Fluoride-Salt-Cooled, High-Temperature Reactor (FHR) Methods and Experiments Program White Paper

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UCBTH-12-002
Final
May 2013
Department of Nuclear Engineering
University of California, Berkeley

This research is being performed using funding received from the U.S. Department of Energy Office of Nuclear Energy Nuclear Energy University Programs.

Preamble

The University of California, Berkeley; Massachusetts Institute of Technology; and University of Wisconsin, Madison, hosted a series of four workshops during 2012 under a U.S. Department of Energy-sponsored Integrated Research Project (IRP) to review technical and licensing issues for fluoride-salt-cooled, high-temperature reactors (FHRs). This white paper reports results from the second workshop, reviews key thermal hydraulic, neutronic, and structural response phenomena unique to FHRs, and identifies system response codes that are appropriate to predict the response of FHRs under steady-state operation and design basis events, along with experimental data needs to validate these models. Additionally, the four workshops provided an opportunity to receive critical feedback from technical experts in relevant fields.

The four workshops are a central element in developing an FHR preliminary conceptual design report to be completed in 2014. This second white paper focuses on materials covered by the second workshop. The white paper is divided into six chapters. The first chapter provides a brief overview of the IRP and key goals of this white paper. The second chapter reviews general issues for developing, verifying, and validating evaluation models for advanced reactors and specific issues for the FHR. The third through fifth chapters review specific issues and codes for modeling FHR thermal hydraulics, neutronics, and structural mechanics. The sixth chapter reviews issues for coupled and multiphysics modeling of FHR phenomena. Appendices elaborate on certain issues in Chapters 3 through 6.

The comments of the experts attending the workshop, who are listed on the title page, were also integrated into this white paper. The IRP team sincerely appreciates the input of all of the experts who attended and contributed to the second FHR workshop, as well as the hard work of the graduate students and postdoctoral scholars who organized it, facilitated the sessions, and drafted the major sections of this white paper based on their research and the review and input of the workshop experts.

Executive Summary

Fluoride-salt-cooled, high-temperature reactor (FHR) technology uses a novel combination of high-temperature coated-particle fuel, fluoride-salt coolant, and a low-pressure primary system to deliver heat in the temperature range from 600°C to 700°C or higher. FHRs exhibit different thermal hydraulic, neutronic and structural mechanics phenomena compared to conventional – and more extensively studied – advanced nuclear reactor concepts. This white paper reviews the results from a 2-day expert workshop hosted by the FHR Integrated Research Project (IRP) and held in Berkeley, California, in April 2012. This workshop reviewed and discussed simulation and methods development requirements for FHRs. This document includes a review of characteristic phenomena in FHRs and existing modeling and experimental basis for FHR technology. It identifies additional experimental efforts required to validate simulation tools in the domains of thermal hydraulics, neutronics, structural mechanics and multiphysics, to develop the design of – and eventually license – future FHR power plants.

The US Nuclear Regulatory Commission (NRC) has laid the foundation for the development of evaluation models (EMs) for reactor licensing safety calculations in Regulatory Guide 1.203, including verification and validation (V&V) of safety analysis codes. This foundation has been used successfully to develop EMs for licensing of advanced light water reactors (ALWRs) with passive safety systems. The same foundation is now being applied in the licensing of LWR small modular reactors.

The figures of merit calculated by the licensing codes are specific to a given reactor technology and are selected to ensure that high level safety requirements are met and comply with NUREG-0800 and NUREG-1537 guidance. Development of phenomena identification and ranking tables (PIRTs) is a key exercise in the EM development and assessment process (EMDAP) as PIRTs systematically identify phenomena that must included in EMs and phenomena that have not yet been well characterized. The panel of experts present at the workshop emphasized that selecting figures of merit and performing a PIRT exercise should be key deliverables of the FHR IRP, and further recommended that the FHR IRP adopt a baseline design on which to perform the figures of merit selection and PIRT exercise. The strategy adopted by the FHR IRP is to utilize existing general-purpose thermal hydraulics, neutronics and structural mechanics codes that have a significant, existing V&V basis for design and NRC licensing. However, the EMDAP must be followed to ensure that these codes also have a sufficient V&V basis for specific application to the FHR technology.

