file (named “mdif.in”) and produces:

- a file containing COR/HS steady-state temperatures (“Tifile.inp”)
- a file containing steady-state fission product (Cs) distribution/release for TRISO (“init.out”)

Note a few relevant features of the diffusion calculation input:

- burnup time of 900 days
- Diffusion calculations in all fuel-bearing COR cells
- 3 “models”, one each for: intact TRISO, initially failed SiC TRISO, matrix
- 1.45e+4 fuel particles per unit of fuel (i.e. per fuel pebble)
- Initially failed fuel fraction of 1.0e-5
- 5-zone intact fuel model, 2-zone failed fuel model, 2-zone matrix model
- Different Arrhenius equation parameters for Cs diffusion coefficients
- Zone-wise material property definitions (Cs, graphite, UO_2, etc.)

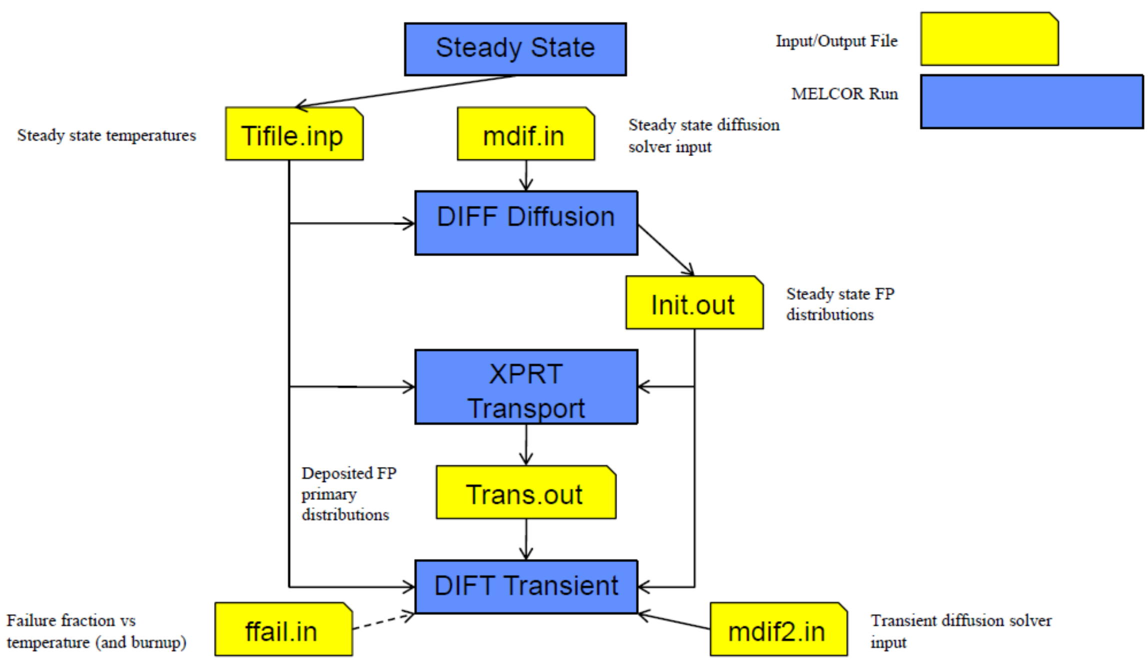

Figure A-14. Flow chart of calculations and input/output files for an HTGR transient run

Second, a single calculation was performed to ascertain steady-state fission product (Cs) and graphite dust transport/settling/deposition. This is the blue block labeled “XPRT Transport”. The output from the steady-state diffusion calculation is read and DCH/RN1 input for the graphite dust DCH/RN class is used to run a MELCOR calculation from time 0 s to about 2000 s when it is observed that inter-volume transport and HS depositions have settled out to constant, unchanging values as a function of time. The results are printed to a file (“Trans.out”) for use in the transient stage of the calculation. Note that the results recorded for transport/distribution in “Trans.out” may be scaled to some desired operating time. This scaling is governed by 1) the time for which the XPRT stage is run, and 2) the actual operating time of the reactor. Dividing the latter by the former results in a scale factor that can optionally be applied to the amounts distributed/transported in order to reflect the actual time the system operates at steady-state before a transient occurs.

Third, the rest of the calculation is run with COR_DIFT input along with information included in “mdif-f2.in”, “Tifile.inp”, “init.out”, “Trans.out”, and possibly “ffail.inp” which provides one way of specifying fuel failure fraction as a function of independent variables like fuel temperature and burn-up. Note that “mdif-f2.in” is not necessarily the same as “mdif-f.in”, e.g. the analytical convolution integral approach to fuel failure modeling may be invoked in “mdif-f2.in”. The transient starts at time 0 with results obtained from steady-state DIFF and XPRT runs. From there, the transient is run in real time with whatever user-prescribed conditions, e.g. those of a PLOFC event. A PLOFC scenario entails a loss of the flow driver (the compressor) in the primary side, yet without any breach in the primary pressure boundary. Thus, primary pressure isn’t lost due to a break but heat removal by forced circulation does not occur. Fission thermal energy generation is assumed to cease coincident with loss of forced circulation, but decay heat remains. A pressurized conduction cool-down ensues wherein core temperatures will redistribute axially/radially and heat transfer to the core periphery (ultimately to the RCCS panels) ought to cope with core decay heat. As temperatures and flow patterns change, fission product and graphite dust transport may be observed.

Results are presented by calculation stage below. The thermal steady-state was the same as presented above (Figure A-7 through Figure A-9) as obtained with the accelerated steady-state option with constant fission power of 400 MW, compressor pressure boost of 2.97e+5 Pa, and primary-to-secondary heat exchange as defined by the integral heat exchanger model assuming a coefficient of 1000 W/m^2/K.

A representative COR cell (a diffusion cell) in axial level 6, radial ring 2, was chosen as an instance of steady-state diffusion calculation results. The results excerpts (Table A-1 and Table A-2) below are taken from the INITFILE generated upon completion of the calculation specified by COR_DIF and an MDIFFILE. COR component temperatures and coolant temperatures remain constant at the thermal steady-state values because fission power, compressor pressure boost, and primary-to-secondary heat exchange are held constant. Note that the comments appearing in Table A-1 and Table A-2 were recently added in to the source code blocks responsible for INITFILE reading/writing.

Table A-1. INITFILE excerpt, steady-state diffusion calculation results, block 1

```
******************BLOCK FORMAT******************
cell   #      ia       ir
specie #      relCell      amtCell      frctCell
************************************************
          1            6            2
    1  1.76043E-16  1.33975E-04  1.02177E-04
```

Table A-2. INITFILE excerpt, steady-state diffusion calculation results, block 2

```
********************************BLOCK FORMAT********************************
cell  #      ffail
model #      nzones      each species : zoneamt(1..nzones)    sumrel    totamt
****************************************************************************
          1  1.000000000000000E-005
          1           5
 1.26235E-12  1.03290E-12  4.74173E-13  1.16303E-13  1.76730E-15  1.92600E-15  2.88942E-12
          2           2
 6.78551E-13  3.05077E-14  2.18036E-12  2.88942E-12
          3           2
 2.08265E-11  3.13157E-12  4.28377E-12  2.82419E-11
```

The first excerpt from INITFILE in Table A-1 indicates that COR cell IA=6, IR=2 is diffusion cell number 1 and has a release rate of $1.76043*10^{-16}$ kmol/s (release of Cs species to coolant), a total Cs amount of $1.33975*10^{-4}$ kmol, and a release fraction of $1.02177*10^{-4}$. The second excerpt from INITFILE in Table A-2 indicates that diffusion cell number 1 has an initial failed fraction of 1.0e-5 (user input quantity), and has 3 regions/models of 5, 2, and 2 zones, respectively. The first model/region represents intact TRISO and the five zones are UO2, buffer, inner PyC, SiC, and outer Pyc (known from diffusion calculation input definition of this model/region). The second model/region represents failed TRISO and the third model/region represents carbonaceous matrix that holds TRISO fuel particles in suspension. For each model/region in turn, the amounts (in kmol) of Cs are listed above in zone-wise order (inner to outer). Following those numbers is the summed release from the cell (species Cs, total release) and the total amount present in the cell (species Cs, includes total release). Those quantities are obviously on a per-model/region basis because there are distinct listings for each model/region. Thus, the diffusion calculation predicts Cs presence in all zones of all models/regions with the trend of decreasing concentration in the radially outward direction.

The steady-state transport calculation results are presented below using selected heat structures and control volumes. Graphite dust (user-defined RN class 'GR') is predicted in CVs and on HSs. Cesium (RN class 'CS') is observed in CVs. The first excerpt from TRANSFILE in Table A-3 below shows graphite dust interaction with the HS named 'COMP-RISER-FLOOR' (HS object number 53). Note the ellipsis indicate an omission of certain other output. The 18th RN class (user-defined for graphite dust, mnemonic 'GR') deposits on the HS surface as an aerosol (ADEP and Adeprate nonzero, VDEP and Vdeprate zero) in the amount of $1.207*10^{-3}$ kg and at a rate of $4.242*10^{-8}$ kg/s. Then, the table indicates graphite dust mass deposited on the HS surface as a function of aerosol section. The 4th aerosol section (the size section covers the range 0.65-1.2 microns) is where the user-defined graphite dust source is "born" by assumption. Thus, this section has the greatest graphite dust mass deposition of $1.207*10^{-3}$. Aerosol sections 5 through 10 (bins/sections of larger aerosol size) have graphite dust mass but in considerably smaller amounts. There is no radioactive graphite dust, so RADEP, RVDEP, etc. are zero.

Table A-3. TRANSFILE excerpt, steady-state transport calculation results, block 1

```
******************BLOCK FORMAT******************
 HS order #     HS side ID     HS name
 for each RN class, deposition quantities:
 Cls #     Cls Name
 ADEP     VDEP     Adeprate     Vdeprate  (total)
 Adepsize
 RADEP     RVDEP     Adeprate     Vdeprate  (radioactive)
 ************************************************
 ...
          53            1 COMP-RISER-FLOOR
 ...
           18 GR
  1.207517575371950E-003  0.000000000000000E+000  4.242080888741289E-008
  0.000000000000000E+000
  0.000000000000000E+000  0.000000000000000E+000  0.000000000000000E+000
  0.000000000000000E+000  1.206883658459143E-003  6.339095510390441E-007
  7.361817569961779E-012  2.685269457968741E-017  3.981711227129161E-023
  8.513215806807155E-030  9.783769773156198E-037
  0.000000000000000E+000  0.000000000000000E+000  0.000000000000000E+000
  0.000000000000000E+000
```

Table A-4. TRANSFILE excerpt, steady-state transport calculation results, block 2

```
 *****************BLOCK FORMAT*****************
CV order #     CV Name
for each RN class, aerosol mass quantities:
TOT:
for each aerosol section:
Sec #     AER1G     Arate
VAP1G Vrate
RAD:
for each aerosol section:
Sec #     RDA1G     Arate
RDV1G Vrate
**********************************************
...
         65 CV630
...
         2 CS
TOT
         1  0.000000000000000E+000  0.000000000000000E+000
         2  0.000000000000000E+000  0.000000000000000E+000
         3  0.000000000000000E+000  0.000000000000000E+000
         4  0.000000000000000E+000  0.000000000000000E+000
         5  0.000000000000000E+000  0.000000000000000E+000
         6  0.000000000000000E+000  0.000000000000000E+000
         7  0.000000000000000E+000  0.000000000000000E+000
         8  0.000000000000000E+000  0.000000000000000E+000
         9  0.000000000000000E+000  0.000000000000000E+000
        10  0.000000000000000E+000  0.000000000000000E+000
 8.483732183907432E-010  2.711545190416119E-014
RAD
         1  0.000000000000000E+000  0.000000000000000E+000
         2  0.000000000000000E+000  0.000000000000000E+000
         3  0.000000000000000E+000  0.000000000000000E+000
         4  0.000000000000000E+000  0.000000000000000E+000
         5  0.000000000000000E+000  0.000000000000000E+000
         6  0.000000000000000E+000  0.000000000000000E+000
         7  0.000000000000000E+000  0.000000000000000E+000
         8  0.000000000000000E+000  0.000000000000000E+000
         9  0.000000000000000E+000  0.000000000000000E+000
        10  0.000000000000000E+000  0.000000000000000E+000
 7.521231820468942E-010  2.403913693453286E-014
 ...
          18 GR
TOT
         1  0.000000000000000E+000  0.000000000000000E+000
         2  0.000000000000000E+000  0.000000000000000E+000
         3  0.000000000000000E+000  0.000000000000000E+000
         4  2.500556883208720E-005 -1.081788625414400E-009
         5  1.283472980771208E-008 -9.674095371736014E-014
         6  1.056522624863289E-013  3.308387204750149E-017
         7  1.811663570287084E-019  1.807077313621613E-022
         8  9.417274609092634E-026  2.131131883232626E-028
         9  6.238190392017547E-033  1.160278029126469E-034
        10  2.188904363476908E-040  4.881596580732126E-041
 0.000000000000000E+000  0.000000000000000E+000
RAD
         1  0.000000000000000E+000  0.000000000000000E+000
         2  0.000000000000000E+000  0.000000000000000E+000
         3  0.000000000000000E+000  0.000000000000000E+000
         4  0.000000000000000E+000  0.000000000000000E+000
         5  0.000000000000000E+000  0.000000000000000E+000
         6  0.000000000000000E+000  0.000000000000000E+000
         7  0.000000000000000E+000  0.000000000000000E+000
         8  0.000000000000000E+000  0.000000000000000E+000
         9  0.000000000000000E+000  0.000000000000000E+000
        10  0.000000000000000E+000  0.000000000000000E+000
 0.000000000000000E+000  0.000000000000000E+000
```

The second excerpt from TRANSFILE in the table above indicates the presence of ‘CS’ and ‘GR’ in control volume ‘CV630’ (object number 65). The ‘CS’ RN class is not present as aerosol, but rather as vapor. Hence, all aerosol quantities (AER1G, arate) for all aerosol sections are zero. However, all vapor quantities (VAP1G, vrate) are nonzero. In this case, there is radioactive and nonradioactive Cesium mass in ‘CV630’ and both types evolve at a rate on the order of 10^{-14} kg/s. The ‘GR’ RN class is present as an aerosol and not a vapor, so the situation is reversed with respect to the ‘CS’ RN class. Graphite dust mass is present in sections 4 through 10, though exclusively as a nonradioactive aerosol. Figure A-15. CS vapor mass contents of primary loop CVs outside the core shows plot variables for ‘CS’ vapor mass by control volume. The cesium mass in the primary loop is approaching a constant, steady value near the end of the steady transport run. Figure A-16 shows plot variables for total (radioactive plus non-radioactive) aerosol mass by control volume. Most of the aerosol mass in a given CV is comprised of non-radioactive graphite dust which is sourced into the lower plenum (red line labeled “Lower Plenum – CV 100” in Figure A-16). The greatest amount of aerosol mass is found in the riser (blue line labeled “Riser – CV 181” in Figure A-16). Since no aerosols are “born” in the riser, inter-volume aerosol transport (including that of graphite dust) is clearly occurring.

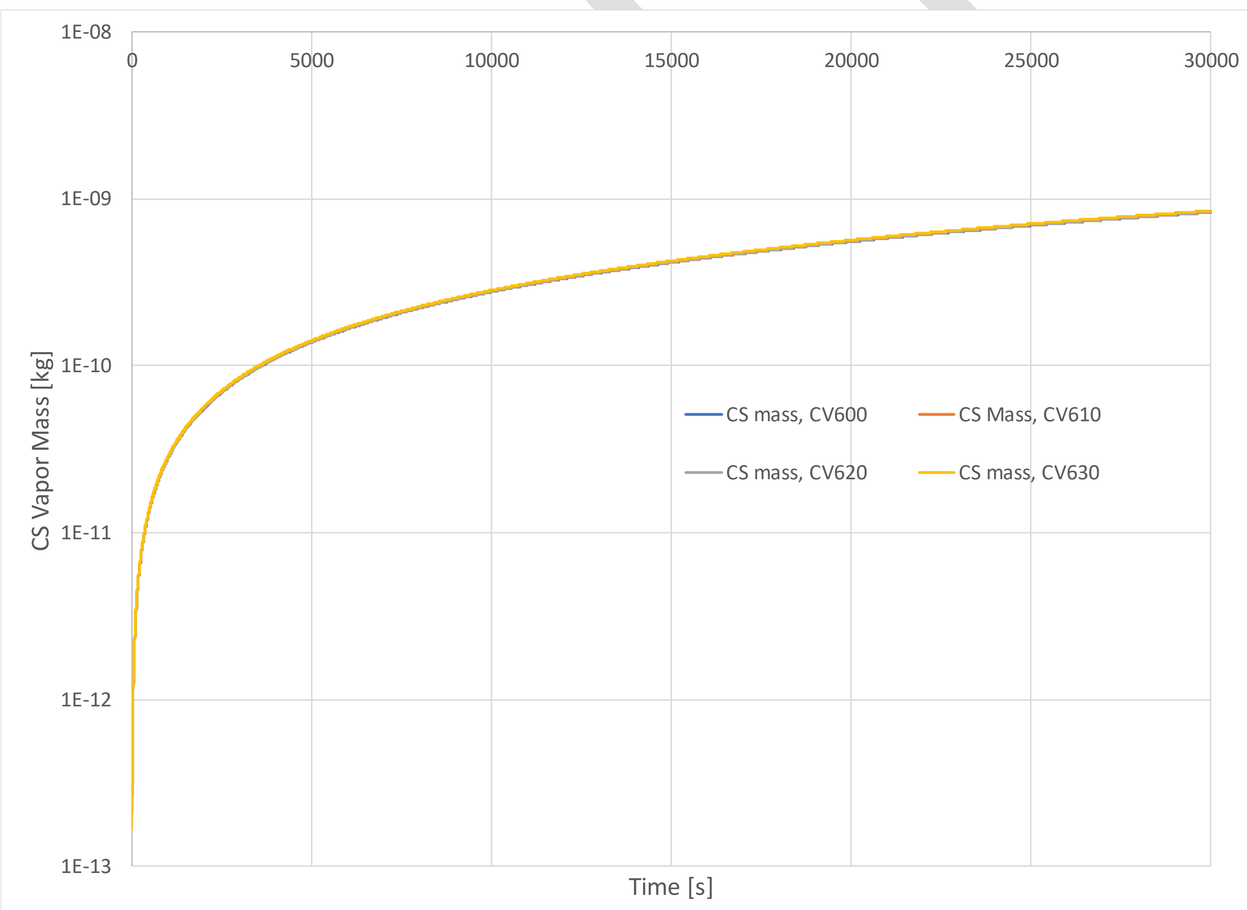

Figure A-15. CS vapor mass contents of primary loop CVs outside the core

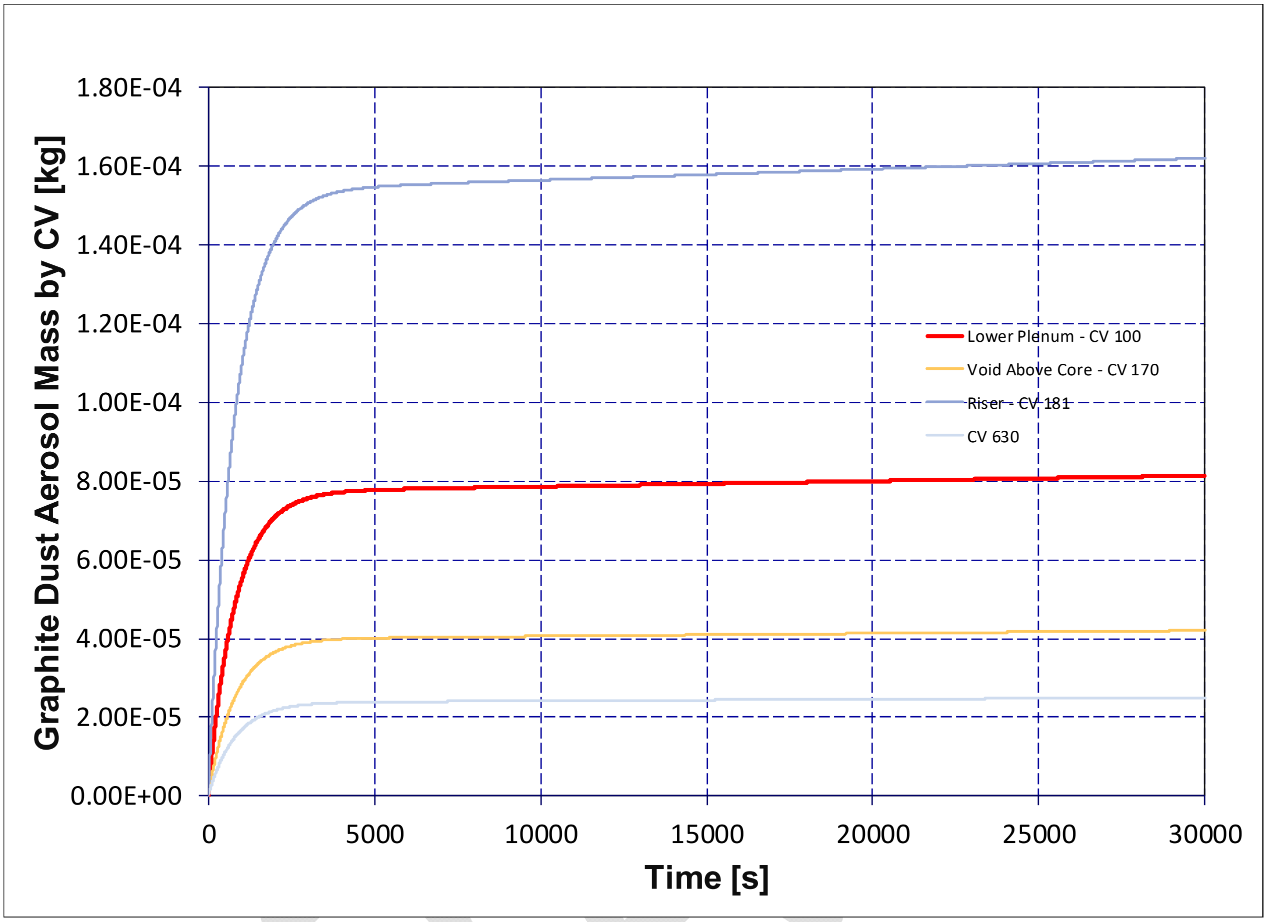

Figure A-16. Graphite dust aerosol mass contents (total, all non-radioactive), select CVs

The results for the actual PLOFC transient with diffusion and graphite dust transport are presented below by way of core component temperatures, cesium vapor mass content of select CV's, and aerosol mass content of select CV's.