This white paper discusses FHR thermal hydraulic simulation requirements, candidate codes and their validation basis. A requisite set of figures of merit (FOMs) must be calculated by thermal hydraulic codes for the FHR, including metrics such as time at temperature, peak temperature and peak thermal gradients for fuel and structural components, peak bulk coolant outlet temperature, minimum coolant temperature and temperature rise in the direct reactor auxiliary cooling system (DRACS), peak local power density, and time to establish natural circulation in following loss of forced circulation. Additionally, key thermal hydraulic phenomena must be modeled in FHRs, such as high Prandlt number fluid flow and heat transfer; thermal shock, striping and ratcheting; multi-dimensional porous media flow for a pebble-bed FHR; transition to natural circulation for passive decay heat removal; potential for freezing of the

salt coolant; conduction through ceramic structural materials; and radiative heat transfer with high-temperature fluoride salts.

The RELAP5 systems analysis code has been – and will continue to be – an important tool for design and safety analysis of FHRs. However, based on expert recommendation, after the workshop the FHR IRP acquired the Flownex code previously used by the High-Temperature Gas Reactor (HTGR) and Pebble Bed Modular Reactor programs, to use to perform design analysis and to benchmark RELAP5 results. Code scaling, applicability and uncertainty and hierarchical two-tier scaling analyses are utilized to assess the applicability of existing experimental data and design new scaled facilities using simulant fluids to develop the FHR technology. Moreover, a credible quality assurance program must be implemented for a nuclear regulatory body to accept collected experimental data as a validation basis for licensing the FHR. Many integral effects test (IET) facilities exist or are in the development or construction phase, which will provide data applicable to the FHR technology. The Chinese Academy of Sciences' Thorium Molten Salt Reactor (TMSR) program at the Shanghai Institute of Applied Physics is committed to constructing a 2-MWt fluoride-salt-cooled pebble-bed critical test reactor and supporting an experimental program to license it. Most of this work will be directly applicable to the development of a technical basis for design and licensing of commercial FHRs.

This white paper also discusses FHR neutronic simulation requirements, candidate codes and their validation basis. Four major capabilities are required to calculate all the FOMs for design and licensing of an FHR: high-fidelity criticality analysis (HFCA); depletion analysis; transient analysis; and sensitivity, uncertainty and representivity analysis (SURA). These capabilities must accurately model key FHR neutronic phenomena, including double heterogeneity self-shielding, flibe neutronics, coated-particle in annular pebble- and slab compact-geometry, stochastic pebble recirculation, and internodal leakage. MCNP and SCALE have previously been used for HFCA. The expert panel recommended that the continuous energy Monte Carlo neutron transport code Serpent also be used, because it can generate nuclear data for deterministic transient analysis and couple to point depletion solvers for depletion analysis, in addition to its primary function, which is to perform HFCA. The capability to compare results of different codes creates additional confidence in the accuracy of the results, and the different capabilities of the codes (for example, Serpent is not designed to search for equilibrium compositions) can complement each other.

SURA is an emerging field and new versions of MCNP will include updated methods to perform SURA. It should be noted that much of the methods development work for the Next Generation Nuclear Plant program is applicable to the FHR technology, because both systems are graphite moderated and utilize coated-particle fuel. Literature for HTGR reactor physics shows that nuclear data for graphite introduces significant uncertainty in neutronic calculations. Furthermore, preliminary sensitivity and uncertainty analysis shows that uncertainty in the ^{7}Li nuclear data is a major source of uncertainty for FHRs. The similitude of reactor physics experiments will be assessed based on the sensitivity and uncertainty methodology developed by Oak Ridge National Laboratory. The NRC recommends heavily peer reviewed benchmarks with a high degree of quality assurance, explicitly recommending utilization of the International Criticality Safety Benchmark Evaluation Project (ICSBEP). Therefore, the US FHR program should facilitate the development of an ICSBEP benchmark for the TMSR test reactor. Other recommended activities include quantifying acceptable levels for impurities in FHR primary coolant salts.

Important structural mechanics phenomena for FHRs are highlighted in this white paper, including radiation- and thermally-induced stresses on graphite and ceramic composite structural materials, time-dependent structural behavior of metallic components, and coated-particle fuel performance. Based on expert recommendation, ABAQUS and ANSYS have been recommended as candidate codes for structural analysis of the FHR. Additional experimental data on temperature- and radiation-induced degradation of FHR structural materials is needed. However, detailed experimental requirements cannot be defined until design decisions for FHR structural materials have been solidified. Continued work to develop ASME Code Section III, Division 5 on high-temperature design rules is directly applicable to the FHR technology basis.

Multiphysics and coupled physics modeling are emerging topics in the FHR methods program. Codes in different physics domains provide source terms (power, deformation, temperature distribution, etc.) for simulation. For example, coupled neutronics and thermal hydraulic simulations are important for assessing FHR response to anticipated transient without scram accidents. Prototypical scale facilities such as the TMSR or other IETs will provide the validation basis for these methods.

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Acronyms and Abbreviations

AHTR – Advanced High-Temperature Reactor
APEX – Advanced Plant Experiment
ASCE – American Society of Civil Engineering
ASME – American Society of Mechanical Engineers
ATWS – Anticipated Transient Without Scram
BDBE – Beyond Design Basis Event
BEAU – Burnup Equilibrium Analysis Utility
BOEC – Beginning of Equilibrium Cycle
CFD – Computational Fluid Dynamics
CIET – Compact Integral Effects Test
CSAU – Code Scaling, Applicability, and Uncertainty
DBE – Design Basis Event
DEM – Discrete Element Methods
DHX – Dynamic Heat Exchanger
DOE – U.S. Department of Energy
DPA – Displacements per Atom
DRACS – Direct Reator Auxiliary Cooling System
EM – Evaluation Model
EMDAP – Evaluation Model Development and Assessment Process
EOEC – End of Equilibrium Cycle
FHR – Fluoride-salt-cooled, High-temperature Reactor
FHTR – FHR Test Reactor
GT-MHR – Gas Turbine Modular Helium Reactor
H2TS – Hierarchical Two-Tier Scaling (analysis)
HFCA – High-Fidelity Criticality Analysis
HTGR – High-Temperature Gas Reactor
HTTF – High Temperature Test Facility
ICSBEP – International Criticality Safety Benchmark Evaluation Project
IET – Integral Effects Test
IHX – Intermediate Heat Exchanger
IRP – Integrated Research Project
IRPhEP – International Reactor Physics Experiment Evaluation Project
KMART6 – KENO-VI Module for Activity-Reactivity Rate Tabulation
LBE – Licensing Basis Event
LEU – Low-Enriched Uranium
LIFE – Laser Inertial Fusion Energy
LNC – LIFE Nuclear Control
LOFC – Loss of Forced Circulation
LSPBR – Liquid-Salt-Cooled Pebble Bed Reactor
LS-VHTR – Liquid Salt Very-High Temperature Reactor
LWR – Light-Water Reactor
MHR – Modular Helium Reactor
MHTGR – Modular High Temperature Gas-Cooled Reactor