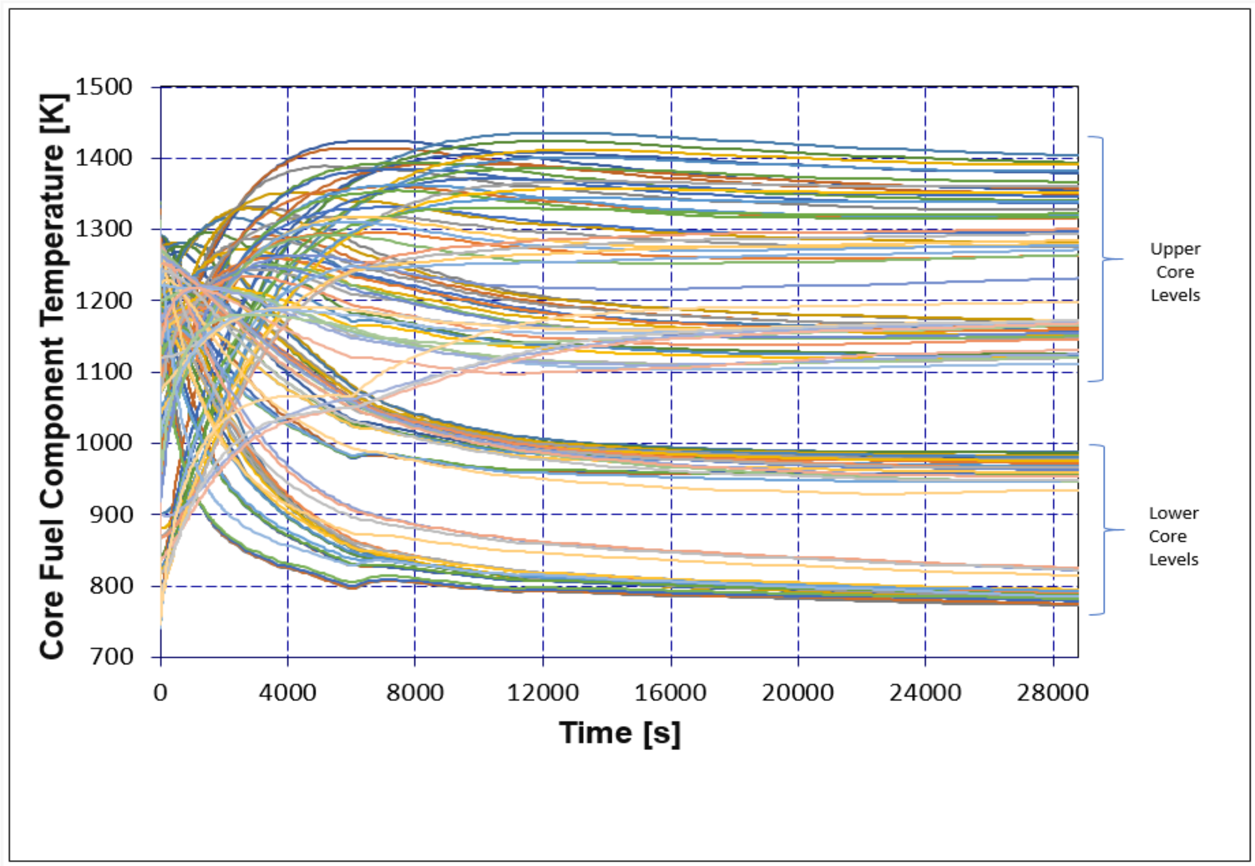

Figure A-17. Core fuel (FU component) temperatures during first 8 hours of PLOFC event

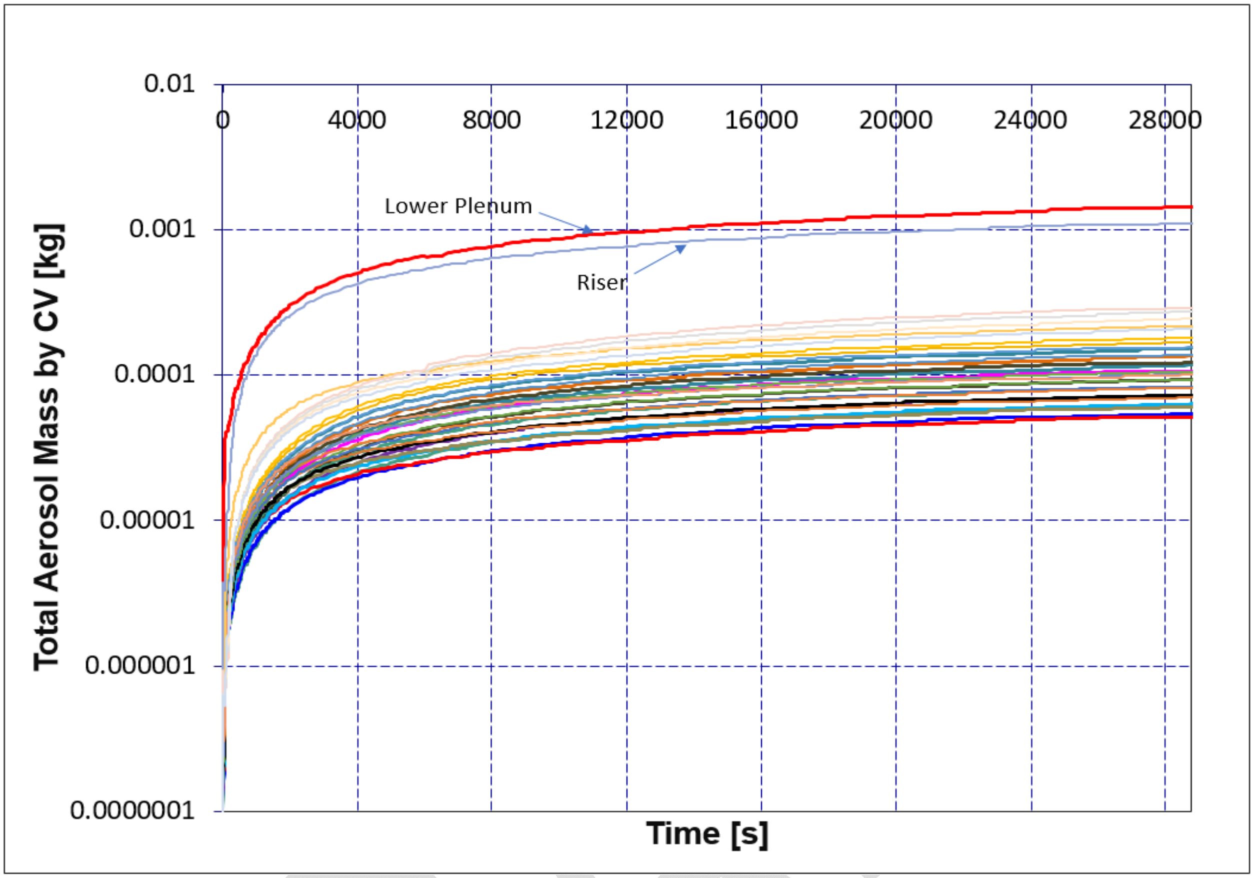

Figure A-18. Total aerosol mass by CV during PLOFC

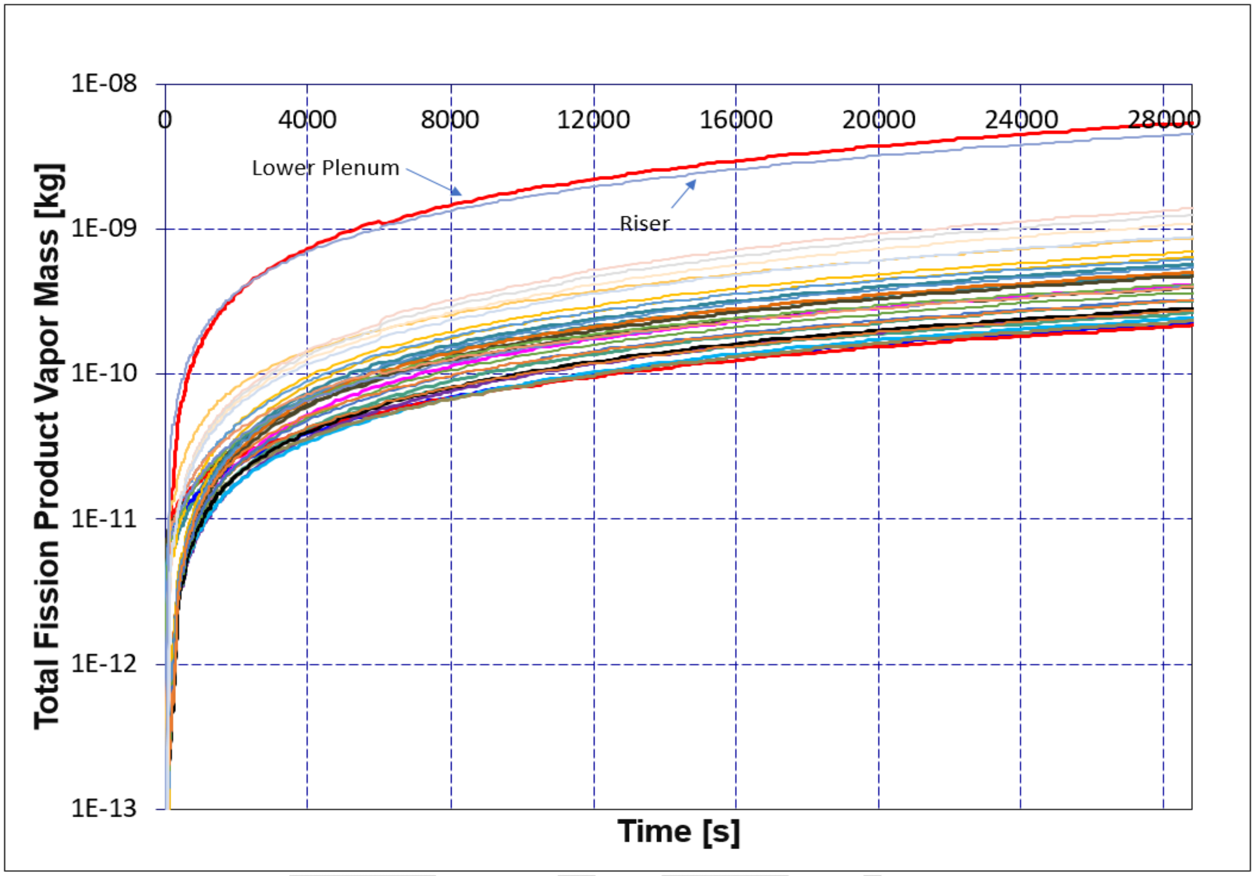

Figure A-19. Total fission product vapor mass by CV during PLOFC

The COR temperatures in Figure A-17 show the expected re-distribution of thermal energy in the active core during the PLOFC event. The hotter fuel near the core outlet (at the start of the PLOFC) tends to transfer thermal energy (via conduction and natural circulation) to the cooler fuel near the core inlet. Temperatures are higher near the core interior and cooler near the core periphery, which facilitates thermal conduction to the reactor pressure vessel and, ultimately, the RCCS panels. Figure A-19 shows that fission product vapor escapes from the fuel as predicted by the TRISO failure models. Figure A-18 shows that aerosol mass – in large part consisting of graphite dust – is present all around the primary loop because of the user-defined source.

Future Development Work

Test problems from years ago were revisited and checked for any regressions or degradations with satisfactory results. The recently-implemented turbulent deposition and resuspension models should also be exercised with graphite dust in the context of appropriate HTGR demonstration problems.

A few modeling features ought to be checked for completeness and further-developed if need be. These include:

- Heat structure and graphite dust interactions (deposition, resuspension, coverage, and size distribution modeling)
- Aerosol and graphite dust interactions

- Fragmentation of aerosols at high velocity
- Machinery models (improvements, more mechanistic alternatives, etc.)

Additionally, some of the models meant for HTGR applications require further refinements to the documentation in the user manuals. Part of the work accomplished in reviewing the readiness of the HTGR models was spent on aggregating all model descriptions and updating the user manuals for the existing modeling capabilities.

APPENDIX B. MELCOR MODELING OF SFRS

B.1. INTRODUCTION AND BRIEF HISTORY

The sodium fast reactor (SFR) is among the most well-developed of the generation IV, non-LWR concepts due to its advanced technology base and accumulated world-wide operating experience. France, Japan, Russia, the United Kingdom, Germany, the U.S. and a few other countries have some operating experience with SFR installations. In the U.S., EBR-II, FERMI-I, and the FFTF are some past and present SFR installations. There are a few relatively mature SFR design proposals in existence e.g. SAFR, PRISM, and the Integral Fast Reactor (IFR) - formerly known as the Advanced Liquid Metal Reactor (ALMR). SFR design philosophy in the U.S. tends toward metal alloy fuel (as opposed to oxide fuel) and liquid sodium pools for cooling (as opposed to loop cooling).

A couple of SFR designers have made progress in the licensing process, thus the impending need for computational tools capable of SFR licensing analyses. Several SFR studies have been conducted in the way of PIRT-like analyses, mechanistic source term development, and safety/licensing support (e.g. preliminary safety information/evaluation documents/reports). Thus, the most immediate SFR modeling needs are reasonably well-defined.

B.2. DESIGN ASPECTS

For present MELCOR modeling purposes, the reference SFR design will be taken as the metal alloy fueled, pool-type variant as illustrated in Figure B-1 below. To list a few characteristics of this design:

- U-Zr or U-Pu-Zr alloy fuel fabricated in a solid slug with bond sodium between the slug and stainless-steel cladding
- Conventional gas plenum in the fuel rod or an alternative vented fuel design
- Tightly-packed, hexagonal, canned fuel assemblies with or without wire-wrapped pins
- Large liquid sodium pool containing plant components
- Inert cover gas over pool in a sealed vessel (within a guard vessel) at atmospheric pressure
- High core power density relative to LWRs
- Fast neutron spectrum with large mean free paths
- Indirect Rankine power cycle with intermediate sodium heat transfer loop
- Sodium coolant
    - Excellent heat transfer properties, low Prandtl number
    - Good stability (thermal, chemical, radiation)
    - Favorable neutronic properties for a hard neutron spectrum
    - Exothermal reactions with air (oxygen) and water
    - Large margin to boiling (high boiling point)
    - Slight positive void coefficient of reactivity due to sodium absorption

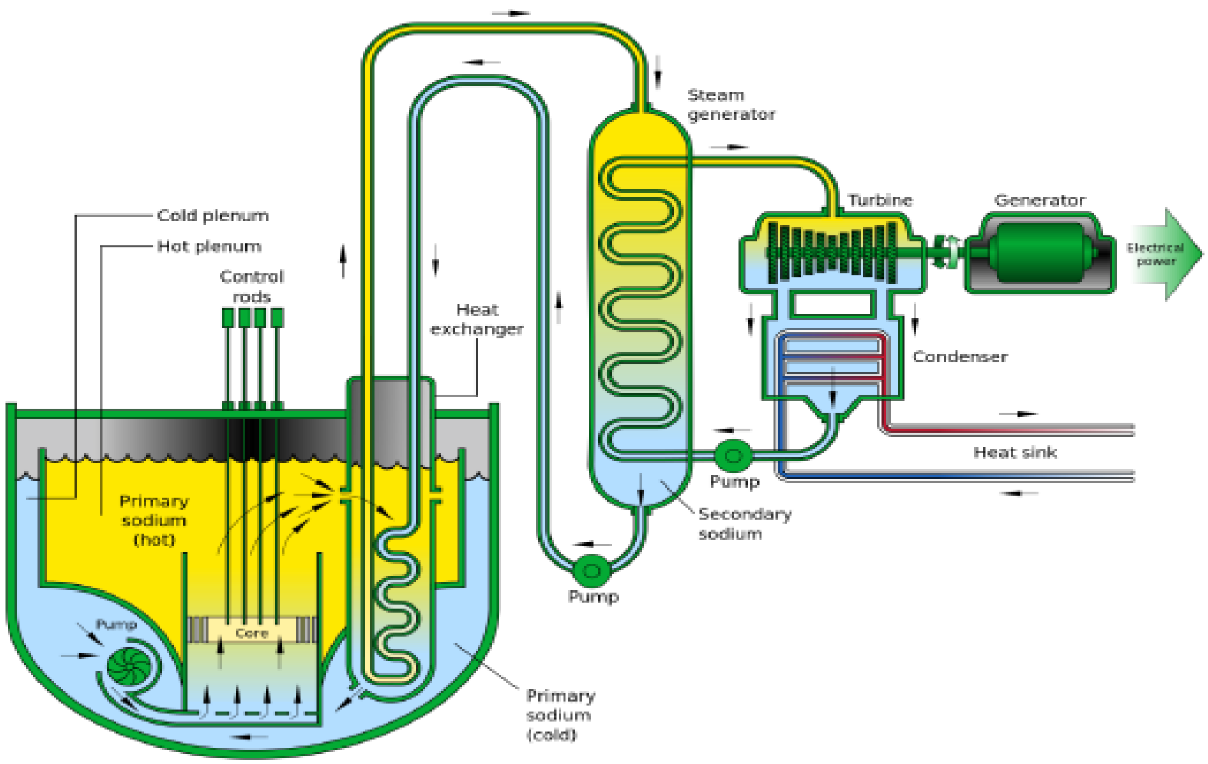

Figure B-1. Sodium pool-type SFR conceptual design [71]

The metal alloy fuel melts at a low temperature, is compatible with liquid sodium coolant, and poses a minimal threat to the reactor vessel under accident conditions. It has a high thermal conductivity which minimizes the severity of the temperature gradient across the fuel slug radius. The fuel itself has a strong, negative Doppler reactivity feedback. There is also a negative feedback from fuel slug axial thermal expansion.

Safety concerns do exist despite the several passive safety features of SFR designs. Sodium is combustible in the presence of even small quantities of air and water, so spray fires, pool fires, and hydrogen production are of concern in licensing analyses. Such hazards pose a threat on the primary side, in the intermediate loop, and on the power-production side.

B.3. MELCOR MODELING

B.3.1. PREVIOUS DEVELOPMENT WORK

The United States DOE has funded efforts to enhance MELCOR's modeling capabilities for sodium reactors by adding models for simulating containment accidents involving sodium fires (WP No. AT-17SN170204). Such models were previously developed for the CONTAIN/LMR code, have received validation, albeit limited, against experiments, and have been used by international code users for more than a decade. However, since the CONTAIN/LMR code is no longer actively developed, it was prudent to add these models to an actively developed systems level code for severe accident modeling, such as MELCOR. In addition, sodium has been added to MELCOR as a working fluid. Finally, new heat pipe modeling capabilities have been added to the code (see Section B.4) using NRC FY18 funding.

In summary, the following tasks have been completed:

- Addition of a sodium working fluid equation-of-state plus other property data
    - Verification of the working-fluid-equation of state models
- Transfer of CONTAIN-LMR sodium models, including:
    - Pool fires
    - Spray fires
    - Aerosol/chemical reactions
- Inclusion of the above models into a managing “NAC” physics package
- Validation/demonstration problems exercising the models listed above
- A survey of in-vessel SFR phenomena from SAS4A computer code manuals
- Consideration of miscellaneous, important ex-vessel phenomena

Sodium Equation-of-State and Properties

To accommodate sodium as the working fluid field in MELCOR, sodium thermophysical properties, such as enthalpy, heat capacity, heat of fusion, vapor pressure, heat of vaporization, density, thermal conductivity, thermal diffusivity, viscosity and thermal expansion have replaced those currently used for water. The equation of state (EOS) for water is based on polynomials in a tabular format. These polynomials relate pressure, specific internal energy, specific entropy and heat capacity to temperature and density, and are expressed analytically in terms of the Helmholtz free energy. In MELCOR, additional thermodynamic properties are derived from the thermodynamic relationships involving Helmholtz free energy, such as fluid internal energy, enthalpy, entropy, specific heat, and derivatives of pressure with respect to temperature and density. The resulting EOS for water is valid for temperature ≥ 273.15 K and for pressure ≤ 100 MPa. With this current implementation, the working fluid (condensable fluid) is either sodium or water and the user cannot have multiple working fluids both in the same problem. However, this limitation can be overcome through additional code development to allow at least two condensable fluids defined within a calculation as long as they reside in control volumes not connected by flow paths. This approach was taken with the CONTAIN/LMR code.

Sodium properties for the SIMMER-III code were incorporated into MELCOR as an alternative EOS [72, 73]. Furthermore, an alternative EOS model was implemented into MELCOR 2.1 to provide a more general means of specifying alternate working fluids. In support of fusion safety research, Idaho National Laboratory (INL) modified MELCOR 1.8.5 to include lithium and other metallic fluid [74]. This database is called herein the Fusion Safety Database (FSD). A soft-sphere model [75] is used to fit thermodynamic equations to an experimental database. This model starts with the Helmholtz equation for free energy and adjustments to parameters are made in fitting the equation to data.