MSRE – Molten Salt Reactor Experiment
NDHX – Natural Draft Heat Exchanger
NGNP – Next Generation Nuclear Plant
NLRM – Non-Linear Reactivity Model
NRC – U.S. Nuclear Regulatory Commission
ORNL – Oak Ridge National Laboratory
OSU – Oregon State University
PB-FHR – Pebble Bed variant of the FHR
PBMR – Pebble Bed Modular Reactor
PIRT – Phenonema Identification and Ranking Table
PNNL – Pacific Northwest National Laboratory
PREX – Pebble Recirculation Experiment
PRISM – Power Reactor Innovative Small Module
PWR – Pressurized Water Reactor
RPT – Reactivity-equivalent Physical Transform
RSICC – Radiation Safety Information Computational Center
SCALE – Standardized Computer Analyses for Licensing Evaluation
SEAU – SCALE Equilibrium Analysis Utility
SET – Separate Effects Test
SFR – Sodium Fast-cooled Reactor
SGGP – SCALE Generalized Geometry Package
SmAHTR – Small modular Advanced High-Temperature Reactor
TLDC – Top-Level Design Criteria
TRISO – Tristructural-Isotropic
UCB – University of California, Berkeley
V&V – Verification and Validation

1 Introduction

Fluoride salts have unique thermophysical properties compared to other reactor coolants, which make them potentially attractive to use as coolants for high-temperature, low-pressure reactors called fluoride-salt-cooled, high-temperature reactors (FHRs). The U.S. Department of Energy (DOE) initiated an Integrated Research Project (IRP) in January 2012 with University of California, Berkeley (UCB); the Massachusetts Institute of Technology; and University of Wisconsin, Madison, to develop the technical basis to design, develop, and license commercially attractive FHRs. To initiate this project, UCB organized a series of four workshops in 2012 to engage reactor technology experts in identifying and reviewing key FHR development issues.

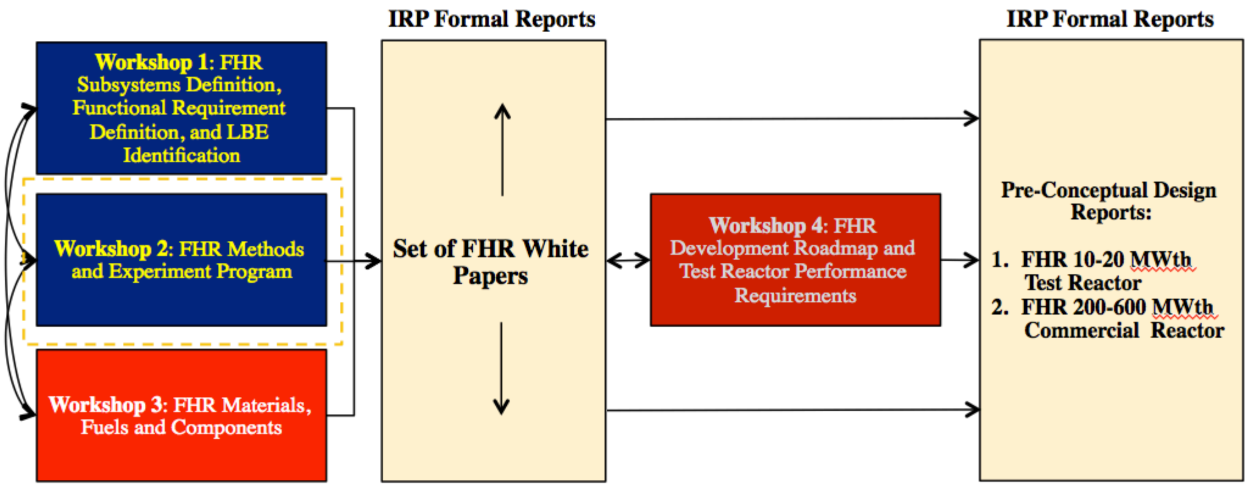

Figure 1-1. IRP Structure Illustrating Workshop Rationale and Key IRP Objectives (this white paper focuses on the second workshop)

The first workshop white paper discusses the major technical characteristics that differentiate FHRs from other power reactor technologies, the major systems and subsystems expected to be used in FHRs, high-level functional requirements for these systems and subsystems, and licensing basis events (LBEs) that should be considered in FHR design and licensing.

This white paper provides results from the second workshop, which took place in April 2012 and focused on reviewing key thermal hydraulic, neutronic, and structural response phenomena unique to FHRs. The second workshop also identified system response codes that are appropriate to predict the response of FHRs under steady-state operation and design basis events (DBEs), along with experimental data needs to validate these models. The experts who contributed to the second workshop, listed on the cover, have experience spanning a range of relevant areas:

- Code scaling, applicability, and uncertainty (CSAU) methodology application including phenomena identification and ranking
- Thermal hydraulic modeling and experiments on separate effects tests (SETs) and integral effects tests (IETs), particularly for single-phase, incompressible high Prandtl number liquids, for design and licensing

- Neutronic modeling and experiments for design and licensing (a key issue is defining neutronic validation experiments to be performed during startup testing of the FHR Test Reactor or FHTR)
- Transient thermal stress and structural response for high-temperature, low-pressure vessels, heat exchangers, pumps, and core internals.

A draft of this white paper was made available to participants prior to the workshop to provide background material on the topics to be covered during the workshop. This final white paper incorporates changes resulting from discussion at the workshop. The key goals for this workshop and white paper include the following:

- Identify a set of goals specific to the IRP (design for commercially attractive FHRs): methods should be usable for design purposes and licensing purposes
- Identify modeling codes to use in FHR design and licensing (thermal hydraulics, neutronics, structural, coupling, and multiphysics)
- Identify gaps in existing codes and recommend subsequent development needed between pre-conceptual design and pre-application review
- Identify modeling efforts and experiments needed for design and licensing of FHRs.

The second chapter of this white paper reviews general issues for developing, verifying, and validating evaluation models (EMs) for advanced reactors and specific issues for FHRs. The third through fifth chapters review specific issues and codes for modeling FHR thermal hydraulics, neutronics, and structural mechanics, respectively. The sixth chapter reviews issues for coupled and multiphysics modeling of FHR phenomena. Appendices elaborate on certain issues in the third through sixth chapters.

2 Requirements for Modeling and Experiments

This chapter reviews the major requirements for models and codes used for the design and licensing of FHRs. The U.S. Nuclear Regulatory Commission (NRC) defines an EM as the "calculational framework for evaluating the behavior of the reactor system during a postulated [transient or design basis accident] (pg. 3)" (NRC 2005). This chapter reviews the NRC's recommended approach to developing and validating EMs.

2.1 EM Development Analysis Process

The NRC Regulatory Guide 1.203 (NRC 2005) defines a systematic process for developing EMs for the analysis of transient and accident behavior of reactors, referred to as the Evaluation Model Development and Assessment Process (EMDAP). The process uses the CSAU methodology originally developed under NRC research to study severe accidents at light-water reactors (LWRs) (Boyack et al. 1990). The methodology outlined in Regulatory Guide 1.203 applies a systematic approach to develop models that are appropriate for a specific system and specific transient, and incorporate a sufficient knowledge base to generate confidence in the analysis. This process is composed of four major elements:

1. Establish requirements for EM capability
2. Develop an assessment base
3. Develop an EM
4. Assess EM adequacy.

These major elements can be further divided into 20 steps, as presented in Figure 2-1.