The implemented EOS models were verified by performing simple tests running the calculation over a wide range of thermodynamic conditions to verify that the code could reproduce the database upon which the model was built. Simple test cases containing a single test volume with a working fluid in a closed system was subjected to external enthalpy sources. These tests were particularly challenging because they covered a very broad range of test conditions extending from very low pressure near the freezing point to near critical pressures. Although the test problems did not run to completion for all three cases due to small time steps, the resulting plots from these runs demonstrate that the addition of working fluid other than water is possible for MELCOR. Note these problems were created to test extreme conditions of fluid properties and they demonstrate that the database for viscosity, thermal conductivity, compressibility, saturation curve, and saturation densities is well modeled (Figure B-2 to Figure B-7).

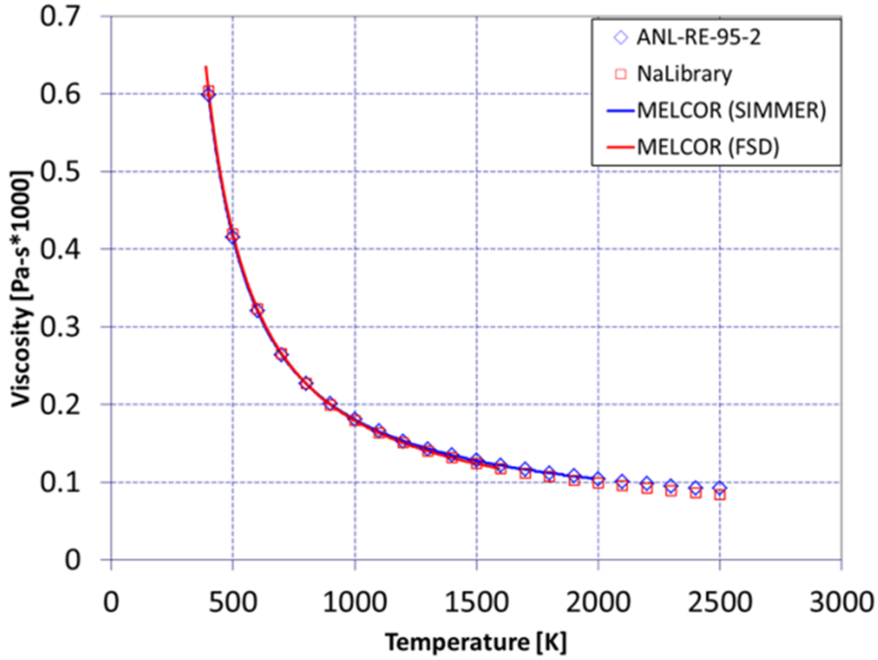

Figure B-2. Sodium viscosity

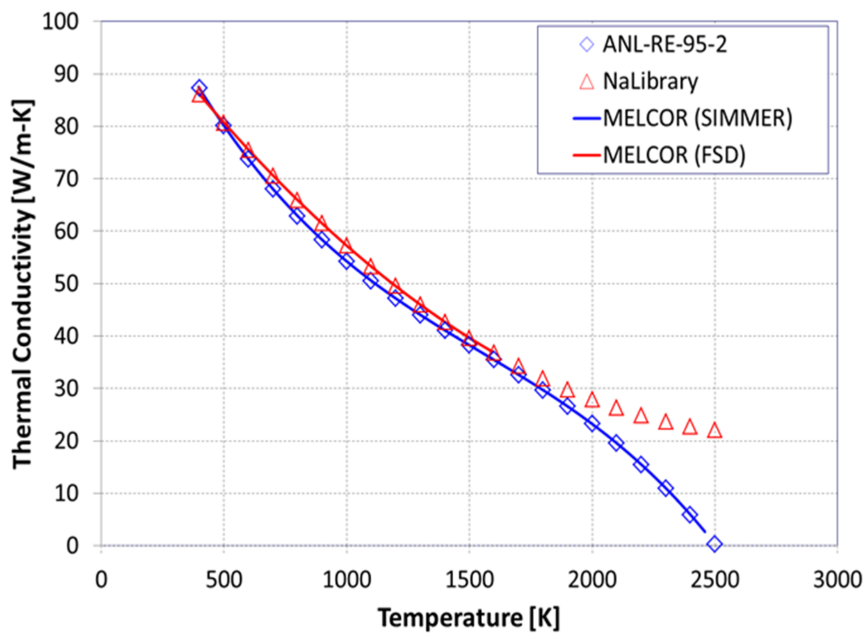

Figure B-3. Sodium thermal conductivity

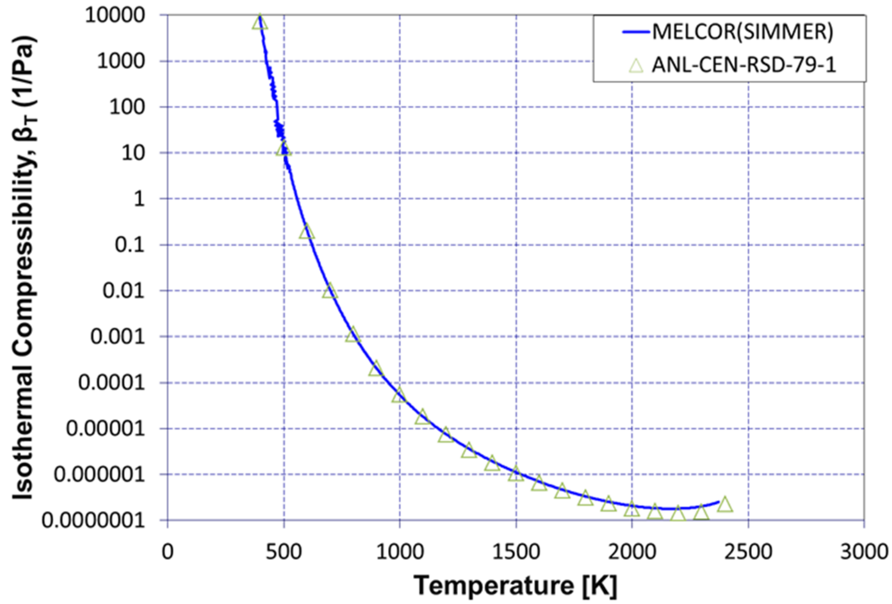

Figure B-4. Isothermal compressibility

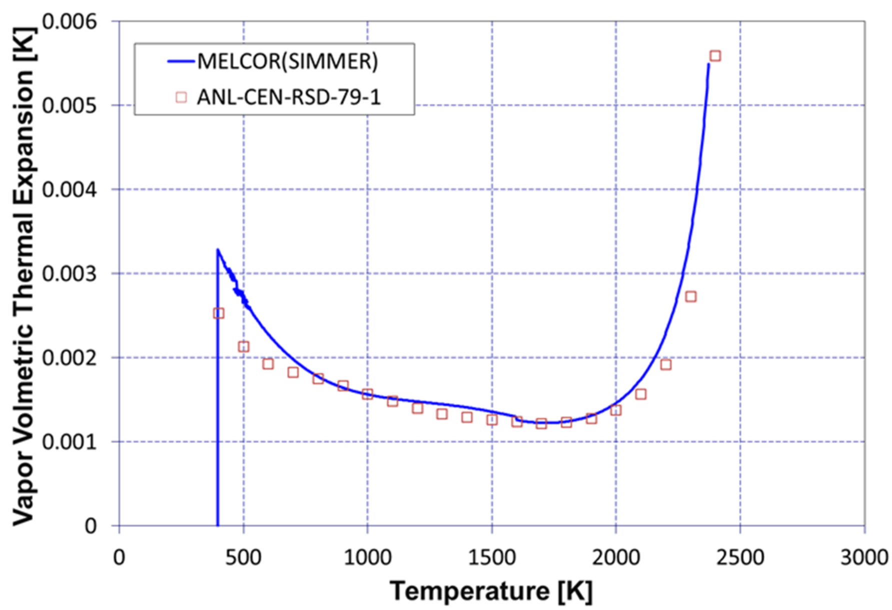

Figure B-5. Volumetric thermal expansion

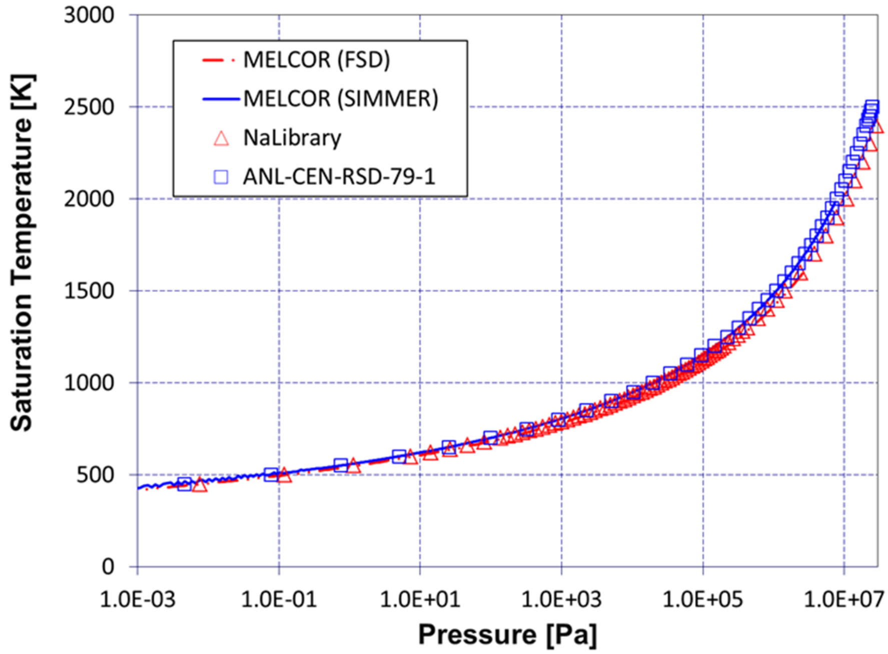

Figure B-6. Sodium saturation temperature

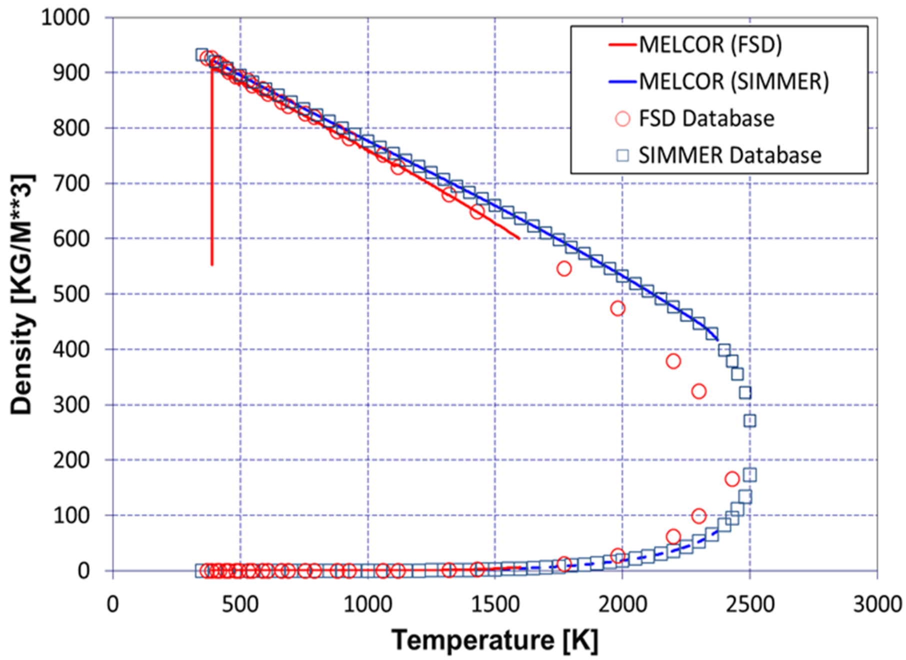

Figure B-7. Sodium density

<u>Containment Sodium Physics Models</u>

Models for containment sodium physics (sodium pool fires, sodium spray fires, sodium atmospheric chemistry) have been added to the MELCOR code. These models are based on those developed or implemented into the CONTAIN/LMR code. A more detailed description has been previously documented [76].

Sodium Pool Fire

This sodium pool fire model is taken from CONTAIN/LMR which is based on the SOFIRE II code developed from the results of pool fire tests. This model predicts the rate of oxygen and sodium consumption as well as the heat of reaction as follows:

$$\mathbf{(1+f_1)\cdot 2\cdot Na + O_2 \rightarrow 2\cdot f_1\cdot Na_2O + (1-f_1)\cdot Na_2O_2 + q(reaction)}$$

Where: $\mathrm{f_1}$ is the fraction of total oxygen consumed that reacts to form monoxide, and $\mathrm{q(reaction)}$ is 9.04540×10^6 J/kg and 1.09746×0^7 J/kg for the monoxide and peroxide, respectively. The sodium burning rate calculated by this model depends on the rate of diffusion of oxygen from the atmosphere to the sodium pool which is a function of the temperature differences between the pool and atmosphere. This difference is assumed to set up turbulent natural convection above the pool. Radiative heat transfer between the pool surface and its surroundings may affect the burning rate.

Sodium Spray Fire

The sodium spray fire model is also taken from CONTAIN/LMR and is based on the NACOM model developed and tested at Brookhaven National Laboratory. In this model, an initial size distribution with eleven size bins is determined from a correlation using a specified mean droplet diameter that is specified by the user. A downward flow of drops falling at the terminal velocity is assumed and it is assumed that there is no interaction between droplets. The combustion rate of the spray fire is integrated over the droplet's fall to obtain the total sodium burned mass, as functions of droplet size, fall velocity and atmospheric conditions. An enhancement was added allow the user to specify the initial velocity for the droplets, making it possible to model an upward directed sodium spray. A droplet acceleration model then calculates the droplet velocity as a function of time in the Lagrangian integration.

Atmospheric Chemistry Models

The sodium chemistry models from CONTAIN/LMR are also implemented in MELCOR 2.2. These models do not explicitly model reaction kinetics. The intimate contact of the reactants in the atmosphere would result in very fast reaction times and it is expected that the assumption is valid there. For reactions between the atmosphere and aerosols deposited on surfaces, kinetics is also ignored for simplicity and may be justified in that such interactions are not significant. For the reaction of atmospheric sodium and surface water, the reaction rate is limited by the evaporation rate of water.

The following reactions are considered for sodium chemistry:

- $\mathrm{Na(l) + H_2O\ (l) \rightarrow NaOH(a) + \frac{1}{2}H_2}$
- $\mathrm{2\ Na(g,l) + H_2O\ (g,l) \rightarrow Na_2O(a) + H_2}$
- $\mathrm{2\ Na(g,l,a) + \frac{1}{2}O_2\ or\ O_2 \rightarrow Na_2O(a)\ or\ Na_2O_2(a)}$
- $\mathrm{Na_2O_2(a) + 2\ Na(g,l) \rightarrow 2\ Na_2O(a)}$
- $\mathrm{Na_2O(a) + H_2O\ (g,l) \rightarrow 2NaOH(a)}$
- $\mathrm{Na_2O_2(a) + H_2O\ (g,l) \rightarrow 2NaOH(a) + 0.5O_2}$

These reactions are assumed to occur in hierarchal order, in the order shown above. It is also assumed that reactions in the atmosphere occur before surface reactions.

MELCOR Implementation and the NAC Package

With respect to the status of MELCOR implementation, various physical and chemical models are complete (data structures built, MELGEN input processing code written, physics model subroutines implemented) including atmospheric chemistry and spray/pool fires. These have been implemented into source code via a new physics package (the so-called "NAC" package) developed to handle sodium physics and integration with existing MELCOR physics packages like CVH and RN. The "NAC" package is responsible for managing data structures, acquiring user input, executing physics models, and interfacing with other code packages. This package is activated upon the identification of sodium as the working fluid. The package adds new RN classes required for modeling sodium chemistry, i.e., H_2O, Na, NaOH, Na_2O, and Na_2O_2 (at a minimum). Furthermore, this package manages the execution of various sodium models, such as atmospheric chemistry, sodium spray/pool fires, and generation of by-products from sodium combustions/burns. In addition, input/output processing for all sodium models is managed through the NAC package:

- New input records for users to provide information
  - Tentatively a new record or tabular record for each phenomenological model (to select options, provide parameters, etc.)
  - Includes sensitivity coefficient input capability for the NAC package
  - NAC_INPUT for activation of models
  - NAC_RNCLASS for user-defined mapping of reaction products to RN classes
  - NAC_ATMCHEM to activate sodium chemistry in certain control volumes and to specify certain parameters about sodium/oxygen reactions
  - NAC_SPRAY to handle sodium spray mass/energy source specification in a control volume
  - NAC_PFIRE to handle sodium pool fire and pool heat transfer specification (oxidation product allocation and sensible heat split between pool and atmosphere)
  - Others for the eventual two-condensable model, sodium/concrete models, etc though it may turn out that new capabilities for sodium physics are grafted on to existing physics packages

Note that any physics models added in the future will interface through the NAC package.

Verification/Validation/Demonstration Problems

Testing is underway for the sodium pool fire and spray fire models as part of the DOE funded work. The spray fire model will be validated against the ABCOVE AB5 and SURTSEY T-3 experiments while the pool fire model is being validated against the ABCOVE AB1 experiment. At this point the testing has focused on verification of the model implementation into MELCOR and full model validation will follow. The models implemented in MELCOR are fully derived from the models implemented in the CONTAIN/LMR code so a code-to-code verification is performed. In this regard, there are differences in modeling capabilities for the MELCOR and CONTAIN/LMR codes outside the fire models, and therefore the verification comparisons may not exercise all the optimum modeling choices in favor of obtaining closer comparisons between the two codes. As an example, CONTAIN/LMR is unable to calculate the heat loss from the outer surfaces of heat structures, uses only a constant value of heat transfer coefficient for the convective surfaces of heat structures, and only models radiation from heat structures surfaces and the sodium pool surface and does not model radiation between heat structure surfaces. For verification, rather than exercising such capabilities in MELCOR, these were disabled in favor of generating more similar results to verify proper implementation.

ABCOVE AB1 Sodium Pool Fire Test

The ABCOVE AB1 test, conducted at the Containment System Test Facility (CSTF) facility at Hanford Washington, generated an experimental database for benchmarking models for the simulation of a sodium pool fire. Though the test was 'conducted to develop baseline data for follow-on air cleaning tests,' it provides an invaluable experimental resource for a sodium pool fire under dry conditions, providing data on aerosol behavior as well as thermal and pressure response of the containment. Sodium was burned in a 4.38 m^2 pool for one hour and aerosols generated were monitored both during the fire and up to 50 hours following the termination of the fire. Aerosol depletion was entirely from passive processes.

Table B-1. Boundary conditions for AB-1 test

INITIAL CONTAINMENT ATMOSPHERE	PARAMETER
Oxygen Concentration	19.8%
Temperature (mean)	299.65K
Pressure	0.125MPa
Dew Point	283.15K
Na POOL	PARAMETER
Na Source Rate	11.1 g/s
Source Start Time	0 s
Spray Stop Time	3600 s
Total Na Spilled	410 kg
Initial Na Temperature	873.15 K
Burn Pan Surface Area	4.4 m^2
Burn Time	3600 s
Total Sodium Oxidized	157 kg
OXYGEN CONCENTRATION	PARAMETER
Initial O_2 Concentration	19.8 vol %
Final O_2 Concentration	14.7 vol %
Oxygen Injection Start	60 s
Oxygen Injection Stop	840 s
Total O_2	47.6 m^3 (STD)
CONTAINMENT CONDITIONS DURING TESTS	PARAMETER
Maximum Average Atmosphere	552.15 K
Temperature	366.65 K
Maximum Average Steel Vessel	0.142 MPa
Temperature	233.15 K
Maximum Pressure	39.9 kg
Final Dew Point	0.255
Total Aerosol Released as Na	
Fraction of Oxidized Na Released	

Boundary conditions for this test are summarized in Table B-1. Atmospheric conditions are well characterized by temperature measurements at 44 locations within and outside the containment vessel, transient pressure response by a diaphragm-type transducer with backup measurements from a Bourdon pressure gauge, Pre- and post-test oxygen concentrations, and sodium concentration through in-vessel cluster samplers, through-the-wall filter samples, deposition coupon samples, and cascade impactor samplers throughout the test conduct.

A diagram showing the main features of the CSTF facility as well as the MELCOR representation of the test vessel are depicted in Figure B-8. CSTF test apparatus and single volume MELCOR representation. The vessel is represented by a single control volume in contact with heat structures representing vessel walls, vessel upper head, internal structures, vessel lower head, and the test pan. Note that heat structures not only exchange energy through convection with fluid and radiation to the sodium pool surface, but can also receive aerosol deposition from the atmosphere. A similar representation is made for the CONTAIN/LMR code. A single cell is modeled with radiation between heat structure surfaces and pool surfaces and adiabatic conditions on the outer vessel surfaces. In addition, water vapor was not modeled in the atmosphere to agree with the MELCOR representation.

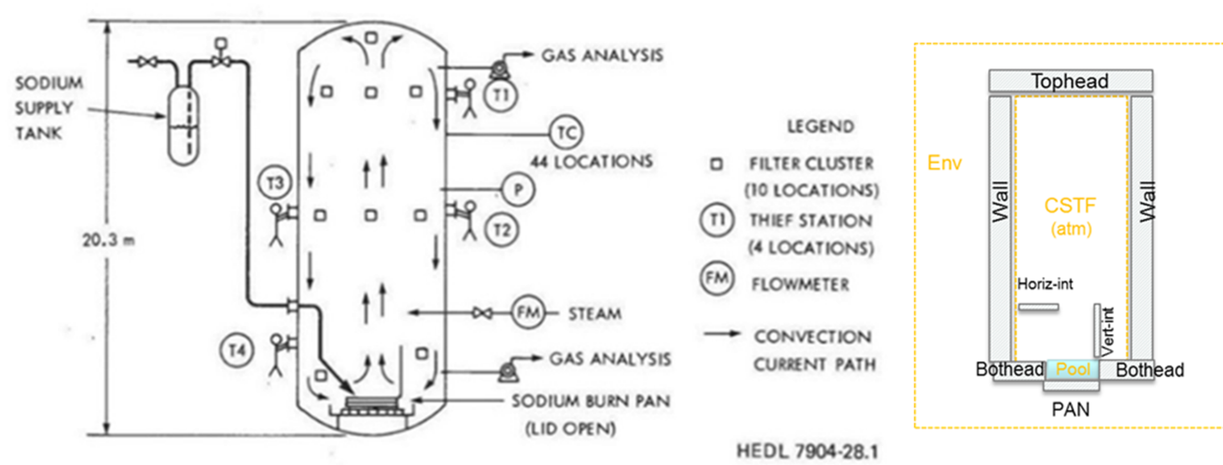

Figure B-8. CSTF test apparatus and single volume MELCOR representation

Results from the two code calculations were compared to show similarities in combustion rate, the containment thermal response, and the aerosol characteristics. The rate of oxygen mass consumption and the combustion energy distribution to the atmosphere and pool show almost exact agreement between the two calculations as indicated in Figure B-9 and Figure B-10. There are slight differences in both the atmospheric temperature as well as the pool temperatures calculated for the two cases. For both atmosphere and pool, MELCOR predicts a slightly higher temperature, possibly indicating a smaller heat loss to heat structures predicted by MELCOR. MELCOR also predicts a slightly higher-pressure response which is consistent with the higher temperatures predicted. It should be noted that both the CONTAIN/LMR and MELCOR temperature responses are within the uncertainty of the measured temperature response. Finally, the suspended aerosol mass is plotted in Figure B-14 (log-log scale) and in Figure B-15 (linear scale). Both codes predict reasonable agreement though the MELCOR prediction more closely follows the trends in the experimental data.

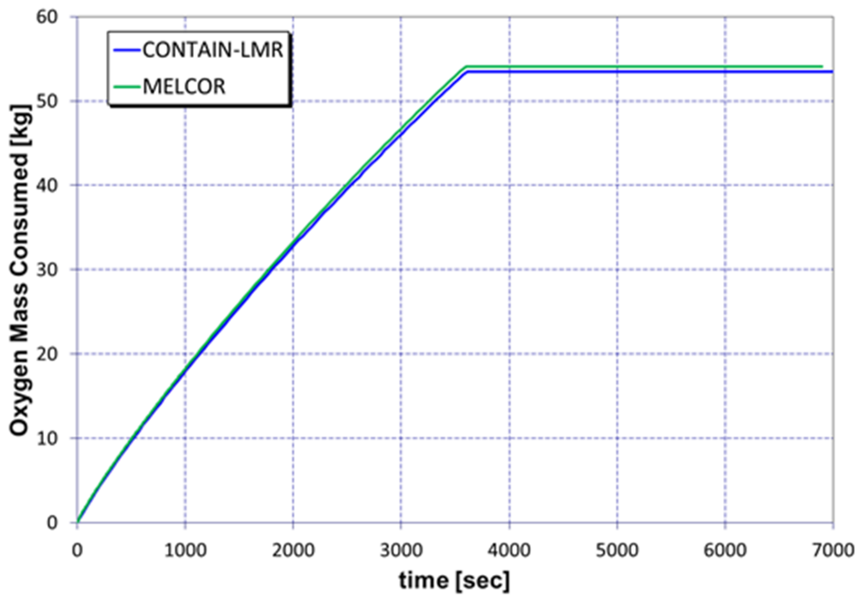

Figure B-9. Oxygen consumption in AB1

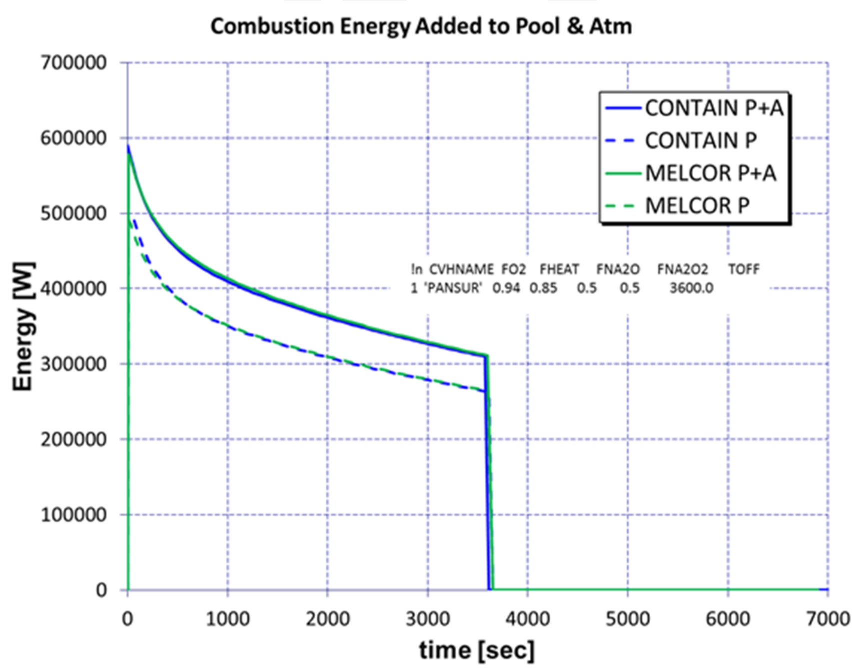

Figure B-10. Combustion energy in AB1

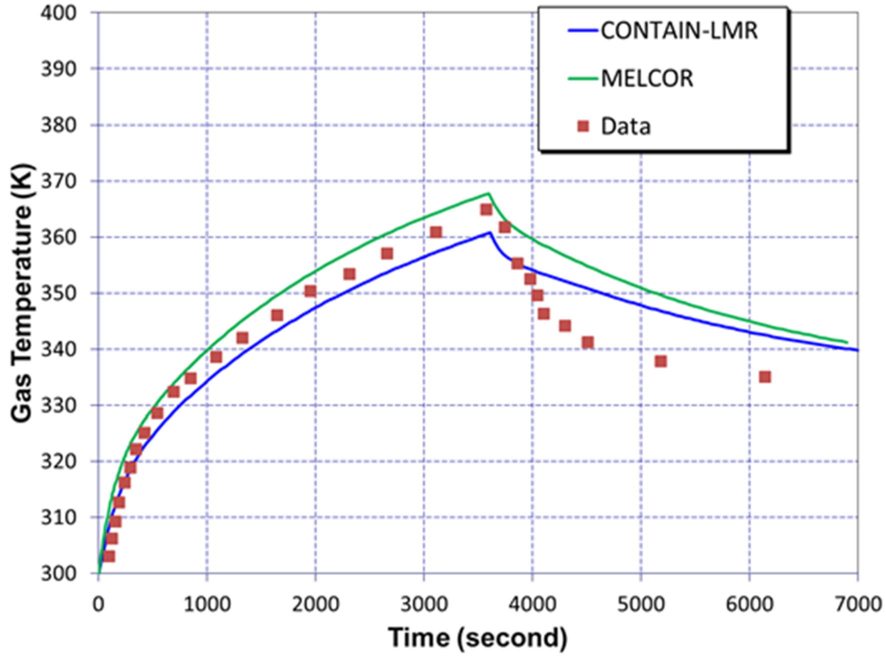

Figure B-11. Atmospheric temperature - AB1

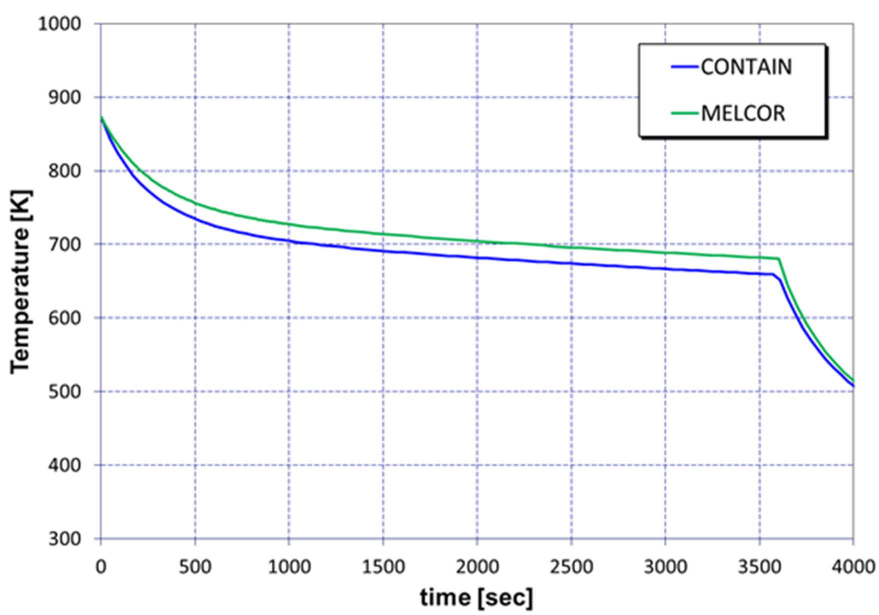

Figure B-12. Sodium pool temperature - AB1

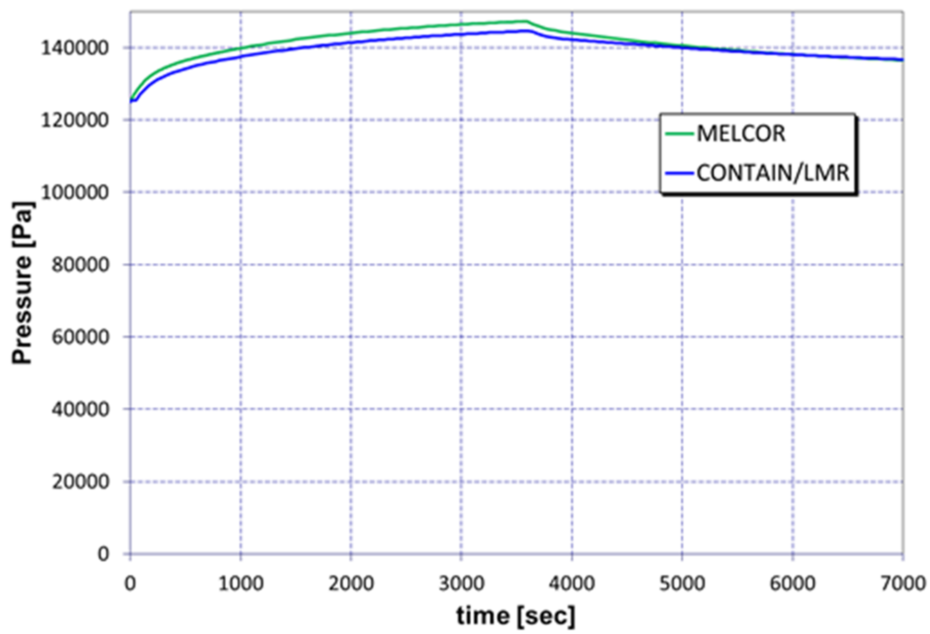

Figure B-13. Containment pressure response - AB1

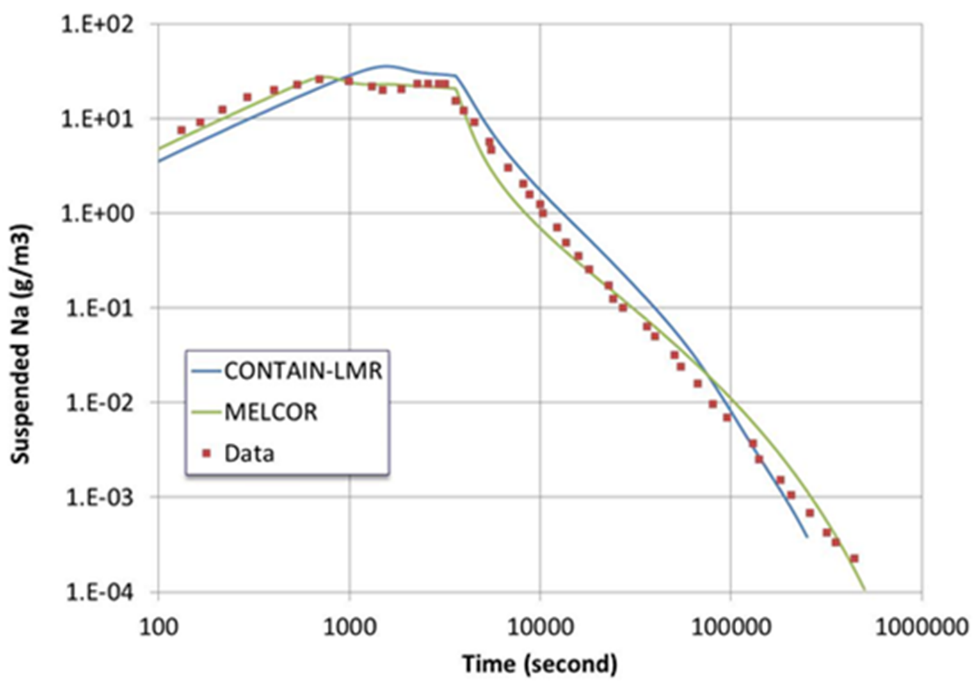

Figure B-14. Suspended Na aerosol mass - AB1

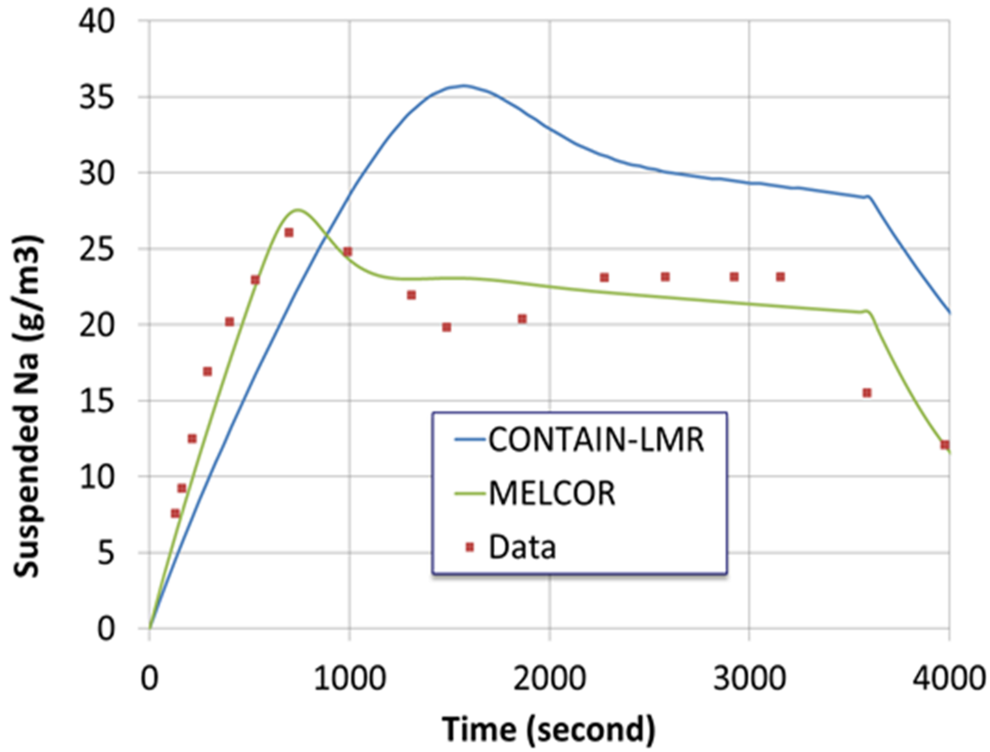

Figure B-15. Suspended Na aerosol mass - AB1

ABCOVE AB5 Sodium Spray Fire Test

The primary objective of the ABCOVE AB5 test was to provide experimental data for use when validating aerosol behavior computer codes for the case of a moderate-duration, strong, single-component aerosol source generated by a sodium spray in an air atmosphere. A secondary objective was to provide experimental data on the temperature and pressure in the containment vessel and its atmosphere for use when validating containment response codes.

Table B-2. Boundary conditions for AB-5 test

AB5	
INITIAL CONTAINMENT ATMOSPHERE	PARAMETER
Oxygen Concentration	23.3±0.2%
Temperature (mean)	302.25K
Pressure	0.122MPa
Dew Point	289.15±2K
Nominal Leak Rate	1%/day at 68.9kPa
Na SPRAY	PARAMETER
Na Spray Rate	256±15g/s
Spray Start Time	13s
Spray Stop Time	885 s
Total Na Sprayed	223±11 kg
Na Temperature	836.15 K
Spray Drop Size, MMD	1030±50 µm
Spray Size Geom. Std. Dev., GSD	1.4
OXYGEN CONCENTRATION	PARAMETER
Initial O_2 Concentration	23.3±0.2 vol %
Final O_2 Concentration	19.4±0.2 vol %
Oxygen Injection Start	60 s
Oxygen Injection Stop	840 s
Total O_2	47.6 m^3 (STD)
CONTAINMENT CONDITIONS DURING TESTS	PARAMETER
Maximum Average Atmosphere Temperature	552.15 K
Maximum Average Steel Vessel Temperature	366.65 K
Maximum Pressure	213.9 kPa
Final Dew Point	271.65 K

As was done for AB1, a single cell is used in the CONTAIN model representation. The walls, floor and roof of the vessel are modeled, including the internal deposition components. A summary of the test conditions for ABCOVE AB5 is provided in Table B-2. Since the aerosol results showed no monoxide formed (60% Na_2O_2 and 40% NaOH), the input value for the peroxide is set to 1.0. In order to model NaOH formation, the water vapor mass of the dew point from the test was included.

Again, results for the spray fire test as calculated by CONTAIN/LMR and MELCOR are very similar. Oxygen consumption rates and energy generation rates are nearly identical. Again, MELCOR predicts a slightly higher atmosphere temperature along with a corresponding higher containment pressure but the differences are still very small. Also, MELCOR produces a more representative sodium concentration in the atmosphere. Overall, the agreement is excellent and the differences are consistent with the AB1 test results.

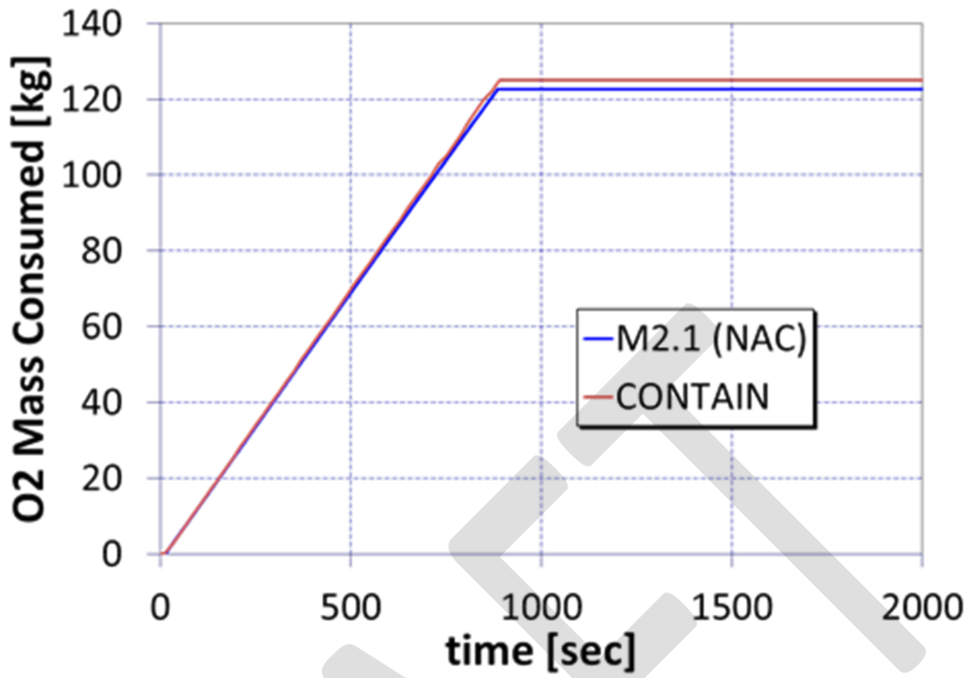

Figure B-16. Oxygen mass consumption for AB5

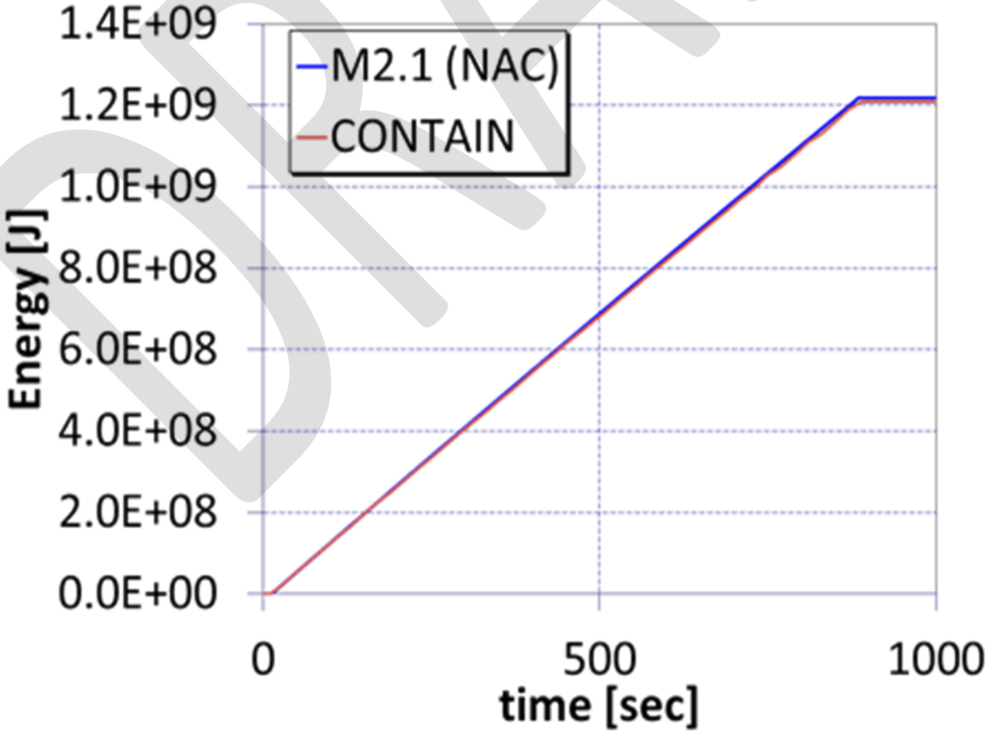

Figure B-17. Combustion energy for AB5

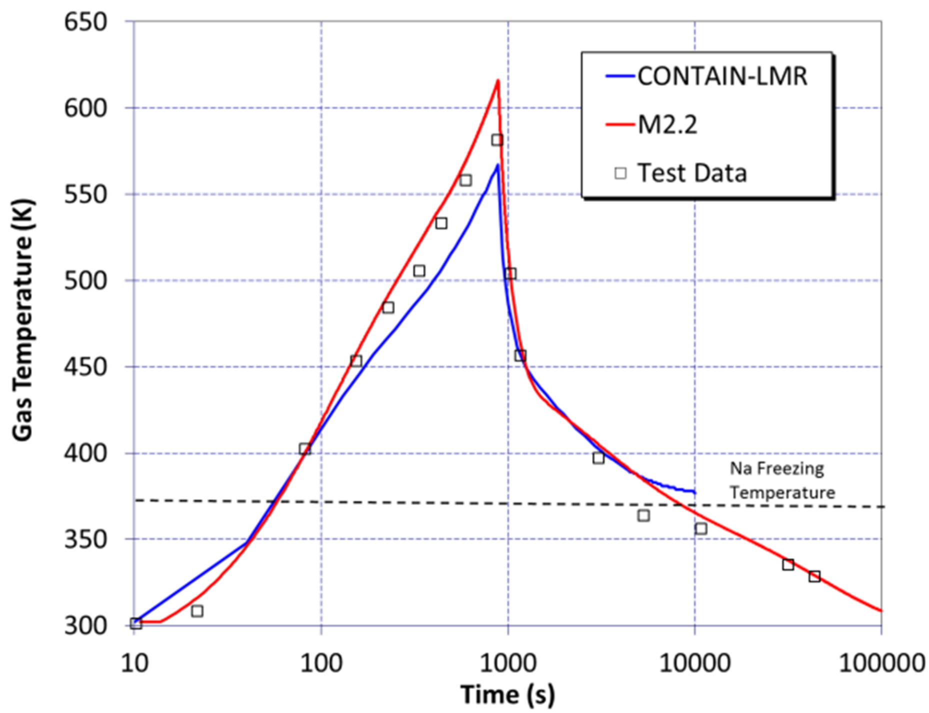

Figure B-18. Atmospheric temperatures for AB5

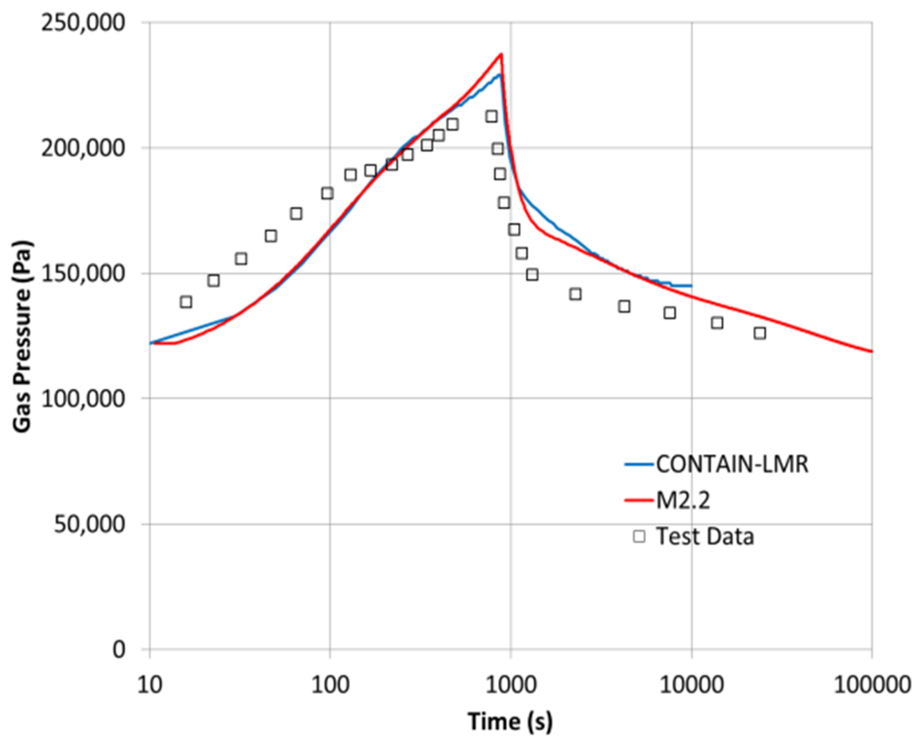

Figure B-19. Atmospheric pressure for AB5

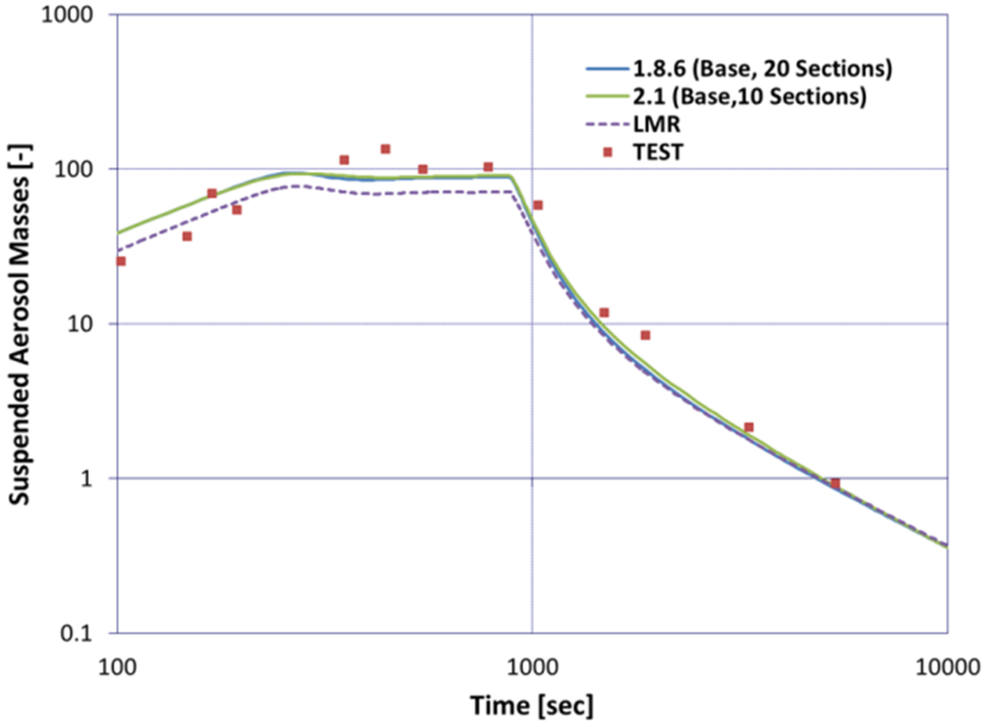

Figure B-20. Suspended aerosol masses for AB5

B.3.2. CURRENT DEVELOPMENT WORK

The previously described containment models were recently added to MELCOR 2.2 and verified under funding from DOE whereas current development work performed under U.S. NRC funding has been related to verification efforts of the equation of state. It is recognized that both verification and validation of these new models for sodium is essential so we are performing code-to-code comparisons with existing codes such as SAS4a for modeling sodium reactors. Initial calculations will investigate steady state performance, followed by recovered accident transients. As newer core degradation models are added, these will also be benchmarked with existing codes. For reference, a brief summary of the SAS4A code is provided in Appendix D.

As an initial steady state benchmark calculation, the Advanced Burner Test Reactor was considered. This proposed reactor was well studied by Argonne National Laboratories with several steady state and transient accident characterizations. A steady state response under design conditions was modeled with MELCOR and compared against SAS4A calculations.

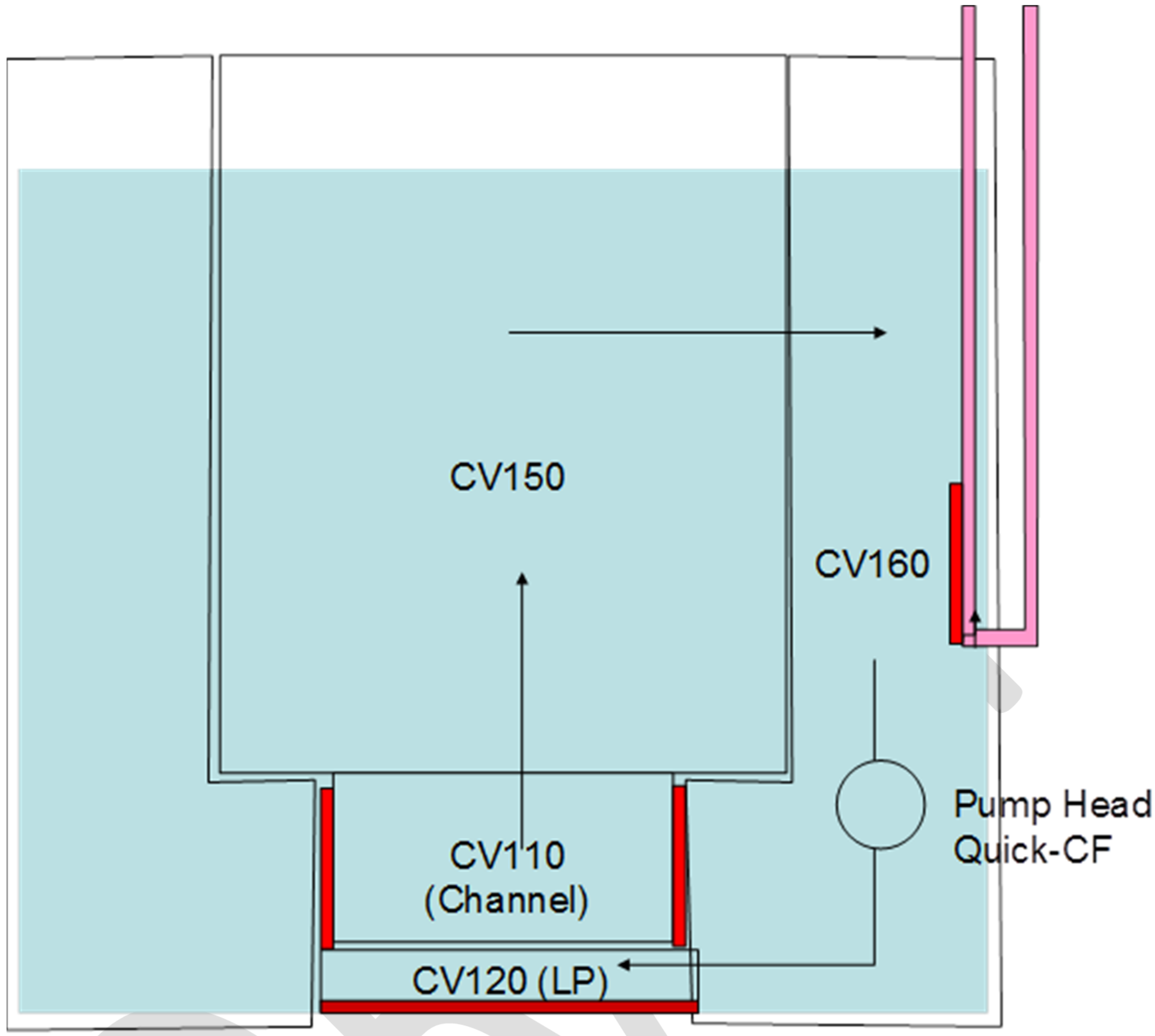

Figure B-21. Nodalization diagram

Parameter	MELCOR	SAS4A
Core		
Rx Power (MW)	252	250
Heavy Metal (MT)	4.03	4.03
Fuel Outer Radius (mm)	3.48	3.48
Clad Outer Radius (mm)	4	4
Gap Thickness (mm)	0	0
Rod/Coolant Area (m^2)	130.89	130.89
Active Core Height (m)	0.8	0.8
Peak linear power, kW/m	50	38.5
Core Flow (kg/sec)	1651	1264
Tinlet	652	628
Toutlet	769	783
Maximum Clad	819	823
Maximum Fuel	872	910
Core Temperature rise (K)	117	155
Core Pressure drop (kPa)	814.119	
D_{eq}	0.003	0.00336
Form Loss Σ K	1.5	1.5
Flow Area	0.32	0.32
L	3	3.05
Q/mdot/dT (Joule/kg/K)	1304.571	1276.031033
Cp (Joule/kg/K)		1258
Density (kg/m^3)	828	828 @ 800 K
IHX		
Heat Transfer Area (m^2)	2.522586	
Primary Flow Rate (kg/sec)	873.5	628
Primary Inlet T (K)	771	783
Primary Outlet T(K)	650	628
Primary Pressure Drop (Pa)	6800	12600
Secondary Flow Rate (kg/sec)	527.5	628
Secondary Inlet T		606
Secondary Outlet T		761
Secondary Pressure Drop (Pa)	6000	5700
	1192.126	1284.158619
Pump		
Flow (kg/sec)	436.75	316.1
Pressure Head (kPa)	814	758

Figure B-22. Steady-state variables

Future Development Work

Future development work should be done for several of the models mentioned in the previous section and validation work should continue for existing models (sodium atmospheric chemistry and sodium spray/pool fires). Work should begin on other in-vessel and ex-vessel phenomenological modeling including construction of data structures, creation of input acquisition code, and actual coding of mathematical models. Any development in the future should be done within the context of the new NAC package. In all likelihood, future development targeting SFR in-vessel phenomena will be informed by SAS4A. Future development targeting SFR ex-vessel phenomena will rely heavily on CONTAIN-LMR. Exploration in these areas is underway and will continue in the future.

There are several models pertaining to source term and/or safety analysis that may require development or adaption from existing models. Among these phenomena are:

- Hot gas layer formation during sodium fires (impacts reaction rates, aerosol transport)
- Radionuclide entrainment near pool surface during sodium fires
- Fission product release models.
- Radioisotope decay (tracking transitions between RN classes due to decay transitions)

B.4. DESIGN SPECIFIC MODELS – OKLO HEAT PIPE REACTOR

In addition to the general models recommended above, specific design concepts may require additional model development. For example, the OKLO heat pipe reactor design is a unique design utilizing heat pipes to remove energy from the reactor core. Heat pipes are placed vertically in the core, extending upward to a heat exchanger situated above the core. The core thermal energy is carried away by sodium heat pipes, based on the principles of evaporation and condensation. As heat from the core is transferred to the liquid sodium at the lower end of the heat pipe the sodium evaporates, rising to the upper end of the heat pipe where heat is then transferred to the heat exchanger as sodium condenses on the wall of the heat pipe. The condensed sodium then flows down the heat pipe wall via a wick structure. Each heat pipe represents a closed system. Decay heat would either be removed by the sodium heat pipes or radially and axially conducted through the reactor vessel into surrounding regions.

COR Package Components

The OKLO fuel cell is designed as an annular fuel region, with a cylindrical core representing the heat pipe. This geometry would require a new fuel component (modification to existing fuel component) since the effective coolant channel is now internal to the fuel cell and the fuel region is not cylindrical and may be interspersed with a sodium bond. The duct surrounding the fuel cell and the heat pipe walls would also need to be represented by a new (or by a modified) COR component.

A third COR package component would be developed to represent the heat pipe which would account for sensible heat, conduction, melting and degradation. Axial radiation for this new component can be modeled using one of several existing radiation exchange generalizations that have been added to MELCOR 2.2.

Failure of a heat pipe within one fuel assembly would result in heat being transferred radially to neighboring fuel assemblies which may challenge boundary condition assumptions in MELCOR's ring models. These new fuel cell components could be extended using the existing multi-rod model for assessment of propagation from localized failures.

Fuel Material

The OKLO reactor uses metallic U-10wt%Zr fuel in a steel alloy heat pipe wall and is surrounded by a steel alloy duct. MELCOR must be modified with new fuel properties and associated models for fuel expansion, foaming, melting, and the fission product release (i.e., gap release). If elevated temperatures can be achieved intermetallic reactions could be important. Initial release fractions for metallic fuels of some volatile fission products such as Cs and I are typically expected to be similar to those of UO_2 fuel, but Ba, Sr, Ce, and La releases from metallic fuel would be expected to be somewhat higher than for UO_2 fuel. However, OKLO's fuel is operated at lower linear power levels and to a lower burnup than historical U-10wt%Zr fuels and may correspond to a lower radionuclide release potential.

Sodium Coolant

The OKLO design is based on sub-atmospheric, approximately 0.8 atm, sodium coolant flowing inside individual vertically oriented closed ended pipes (heat pipes). Recent model development in MELCOR has added both an equation of state as well as thermal-mechanical properties for a sodium fluid though it would need to be verified for sub-atmospheric conditions. While the current code will only treat a single working fluid, future code development could allow the user to specify more than one working fluid for a heat exchanger.

Sodium is strongly reactive with oxygen and moisture in the atmosphere which may become important as sodium may potentially leak from systems under accident conditions. Such reactions will be modeled by the chemistry models which are currently under development funded by DOE. In addition, the potential for sodium fires in the containment exist which can already be modeled with new sodium spray and pool fire models recently developed for DOE.

Primary Heat Removal System

A unique and important feature of the OKLO design are the heat pipes for passively rejecting heat from the reactor core. Failure of a heat pipe will result in local degradation of heat removal and creates the potential for release of sodium and fission products to the atmosphere.

MELCOR is being adapted to incorporate heat pipe (HP) models of differing levels of complexity and fidelity by defining a common interface that is independent of HP model specifics. This approach defines how any HP model will interface with the COR, CVH, and RN packages, what input is required, and what specific quantities will be passed between these packages. Note that in a heat pipe reactor, the HP model is the "pathway" for energy to be transferred from the fuel in the core to the coolant (i.e. the coolant does not interact directly with the fuel). Likewise, if a HP fails, then the HP model also becomes the "pathway" for radionuclides to move from the fuel to the coolant.

To test and exercise the HP model interface, a simple heat pipe model has been written and added to MELCOR for developmental purposes. Activation of this new type of COR component also invokes modifications to the fuel and cladding component heat transfer models so they can represent the geometrical differences of the fuel and ducting. The current simple model has the correct interface requirements and modeling characteristics needed to debug and test the behaviors that should be modeled during both normal operation and during an accident. Ongoing work is exercising the interface under different conditions to debug, test and refine the approach and its interface to other MELCOR models. For example, figure B-23 shows fuel, coolant, three heat pipe wall temperatures, and the bulk temperature of the heat pipe working fluid for a transient-equilibrium test problem of a MELCOR deck representing a simplified OKLO-like heat pipe reactor. As expected the system moves to a steady state where the energy being released in the fuel is all transferred to the coolant, and the temperatures throughout the system stabilize.

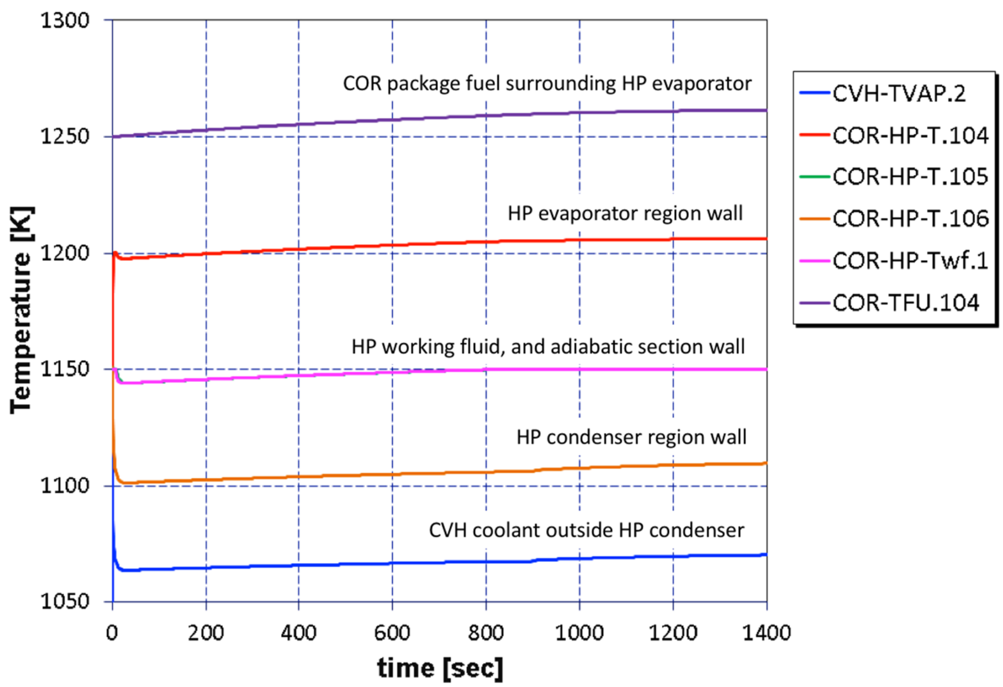

Figure B-23. MELCOR heat pipe temperatures for a transient-equilibrium test problem

The simple heat pipe model currently being used is only of value for development purposes. Using the new heat pipe interface, an improved high-level model (similar to the homologous pump model or counter-current flow model) would be developed using correlations for limits and pressure drops that would give a good approximation of throughput performance and temperature drops, while using simple models for the complicated wick physics. If a higher fidelity model is needed, adding an additional model would be a very straighforward task. As discussed previously, in all cases the heat pipe walls would be modeled by the new "HP" COR component. Heat transfer modeling from the fuel to the heat pipe is important to accurately calculate the heat rejection through the heat pipe. Literature review on MELCOR application to Savannah River K-Reactors in the 90s and EBR-II applications may be needed to refine heat transfer coefficient correlations.

Reactor Kinetics

MELCOR has an internal point kinetics model that can be used in modeling reactivity effects that was developed for HTGR applications. To the extent possible, reactor kinetics would be based on the existing MELCOR models for accident sequences without scram. At this point, no source code changes are envisioned, but the neutronic parameters in the point kinetics model would be re-evaluated to reflect the OKLO reactor application.

B.4.1. DEVELOPMENT STATUS

At present, MELCOR can qualitatively model a transient response of the heat pipe and system to the following transients, up to the point of heat pipe failure: (1) change in system heat loads, (2) sudden loss of heat rejection, (3) sudden power spikes, and (4) slower-time-scale power increases that exceed the heat-pipe heat-transfer limits. Additional work is needed to model failure of the heat pipe walls and subsequent release of degraded material into the COR package and sodium and radionuclides into the CVH package (related to development items M1.2, M1.3, and M1.4 in Table 2-1).

APPENDIX C. MELCOR MODELING OF MSRS

C.1. INTRODUCTION AND BRIEF HISTORY

Molten Salt Reactors (MSRs) - though they date back to the 1950's and though there is limited domestic operating experience - are relatively foreign in concept from a licensing perspective. The international community has shown some interest in MSRs over the years for various purposes, and several design variants have been proposed. Domestically, the Aircraft Reactor Experiment (ARE) and the Molten Salt Reactor Experiment (MSRE) comprise the bulk of experience with molten salt systems. ARE utilized a high-temperature fluoride salt system (fluid-fueled) and the MSRE consisted of a Lithium/Beryllium fluoride (FLiBe) molten salt-cooled/fueled, graphite-moderated core.

In recent years, some private developers of fluid-fueled (i.e. salt-fueled) MSR designs have taken preliminary steps in the licensing process, thus the impetus to develop MELCOR models for purposes of MSR analysis. There are currently no MELCOR models that specifically target MSRs of either the salt-cooled (solid-fueled) or salt-fueled (fluid-fueled) type, but there are existing models that could be leveraged to aid in the modeling process. Solid-fueled and fluid-fueled systems will be addressed separately when discussing MELCOR modeling of MSRs.

C.2. DESIGN ASPECTS

With respect to MSRs in general (regardless of fuel type), design features include:

- Low pressure operation
- Comparatively smaller volume of waste production (vs. LWRs), more utilization of fuel
- Passive cooling by design
- Use of intermediate loops to separate working fluids
- Various power cycles (Rankine, Brayton via helium turbomachinery, etc.)
- Higher outlet temperatures, thermal efficiencies vs currently operating LWRs
- Similarities to SFRs (guard vessel, low pressure system, cover gas, pool type designs, etc.)

Before delving into the two broad types of MSR, general characteristics of molten salts and MSR designs should be discussed. Molten salts tend to have both a higher heat capacity and a larger Prandtl number than water. Thus, they can store more energy than water and they tend to transport energy more readily by convection than conduction as momentum diffusivity dominates thermal diffusivity. This bears relevance for natural circulation cooling strategies. Fluoride salts – a popular choice for fuel salts and/or coolant salts have a long list of desirable properties including [77]:

- Chemical stability, low volatility at high temperature, compatible with air/water
- Stable in a radiation field
- Good fission product retention
- High solubility for uranium/thorium fluorides
- Favorable neutronics (low capture cross sections, good moderation capability)

Turning to salt-cooled (solid-fueled) reactors, the fuel and fuel element designs are similar to those of HTGRs for the most part. Design proposals for this variant of MSR typically rely on carbon moderation (graphite structures) and employ TRISO-fueled elements of either the PBR-type or the PMR-type. Some experimental designs use more unorthodox arrangements such as TRISO-bearing plate fuel elements. To summarize special design features of solid-fuel MSRs:

- Usually graphite-moderated (carbonaceous core structures)
- TRISO fuel in some arrangement (PBR-type pebbles, PMR-type compacts, plate fuel, etc)
- Fluoride salt-cooled (typically FLiBe)
- Thermal spectrum
- Forced circulation or pool-type approaches relying on natural circulation

Considering salt-fueled (fluid-fueled) reactors, fissile/fissionable isotope-bearing salts serve as the nuclear fuel. There is no "fuel element" in a fixed geometry, though fuel salts may flow through designated graphite channels of some given geometry. To summarize special design features of fluid-fuel MSRs:

- Fuel salt and coolant salt flowing together
- Wider range of salts employed (Chloride salts, NaF, ZrF, KF, etc.)
- Thermal or fast spectrum
- On-line fission product clean-up
- Use of freeze plugs and drainage vessels for accident mitigation

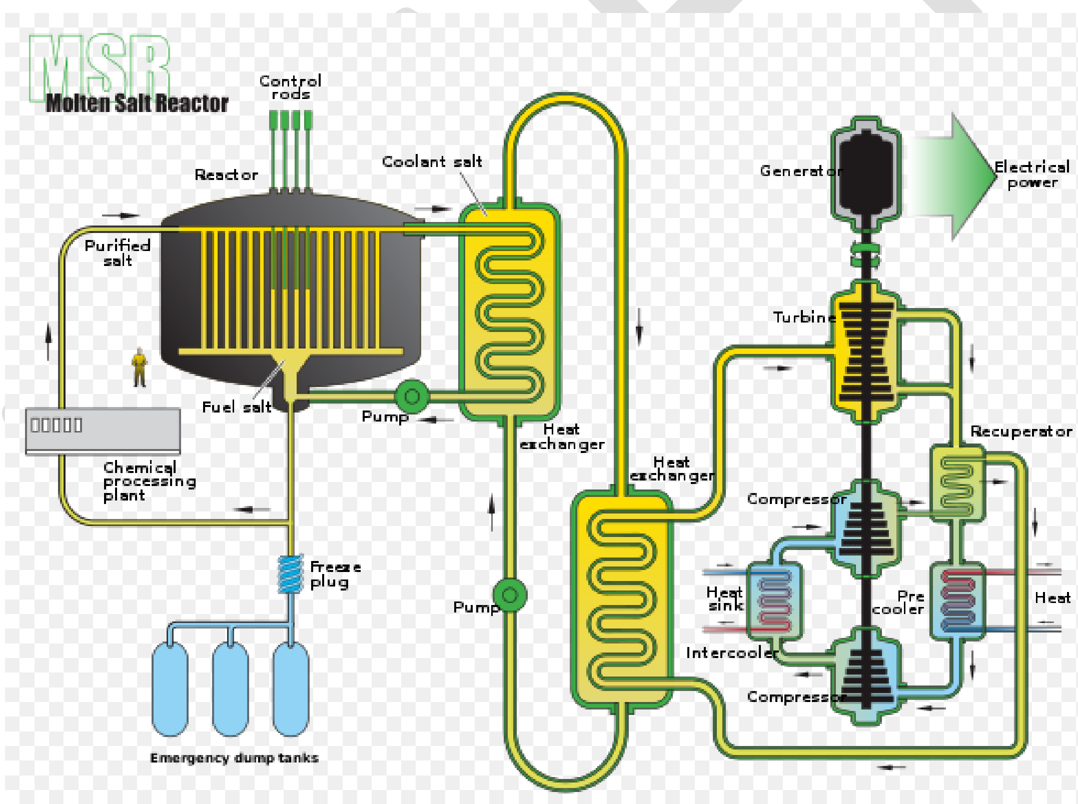

Figure C-1. Salt-fueled MSR conceptual sketch [71]

C.3. MELCOR MODELING

C.3.1. PREVIOUS DEVELOPMENT WORK

Until now, capabilities for modeling MSRs have not existed in MELCOR. Even so, previously developed capabilities for LWRs, HTGRs, and SFRs can be expanded for application to MSRs. As examples, the generic working fluid equation of state libraries which was added for SFRs can be leveraged to develop similar libraries for molten salts. Furthermore, the TRISO fuel models developed for PBR-type or PMR-type HTGRs should be adaptable for use in some salt-cooled (solid-fueled) MSRs.

C.3.2. CURRENT DEVELOPMENT WORK

A working fluid equation of state library was created for LiF-BeF_2 fluids using the soft shell model as described for sodium previously. For molten salts, the Helmholtz equation is modified by an additional term to account for the fact that the original soft sphere model did not adequately model all degrees of freedom of stored energy for Flibe [78]. The property database is based on physical properties published by Oak Ridge National Laboratory [79]. Verification of the EOS library was again performed by a single volume test case that is heated internally at saturation conditions. The test shows that the equations are stable over a large range in pressure from 50 Pa up to 81 MPa where the critical pressure is 1.8 MPa.

<u>Verification</u>

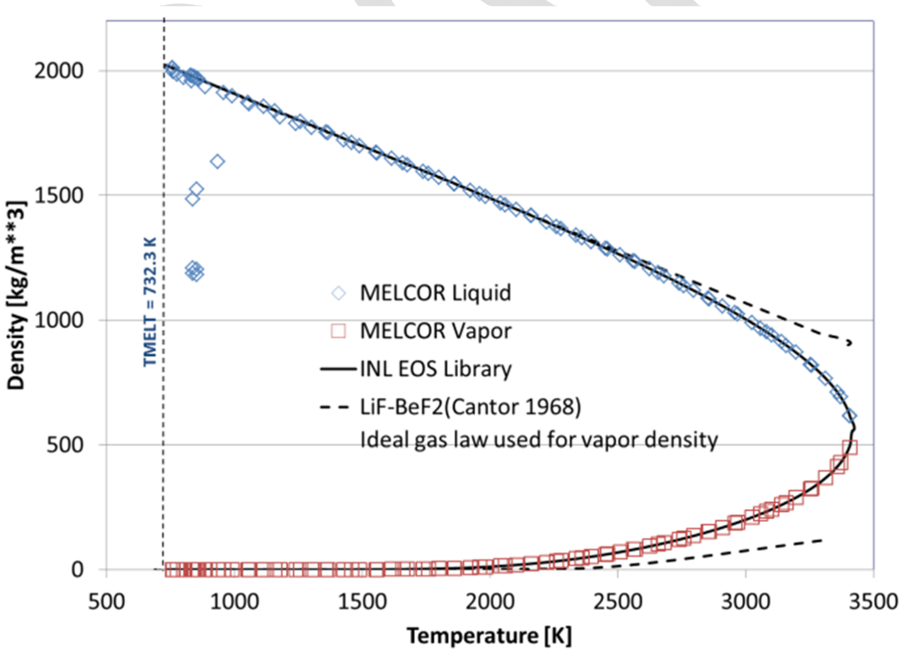

Figure C-2. Li-BeF2 Density curves, saturation

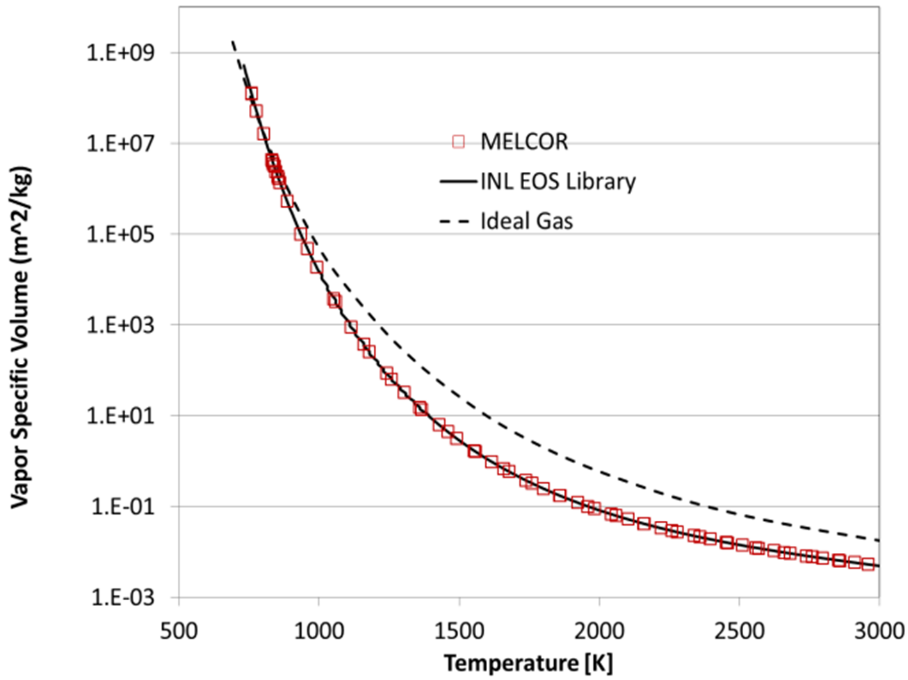

Figure C-3. Vapor specific volume, saturation

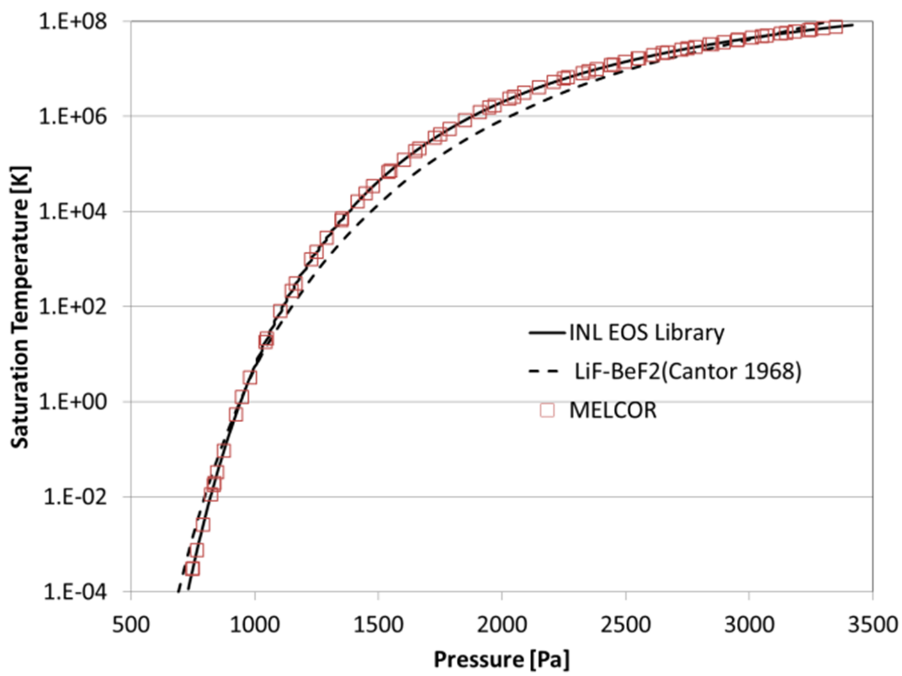

Figure C-4. Saturation curve for LiF-BeF2

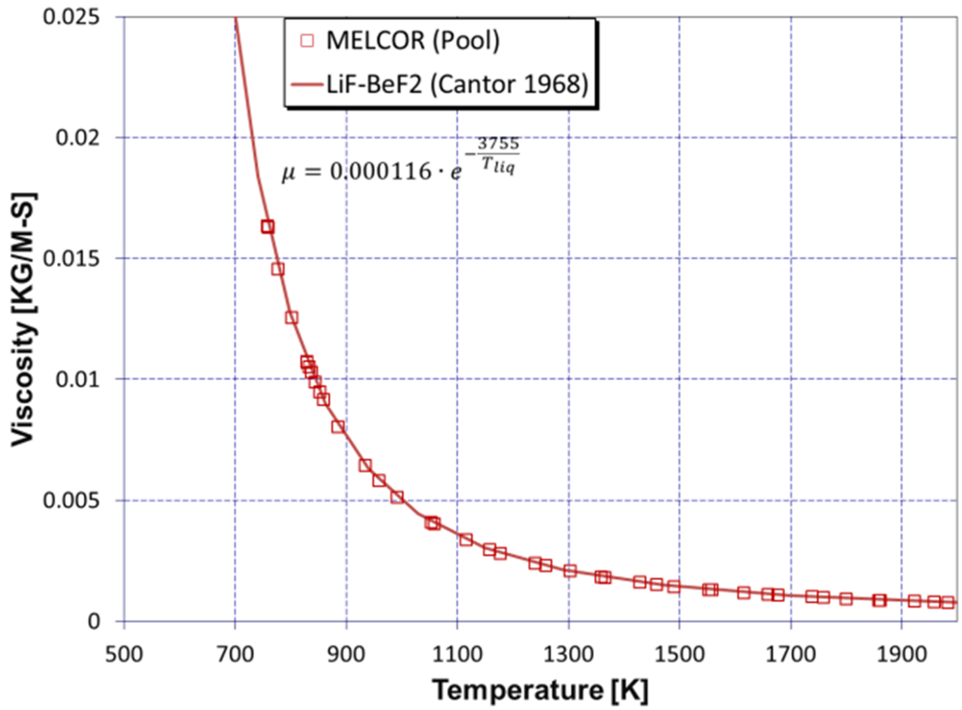

Figure C-5. Viscosity curve for LiF-BeF2

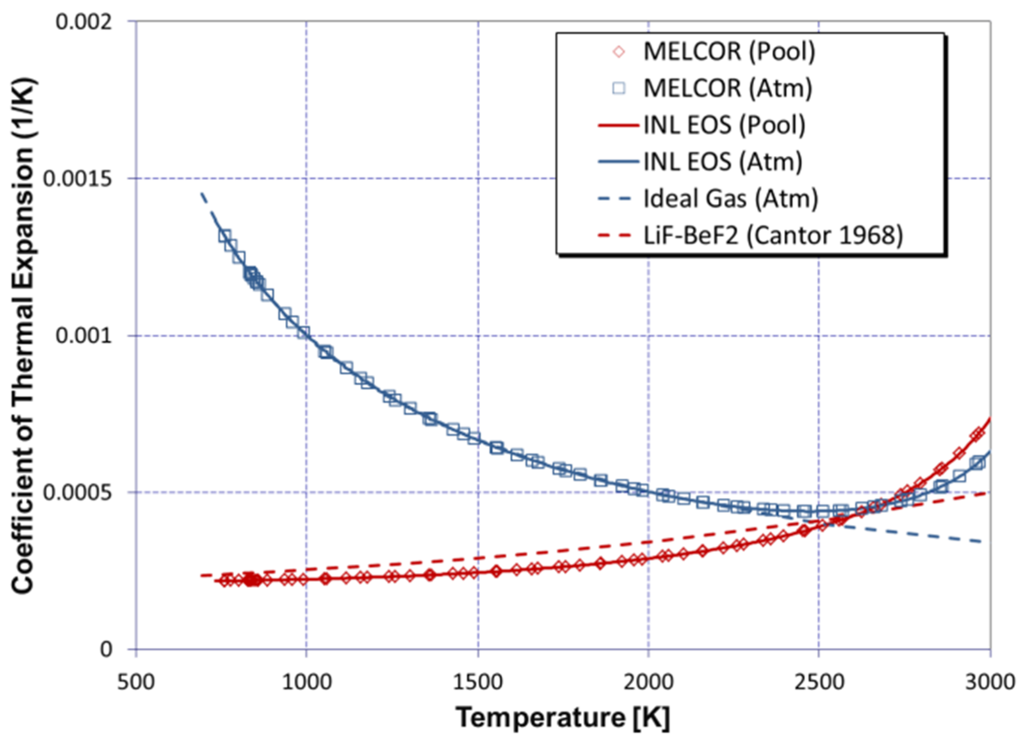

Figure C-6. Coefficient of th. exp. for LiF-BeF2

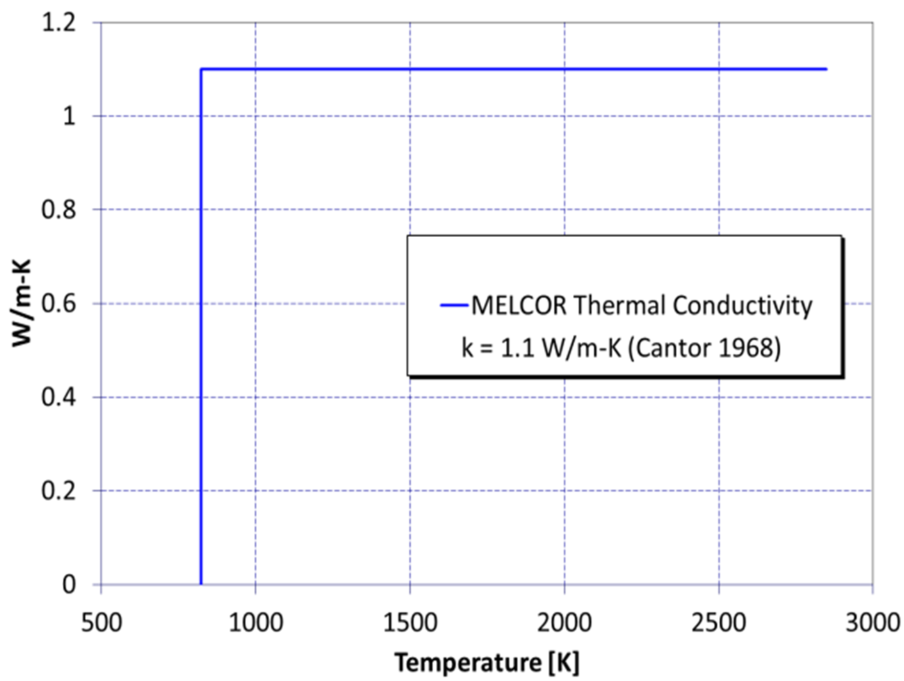

Figure C-7. Th. Cond. for LiF-BeF2

Validation

Validation has not begun on this model. However, the code has sufficient capabilities now to test it against some steady state experiments of the MSRE performed by Oak Ridge National Laboratory (ORNL) between 1965 and 1969. These experiments utilized UF_4 dissolved in a fluoride salt with a power level of ~8MW/s and only considered steady state conditions. This validation test would model the core as control volumes with heat structures representing piping, vessels and graphite moderators.

Future Development Work

Before proposing any future MSR-related MELCOR development tasks, it is helpful to identify some issues particular to MSRs as they will certainly influence modeling efforts. A few concerns include:

- Validation of molten salt and molten salt mixtures as control volume working fluid(s)
- Simultaneous modeling of multiple different working fluids in terms of control volume hydrodynamics, where some or all of the fluids may be condensable species
- Modified chemistry including salt/material interactions
- New aerosol physics that influence radionuclide transport
- Natural circulation modeling with MELCOR control volume and flow path approach
- Special system components and miscellaneous concerns specific to MSRs
  - Power-production side equipment

  - Power-production side exotic working fluids (e.g. supercritical water)
  - In-vessel equipment on the primary side
- Salt-cooled (solid core structure) special concerns
- Salt-fueled (fluid core) special concerns

Modeling the salt-cooled, fixed core geometry reactor fits naturally within the current MELCOR paradigm (rod lattice in a two-dimensional, azimuthally-symmetric cylindrical geometry consisting of a complex of “rings” and “levels). Furthermore, prior work on HTGRs could be leveraged for PBR-type and PMR-type TRISO-fueled MSRs. These HTGR models were described previously and are related to heat transfer, fuel failure, fission product release, etc. Given the fuel designs for some MSR concepts, HTGR MELCOR models could possibly be utilized as-is or after slight modifications. There are perhaps other concerns – generally related to in-vessel and ex-vessel phenomena - that could be identified via a possible PIRT process.

Additional Comments by Dr. Dana Powers

Fission products released from fuel will be trapped, at least temporarily, in the molten salt. To contribute to an accident source term from the nuclear plant, the radionuclides will have to escape from the molten salt to the cover gas that will vent along some leak path to the containment and into the environment. Escape of the noble gases from the molten salt is immediately plausible. I can envisage two primary mechanisms for the escape of other fission products from the molten salt to the gas phase:

- **Entrainment of contaminated molten salt droplets in the gas flow**. The primary mechanism for such entrainment of droplets is of course the rupture of gas bubbles at the molten salt surface. We have not searched for data on the formation of droplets by bubble burst in molten salts other than to know that it occurs in abundance during the “carbon boil” in steel mills. I think that for the purposes of estimation it should be possible to use correlations derived from data for droplet formation during bubble bursting in aqueous systems. These could be employed if we have information on the gas flow through the molten salt.
- **Vaporization of fission products from the molten salt.** Fission products will have, of course, a natural vapor pressure in the molten salt and this can be estimated to infer a partial pressure of fission products in the cover gas over the molten salt. That is, for the simple process:

$CsCl$ (salt) $\rightarrow$ $CsCl$(gas)
We need to solve:

$$K_{eq}(T) = \frac{P_{CsCl}}{[CsCl(salt)]\gamma_{CsCl}}$$

where:

$K_{eq}(T) = \ equilibrium\ constant\ as\ a\ function\ of\ temperature$
$P_{CsCl} = partial\ pressure\ of\ CsCl\ in\ the\ cover\ gas$
$[CsCl(salt)] = \ concentration\ of\ CsCl\ in\ molten\ salt$
$\gamma_{CsCl} = activity\ coefficient\ of\ CsCl\ in\ molten\ salt$

To obtain estimates of the equilibrium constants some model of the molten salt and the solubilities of the fission products in the salt will be needed. I suspect that substitutional or interstitial modeling would be adequate for the molten salt model. The activity coefficient might be estimable, but it would be far better to have data such as might be obtained from transpiration experiments.

There seems to be some interest in how iodine might be retained in the molten salts. My suspicion is that iodine released from the fuel as molecular iodine will be retained in the salt as an ionic species. For example:

I_2 (salt) + Cl^- ↔ I_2Cl^-

My suspicion is that estimation of fission product release under strictly 'thermal' conditions that ignore the radiation field will yield very much a lower bound on the fission product release to the cover gas. Again, consider the case of NaCl as the molten salt for simplicity. In a radiation field, there will be formation of chlorine:

Cl^- + γ or n^o → Cl^o + e^-
Cl^o + Cl^- → Cl_2^-
2 Cl_2^- → Cl_3^- + Cl^-
Cl_3^- ↔ Cl_2 (salt) + Cl^-

The activity of chlorine in the molten salt could lead to vaporization of fission products that might under thermal conditions be considered nonvolatile. Consider the following hypothetical example:

Ru^o(salt) + Cl_2(salt) → $RuCl_2$(gas)

Similar chemistry is available in fluoride molten salts producing fluorine gas. I believe fluorine gas was detected in decommissioning of the Oak Ridge molten salt reactor.

It is easy to dismiss radiolytic effects on molten salts by arguing that "recombination is rapid." There is rapid recombination, but even so a steady-state concentration of radiolytic products will be sustained in the molten salt. Consider the above example for generation of atomic chlorine and a free electron. The production rate is determined by the dose rate, D:

$$Atomic\ chlorine\ production\ rate = D\rho G(Cl^o)$$

The recombination rate is:

$$Recombination\ rate = k[Cl^o][e^-]$$

The overall rate of production of atomic chlorine is:

$$\frac{d[Cl^o]}{dt} = D\rho G(Cl^o) - k[Cl^o][e^-] \sim D\rho G(Cl^o) - k[Cl^o]^2$$

Then, at steady state where ${d[Cl^o]}/{dt} = 0$, there is a steady state concentration of atomic chlorine in the molten salt:

$$[Cl^o]_{steady\ state} = \sqrt{\frac{D\rho G(Cl^o)}{k}}$$

This is, of course, a very simple, hypothetical example. Similar processes for fluoride salts could account for the formation and transport of uranium hexafluoride in the Oak Ridge molten salt reactor system. To account for these kinds of processes we would need to have G values for the various radiolytic products in the molten salt and data for vaporization of radionulcides in a radiation field.

Salt-fueled systems represent a more significant departure from MELCOR COR package modeling assumptions of a fixed, structural reactor core. However, in some ways the modeling is simplified as now the fuel and coolant are mixed and the heat transfer from a rod bundle is no longer required. This would require a paradigm shift in the COR package but new reactor components with thermal-physical properties and degradation characteristics are not required. However, there is a litany of new phenomena to consider with this type of MSR, and development efforts would benefit from a PIRT study and/or some kind of mechanistic source term analysis as has been performed for SFRs. To name a few issues:

- Reactor kinetics considerations
    - Delayed neutron fraction model
    - New feedback effects related to fluid fuel density and fluid fuel flow rate
- Can fluid-fuel fission product transport be modeled with present capabilities?
- Can fluid-fuel clean-up systems be modeled with present capabilities?
- Are new ex-vessel models needed (e.g. for freeze-plugs and drainage tanks)?

A logical progression of salt-fueled MSR modeling/development could be as follows:

- Verify/create the capability to model molten salts and mixtures thereof (EOS)
- Gauge the capability to model fluid-fuel thermal energy production without COR
- Decide on COR package modifications, recognizing that there may be different strategies for different MSR designs
- Develop new capabilities in other code physics packages as necessary
- Come up with a demonstration problem exercising all new capabilities

APPENDIX D. SAS4A COMPUTER CODE

SAS4A is a tool developed by Argonne National Laboratories (ANL) for thermal-hydraulic and neutronic analyses of power and flow transients in liquid-metal reactors (LMRs), a category that includes metal/oxide, pool/loop-type SFRs. It includes rather detailed fuel performance models, a point-kinetics treatment of neutronics, and a sub-channel approach to thermal-hydraulic solutions. It models accident transients to the point where fuel is released from the reactor core whereas severe accident analyses would require source term well beyond core degradation. Debris coolability and source term release are features that are missing from this code.

A comparison of MELCOR and SAS4A code capabilities described in NUREG/KM-0007 [80] shows similar capabilities for modeling SFRs. Consequently, a code coupling between MELCOR and SAS4A is unnecessary and undesirable given past experience with similar efforts to link MELCOR with other codes. The SAS4A physics models/methods are being studied for integration into the MELCOR code.

The DEFORM-4, DEFORM-5, SSCOMP, FPIN2, CLAP, PLUTO2, PINACLE, and LEVITATE modules in SAS4A are responsible for modeling fuel pin/element mechanical response under various conditions and in various stages of a particular transient. The phenomenological models of each module should be studied with particular attention given to the physics of metal-clad, sodium-bonded metallic fuel. These modules likely operate on too detailed of a level for direct inclusion into MELCOR given the COR package modeling paradigm. Nevertheless, it may be possible to formulate MELCOR-friendly methods that capture the most consequential phenomena with respect to metallic fuel mechanics, degradation, and motion. Oxide fuel phenomenology is a lower priority at present, but should not be completely disregarded.

Table D-1. Code capabilities for SFR application (reproduced from NUREG/KM-0007)

Code capability matrix	Code													
	SAS4A	SASSYS 1	SCALE	CONTAIN	SIMMER	SSC L	DIF3D	ANSYS	MELCOR	MELTSPRD	MAACS	ARGO	MC2	SE2
Phenomena														
Reactivity														
Reactivity feedback at high power		x					x		x				x	x
End-of-life prediction of reactivity feedback		x					x		x				x	x
Burnup control swing/control rod worth		x					x		x				x	x
Relative motion of core and control rods								x					x	x
Reactivity effects caused by gas-bubble entrainment	x	x			x				x				x	x
Core reactivity feedback	x	x			x		x		x				x	x
Core reactivity feedback—fuel motion and core restraint		x					x		x				x	x
Recriticality—potential for energetic events	x	x			x		x		x				x	x
Cladding Integrity														
Integrity of fuel with breached cladding		x												
Thermal Hydraulics														
Single-phase transient sodium flow		x				x			x			x		
Thermal inertia		x				x			x			x		
Pump coastdown profiles		x				x						x		
Sodium stratification		x				x			x			x		
Transition to natural convection core cooling		x				x			x			x		
Core flow distribution in transition to natural circulation		x							x			x		
Decay heat removal system phenomena		x				x			x			x		
Effect of subassembly flow distribution		x				x						x		
Coolant heating and margins to boiling		x				x			x			x		
Fuel dispersal and coolability	x			x	x				x	x				
Decay Heat Generation														
Decay heat generation	x	x	x		x				x					

Code capability matrix	Code													
	SAS4A	SASSYS 1	SCALE	CONTAIN	SIMMER	SSC L	DIF3D	ANSYS	MELCOR	MELTSPRD	MAACS	ARGO	MC2	SE2
Mechanical Behavior														
Mechanical changes in core structure		x						x						
Intact fuel expansion		x						x	x					
Relative motion of core and control rods		x						x						
Fuel cladding structural integrity at elevated temperatures		x						x	x					
Cooling system structural integrity at elevated temperatures		x						x						
Containment structural integrity								x	x					
Core restraint system performance		x						x						
Chemical Reactions														
Sodium-steam chemical reactions				x					x					
Pressure pulse impacts from chemical reactions				x					x					
Reaction product formation and deposition	x	x		x	x									
Sodium Ejection and Fires														
Sodium spray dynamics				x					x					
Sodium pool fire on inert substrate				x						x				
Aerosol dynamics				x					x					
Sodium/cavity liner interactions				x					x	x				
Sodium/concrete melt interactions				x					x					
Containment and Severe Accidents														
Containment structural integrity				x				x	x					
Radiation release and transport											x			
Plant Dynamics														
Plant dynamics						x			x					

APPENDIX E. U.S. SODIUM EXPERIMENTS REVIEWED BY SNL

This list includes a summary of experimental test series that SNL consulted in the construction of this report.

E.1. SODIUM CONCRETE TESTS

This section summarizes U.S. sodium concrete tests.

HEDL SC

Summary: Intermediate scale tests, to determine the time dependence of the bulk penetration rate of the sodium-concrete reaction.
Concrete Types: Limestone, magnetite, basalt. Horizontal and vertical sodium-concrete interfaces.
Na Mass: ~24 kg
Na Initial Temp: 549 to 871 °C
Test Durations: 2 to 100 hours
Data Collected: Test cell temperature, pressure, gas composition, penetration of concrete.

HEDL SET

Summary: Intermediate scale tests, to determine important mechanisms associated with sodium-concrete reactions.
SET 1-4: Thermally dehydrated basalt concrete compared to hydrated basalt.
Concrete Types: Basalt, and thermally dehydrated basalt.
Na Mass: 15 to 46 kg
Na Initial Temp: 593 to 871 °C
Test Durations: 8 hr to 50 hr
Data Collected: Test cell temperature, pressure, gas composition, penetration of concrete.

HEDL S

Summary: Small scale tests to measure the rate of reaction between sodium and concrete. Vertical and horizontal interfaces. Magnetite concrete was penetrated at 1 inch/hr, conventional (SiO2), 0.5 inch/hr. Cracking occurred on vertical interface tests, not horizontal.
Concrete Types: Conventional (SiO2), magnetite.
Na Mass: 1 to 10 kg
Na Initial Temp: 204.4 to 677 °C
Test Durations: 1.5 to 24 hr
Data Collected Sodium and concrete temperatures, gas composition, water content of concreate after cooldown, final penetration of concrete, final composition of reaction product.

SNL T

Summary: Large scale tests to examine interaction of molten concrete and sodium. Not all tests exhibited energetic reactions.
Concrete Types: Limestone, total sodium/concrete contact area ~1.0 m2
Na Mass: 100 to 200 kg
Na Initial Temp: 450 to 700 °C
Test Durations: 30+ minutes

Data Collected: Pool, vapor, concrete temperatures, penetration of concrete, atmosphere composition (T4, T9), pressure (T1).

SNL S-CDC

Summary: Intermediate scale tests, to examine interaction sodium with calcite and dolomite aggregate concretes. Both concretes showed similar exothermic reactions with molten sodium. Chemical reaction zone of calcite concrete was 1 cm thick, for dolomite-concrete it was 7 cm thick.
Concrete Types: Calcite-limestone, dolomite-limestone, total contact area 1.0 m2
Na Mass: 45.5 kg
Na Initial Temp: 830°C
Test Durations: 10 to 20 hr
Data Collected: Pool and concrete temperature, hydrogen generation (calcite), pressure (dolomite), total sodium penetration.

E.2. SODIUM SPRAY FIRE TESTS

This section summarizes U.S. sodium spray fire tests.

ATOMICS INTERNATIONAL TA&TB

Summary: Liquid sodium was exposed to environment containing 4% (TB) to 21% (TA) oxygen. Oxidized sodium was released as aerosol in test chamber.
Test Chamber Size: 1.13 m3
Na Spray Rate: 5.3E-6 & 9.3E-6 kg/s
Na Mass: 0.0028 & 0.0048 kg
Na Initial Temp: 537.8°C
Data Collected: Airborne mass concentration, mass deposition rates on floor and walls, particle size distribution, all as function of time.

HEDL AB3 & NT1

Summary: Test AB3 was a short duration test (140 seconds), NT1 was a long duration test (4.8 hours). NT1 consisted of two sprays. Large, stable temperature gradients occurred vertically.
Test Chamber Size: 850 m3
Na Spray Rate: 0.34 kg/s & 0.0034/0.0058 kg/s
Na Mass: 48 & 82 kg
Na Initial Temp: 600 & 545°C
Droplet Size: 670 & 380/320 microns
Data Collected: Only two figures shown for AB3: Airborne mass concentration, aerodynamic settling mean particle diameter. No results for NT1 provided.

HEDL SA1

Summary: Large scale sodium fire code validation test (SOFICOV).
Test Chamber Size: 850 m3
Na Spray Rate: 0.27 kg/s
Na Mass: 658 kg
Na Initial Temp: 541°C
Droplet Size: 5500 microns

Data Collected: Containment atmosphere temperature, pressure, wall temperature, sodium reaction rate with oxygen. Compared with NACOM computer code.

HEDL AC7-10

Summary: Large scale atmosphere cleaning tests to demonstrate performance of submerged gravel scrubber. Demister system removed 99.98% of entering sodium aerosol mass.
Test Chamber Size: 850 m3
Na Spray Rate: ~0.01 kg/s
Na Mass: ~1000 kg
Na Initial Temp: 580°C
Droplet Size: ~ 10 microns
Data Collected: Suspending aerosol concentration in confinement, aerosol capture, atmosphere/wall temperature, gas cooling, pressure drop.

HEDL AI JET TEST

Summary: Sodium jet tests where the sodium jet was directed upwards towards a stainless steel impact plate. Liquid sodium spread across sheet and droplets descended from sheet. Oxygen concentration, droplet diameter, sodium temperature, and sodium injected had significant effect on peak pressure.
Test Chamber Size: 62.3 m3
Na Spray Rate: 0.7 to 1.5 kg/s
Na Mass: 2.4 to 5.6 kg
Na Initial Temp: ~535°C
Droplet Size: ~4.6 mm MMD
Data Collected: Initial O2 concentration, average droplet diameter, initial sodium temp, pressure vs time.

Rockwell International

Summary: Sodium fire tests performed in ambient atmosphere. Released sodium at heights 5 to 6 m and 30 m as a fan or jet. Close-in fallout was observed due to sodium aerosol agglomerating to large particles. Sodium fires produced mainly Na2O.
Test Chamber Size: Infinite
Na Spray Rate: 0.08 to 0.38 kg/s
Na Mass: 22 to 75 kg
Na Initial Temp: 540°C
Droplet Size: 1 to 620 microns
Data collected summary: Maximum fallout deposition, particle concentration, airborne particle size and distribution were made as a function of downwind distance. Note, plots difficult to read.

ORNL

Summary: Sodium oxide aerosol behavior tests. Spray directed upward from bottom of chamber. Purpose was to produce a more instantaneous aerosol that higher concentration than would be produced by a pool fire. Sodium aerosol was not well mixed within the chamber.
Test Chamber Size: 38.3 m3
Na Spray Rate: 0.021 kg/s, 4 min
Na Mass: 5 kg
Na Initial Temp: 500°C

Droplet Size: Average 480 microns
Data Collected: Aerosol mass concentration, fallout and plateout rate, particle size, vessel atmosphere temperatures, thermal gradients near the vessel wall, vessel pressure, final aerosol distribution, and sodium material balances.

ANL TESTS

Summary: Molten sodium was injected into a closed reaction chamber. The pressure-rise rate was used as a measure of reaction rate of atmosphere-sodium. Droplet size has a large effect on reaction rate.
Test Chamber Size: ~ 0.017 m^3
Na Spray Rate: 0.23 kg/s
Na Mass: 10 g
Na Initial Temp: 350 to 425°C
Data Collected: Pressure rise rate, peak temp, reacted oxygen, weight of inflight burning sodium in the spray.

SNL (SURTSEY-OUTSIDE)

Summary: Two outdoor tests, where the droplet diameters of molten sodium were varied. T1, spray droplets burned before they reached the pan. T2, droplets partially burned in pan.
Test Chamber Size: Infinite
Na Spray Rate: 0.23 kg/s
Na Mass: 4 kg
Na Initial Temp: 500°C
Droplet Size: 6 and 10 mm
Data Collected: Temperature data collected. T1 thermocouple failed at 1200°C. Heat flux data collected. Spray + Pool fire.

SNL (SURTSEY IN-VESSEL)

Summary: Two in vessel spray fire tests, initial sodium temperature was varied.
Test Chamber Size: 99 m3
Na Spray Rate: 1.0 kg/s
Na Mass: 20 kg
Na Initial Temp: 200 and 500°C
Droplet Size: 3-5 mm
Data collected summary: Melt generator pressure, vessel pressure, wall temperature, spray droplet characteristics, spray temperature, heat flux. Na-concrete reactions occurred. Inconsistent sodium ignition occurred. In T4 (higher temperature), the port failed, as a result of rapid pressurization of Surtsey vessel.

E.3. SODIUM POOL FIRE TESTS

This section summarizes U.S. sodium pool fire tests.

HEDL AB1-AB2

Summary: Large scale aerosol behavior tests. In both tests, the sodium fire was covered one hour after the initial pour, isolating the sodium fire from the test chamber. Steam injection was during test AB2 starting at 960 seconds and terminating at 4560 seconds. For test AB1, The first sample

taken at 16 minutes was primarily composed of sodium hydroxide, small amounts of sodium peroxide, and trace amounts of sodium carbonate. As the water vapor in the air was consumed, the mass fraction of sodium peroxide in the suspended aerosol samples increased, but on a mole basis, the primary aerosol product was sodium hydroxide, followed by sodium peroxide, small fraction of sodium carbonate and trace amounts of sodium hydride. Test AB2 was predominately wet sodium hydroxide. Additional water vapor caused faster falling out during aerosol release period, slower after. Net effect minor, the test had similar suspending aerosol concentrations.
Test Chamber Size: 850 m3 (20 m in height)
Na Mass: 410 kg (AB1) & 472 kg (AB2)
Na Initial Temp: 600°C
Burn Area: 4.38 m2
Data Collected: Containment temperature and pressure, mass fraction of suspended aerosols, aerosol chemical analysis, mean particle diameter, aerodynamic settling diameter.

FAUNA F-SERIES TEST

Summary: Six tests were performed in the FAUNA test vessel. Selected results are provided in [Cherdron and Jordan 1988], with the actual experimental report written in German [Cherdron and Jordan 1983]. Many of the details of the experiments were lost in translation, or the details were simply not provided. The outer tank walls of the vessel were sprayed with water to keep the walls from exceeding 150°C. For the larger pool fire tests, 10-30% of aerosols were released, and for the smaller pool fire tests, up to 10% of aerosol was released (note that the it is not clear whether "large" and "small" refer to quantity of sodium or area of pool.
Test Chamber Size: 220 m3 (6 m in height)
Na Mass: Ranged from 150 kg to 500 kg
Na Initial Temp: Unknown
Burn Area: Ranged from 2 m2 to 12 m2
Data Collected: Containment temperature and pressure, mass fraction of suspended aerosols, aerosol chemical analysis, mean particle diameter.

ROCKWELL T4

Summary: Sodium fire tests performed in ambient atmosphere. Sodium was burned for 60 minutes as a pool. Wind was 9 m/s and 30% of the combustion products became airborne. Close-in fallout was observed due to sodium aerosol agglomerating to large particles. Sodium fire produced mainly Na2O.
Test Chamber Size: Infinite
Na Mass: 55.3 kg
Na Initial Temp: 540°C
Burn Area: 1.5 m2
Data Collected: Maximum fallout deposition, particle concentration, airborne particle size and distribution were made as a function of downwind distance. Note, plots difficult to read.

ORNL 101-104

Summary: Sodium pool fire experiments ranging from 1 to 10 kg. Maximum sodium oxide aerosol concentrations ranging from 6 to 25 g/m3.
Test Chamber Size: 38.3 m3
Na Mass: 1 to 10 kg
Na Initial Temp: 540°C
Burn Area: 0.81 m2

Data Collected: Aerosol mass concentration, fallout and plateout rate, particle size, vessel atmosphere temperatures, thermal gradients near the vessel wall, vessel pressure, final aerosol distribution, and sodium material balances.

ATOMICS INTERNATIONAL B1

Summary: Large pool fire experiment. 10% of iodine release 20% sodium released.
Test Chamber Size: 3.36 m3
Na Mass: 279 kg
Na Initial Temp: 177°C
Burn Area: 2.21 m2
Data Collected: Temperature profiles, burning/release rate of sodium, I & Na balance.

GE S2 S3

Summary: Investigation of the interface reaction between steam atmosphere and stagnant sodium pool. Goal was to create a worst case scenario situation. Identified that damage mechanism is corrosion, rather than thermal weakening.
Test Chamber Size: 0.089 m3
Na Mass: 0.15 to 0.28 kg
Na Initial Temp: 482°C
Data Collected: Photographs of damage/corrosion, peak and final temperatures, only one temperature plot in report. Do not have the experimental report, limited data available.

SNL (SURTSEY)

Summary: Sodium pool fire experiments were performed outside. Main objective was to observe effect of cooling on oxidation of molten sodium poured onto a cold stainless steel pan.
Test Chamber Size: Infinite
Na Mass: 1 to 11.6 kg
Na Initial Temp: 500°C
Burn Area: 0.03 to 0.28 m^2
Data Collected: Melt generator pressure, pan temperature, thickness ratio of sodium to stainless steel.

E.4. SODIUM WATER TESTS

This section summarizes U.S. sodium-water tests.

ATOMICS INTERNATIONAL

Summary: A fixed volumetric ratio of steam and nitrogen was used to determine any problems that might be seen during a steam/sodium reaction and to determine effects of varying sodium thickness.
Na Thickness: 0.5 to 2 inches
Water Flow Rate: 8E-5 to 4.5E-4 kg/s
Duration of Test: 1 to 16 hr
Na Initial Temp: 116 to 204°C
Data Collected: Sodium temperatures and good black and white annotated photographs of the experimental setup and results.
Open Experimental Report: AI-AEC-Memo-12714 1968

LMEC LARGE LEAK INJECTION DEVICE

Sodium Water: LMEC Sodium Water Reaction (SWR) Series I and II
Summary: Steam Generator Tube Rupture Tests to Support CRBR Licensing.
Tube Characteristics:
Number: 158;
Diameter: 1.59 cm;
Pitch to Diameter Ratio: 1.885
Water Conditions:
Mass Injected: up to 145kgs
Pressure: 1700 psig to 2000pisg
Na Initial Temp: 300 to 530 C
Data collected summary: Flow rates, Temperatures, Pressures, Photographs, Steam Generator Component dimension changes, Combustion product location, N2 leak check results, Ultrasonic results.

APPENDIX F. EXAMPLE OF MELCOR APPLICATION FOR HTGR BY INTERNATIONAL COMMUNITY

NUBIKI NUCLEAR SAFETY RESEARCH INSTITUTE

BEYOND DESIGN BASIS ACCIDENT CALCULATION OF ALLEGRO GASCOOLED FAST REACTOR

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MELCOR European Users Group
ZAGREB 25-27 April 2018

Contents

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- Background of calculations
- ALLEGRO 75 MW reactor
- MELCOR model
- Previous calculations
- 10 inch LOCA Beyond Basis Accident
- Radioactivity release
- Radioactivity release mechanisms
- Extent of radioactivity release
- Tasks to do

Background - Scope

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- ALLEGRO 75MW is under development in the frame of V4 countries (PL,Cz,SL,HU)
- NUBIKI Share: Severe accident calc.
- MELCOR selection has been based on:
  - Experiment recalculations
  - Steady-state calc.
  - Compare to Cathare
- Main goals – study processes in gas cooled reactors:
  - severe accident thermal hydraulics
  - Fission product transport
  - Establish accident management procedures

75 MW Fast Breeder

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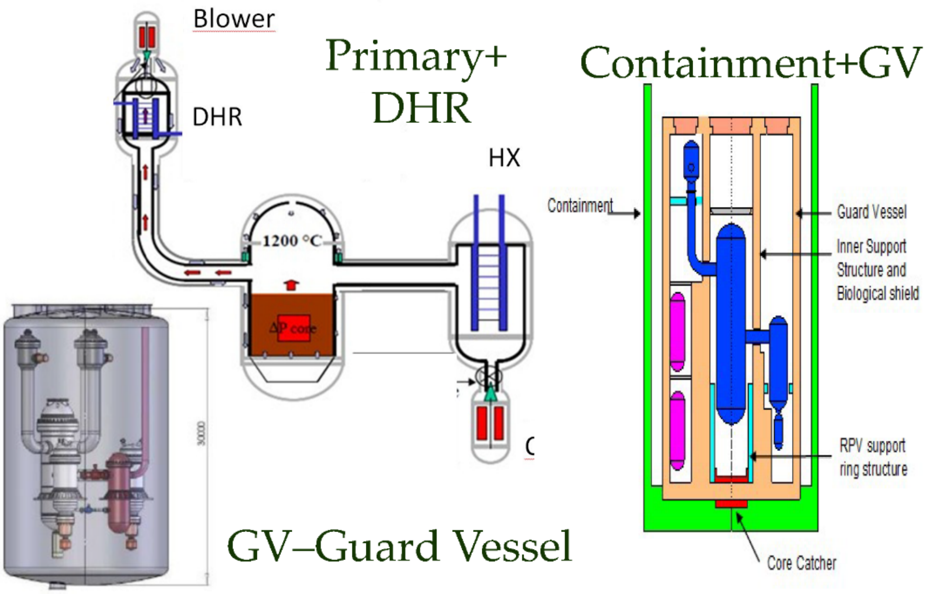

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Allegro 75 MW – model parts

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- 2 loop primary circuit + pony motor
- reactor protection
- Secondary circuit
- DHR heat exchangers + DHR gas blowers
- Nitrogen accumulators

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Allegro 75 MW – Primary + Core model

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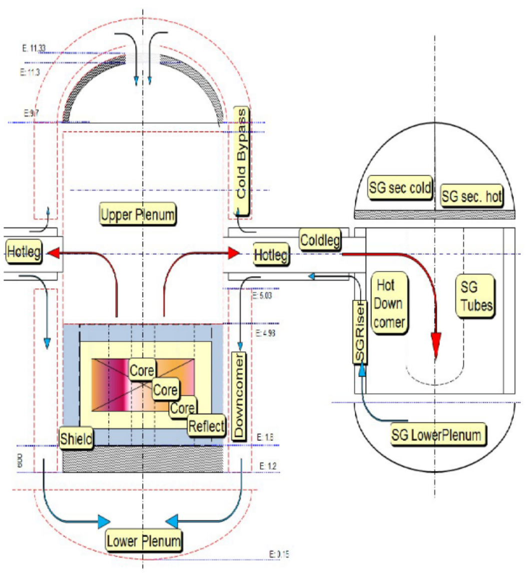

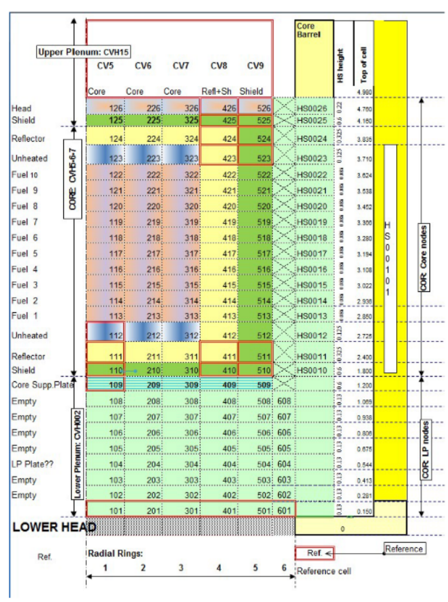

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Allegro 75 MW – MELCOR 1.8.6 vs. 2.2

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- MELCOR core is suitable to calculate 75 MW gas cooled reactor
- MELCOR is able to calculate steady state and transients of ALLEGRO 75 MW reactor
- DBA calculations agree with Cathare results

Allegro 75 MW – Exploratory studies

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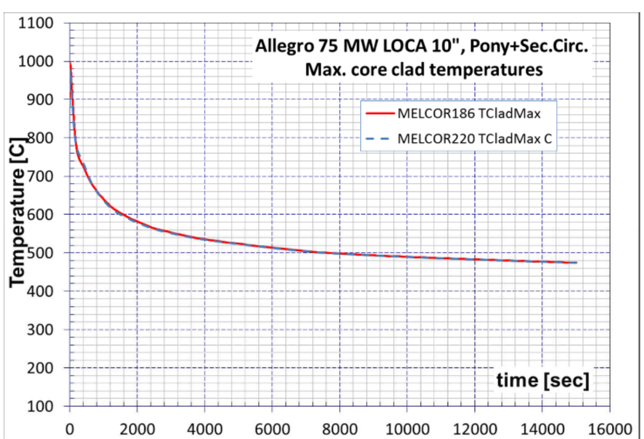
MELCOR 1.8.6 and 2.2 calculations agree well



Allegro 75 MW – BDBA accidents
10 inch Coldleg LOCA initial conditions

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Accident	N2 accum.	Pony Motor+ Sec. Circ.	DHR- HX	DHR-blower	DEC limit
LOCA	On	No	Natural circ.	No	1573 K

N2 accum. M3	GV leak	GV init. pressure	Containment leak	DHR water reserve
2x200	0.1 vol%/d	1 bar	7e-5m2	74m3

Allegro 75 MW – 10inch LOCA events

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Events	Time
Cold leg LOCA d=0.254 m	0.0
N2 accumulator ON	0.15 s
SCRAM	0.2 s
DHR – HX valve ON	20.2 s
Gap release ring 1	209 s
Fuel cladding temperature >1300 K	430 s
Fuel cladding temperature starts to decline	3000 s
Fuel cladding temperature below 1000K	7h
End of calculations	2.3d

Allegro 75 MW – 10 inch LOCA results

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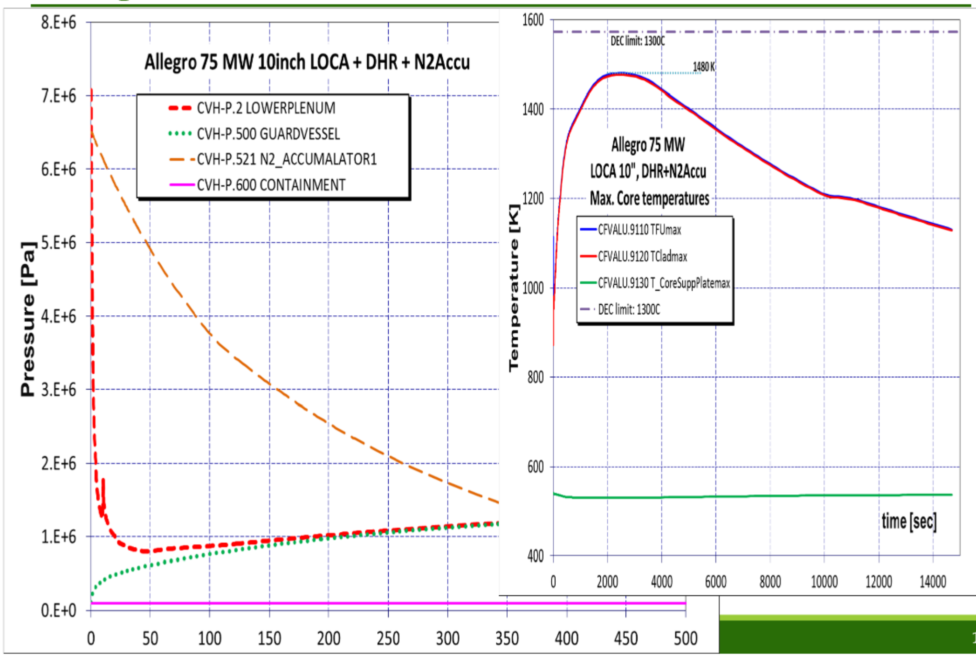

Allegro 75 MW – BDBA accidents
10 inch Coldleg LOCA Main results

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Parameter	
Primary and GV pressure stable after 400s	12 bar
Decay heat after 1 day	1 MW
Max. cladding temperature (below 1573 K DEC limit)	1480 K
DHR HX water saturated	0.5 d
DHR HX water reserve exhausted	8 d
GV max. temperature (around t=0s)	510 K
GV stable temperature after 4-5 days	350 K
Containment initial vacuum is over (leakage starts)	1.4 d

Allegro 75 MW – BDBA accidents
10 inch Coldleg LOCA Activity release

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Gap release =
In 2/3 of core after – 200-300s

Initial gap activity (% of core inventory):

XE: 3%
I2: 1.7%
Cs: 5 %
BA: 0.0004%
TE: 0.01%

Allegro 75 MW – 10inch LOCA activity distribution

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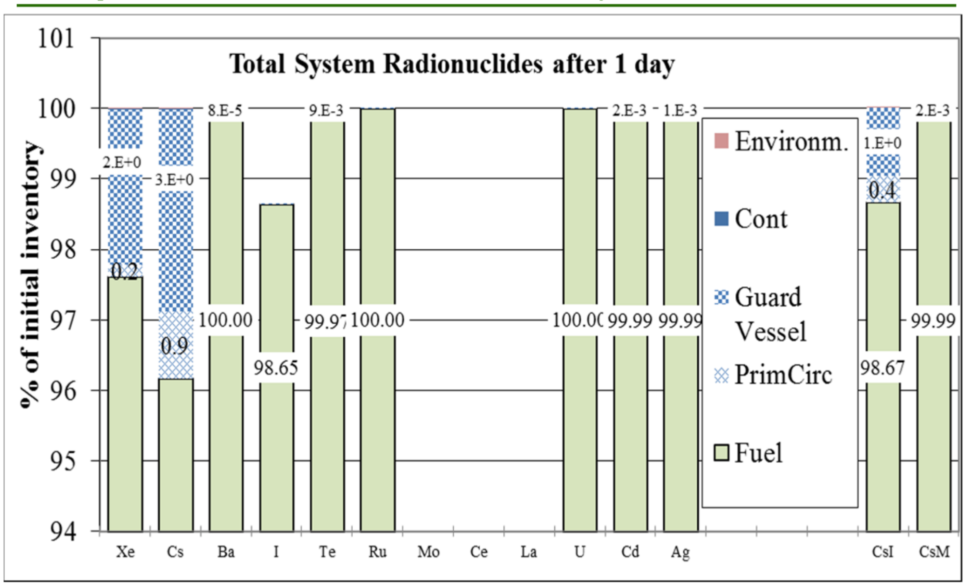

Allegro 75 MW – 10inch LOCA
activity released from fuel

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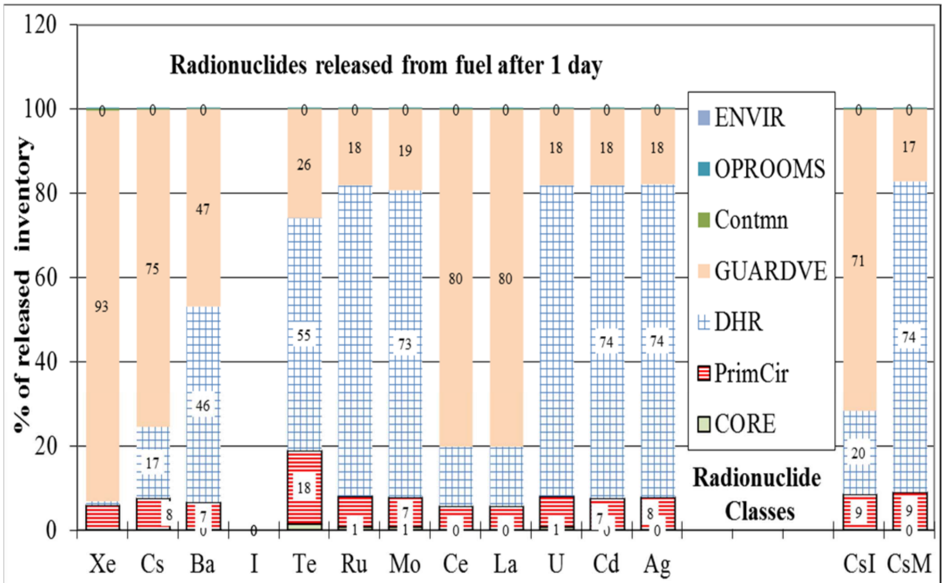

Allegro 75 MW – BDBA accidents
10 inch Cold leg LOCA Activity release

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Most of activity released from fuel (3.8%) stays in:
- primary circuit
- GV and
- DHR

Allegro 75 MW – BDBA accidents
10 inch Cold leg LOCA Main processes

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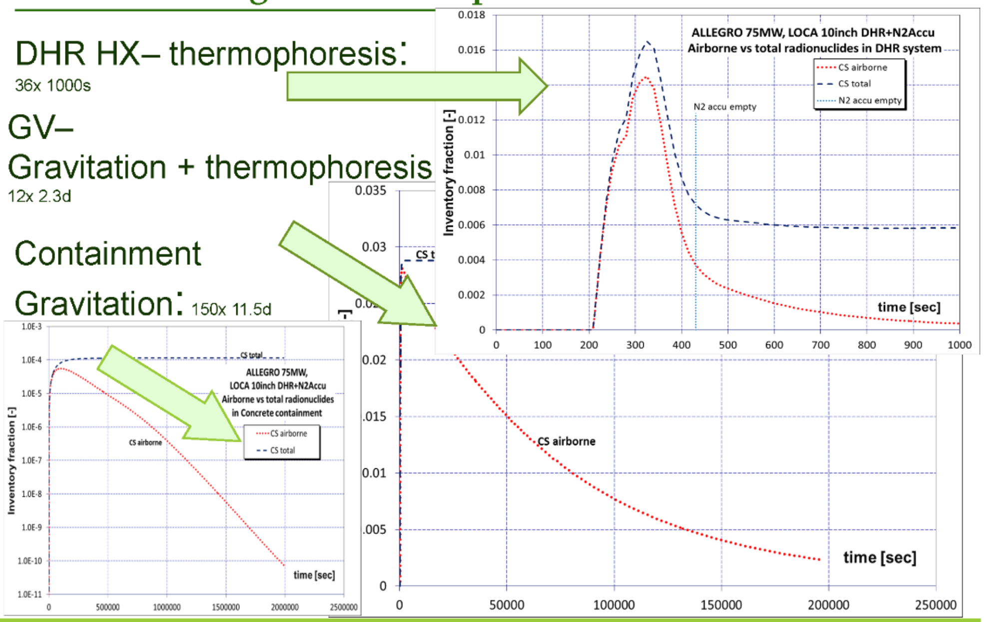
DHR HX– thermophoresis:
36x 1000s

GV–
Gravitation + thermophoresis
12x 2.3d

Containment
Gravitation: 150x 11.5d



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Allegro 75 MW – BDBA accidents
Conclusions

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- 10 inch LOCA is a BDBA accident with N2 accu and DHR HX (natural circulation) without core melt but with core damage
- Max release from fuel is 3.8% of core inventory
- With no water in system (no diffusiophoresis) the aerosol deposition is very slow
- Primary circuit + GV + DHR-HX + Containment gives 5 orders of magnitude radioactivity retention up to 1 day
- Containment gives 2 orders of magnitude retention in 10 days

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Allegro 75 MW – Calculations performed

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No	Accident	N2 accu	Pony Motor+ Sec.Circ	DHR-HX	DHR-blower	T clad. Max.
1	DBA	No	On	No	No	1030 K
2	DBA	No	No	Blower	On	1005 K
3	BDBA	On	No	Natural	No	1480 K

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Allegro 75 MW – BDBA accidents Future

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- Include new design features – ceramic cladding might be a problem
- Calculate severe accidents
- Calculate accident management measures
- MELCOR 2.2 is to be used as it proved to be suitable for gas cooled reactors – use of He is without problem

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Allegro 75 MW

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Thank you for your attention

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