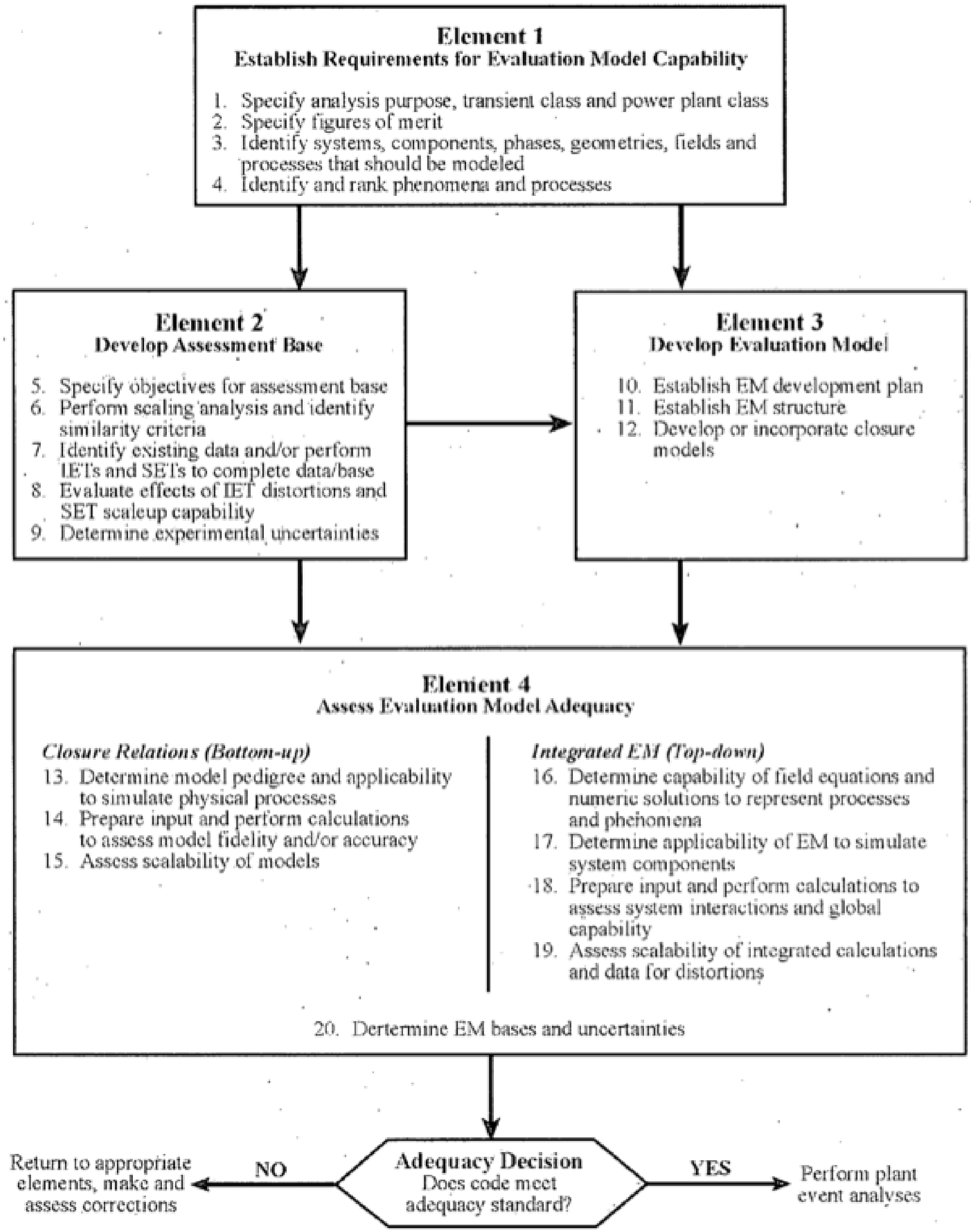

Figure 2-1. NRC EMDAP (NRC 2005)

This white paper focuses predominantly on the first three elements of the EMDAP methodology, based on the needs for FHR development during the pre-conceptual design phase. The EMDAP methodology includes the development of a technical basis for the requirements of an FHR EM (Element 1) and the methods and experimental programs that should be pursued to support those requirements (Elements 2 and 3). The assessment of EM adequacy (Element 4) cannot be discussed in detail until the EM has been completely developed and thus falls outside the scope of this white paper.

2.2 Phenomena Identification and Ranking Tables

Step 4 of the EMDAP outlined in Reg. Guide 1.203 (NRC 2005) is to identify and rank phenomena and processes that influence plant behavior by developing a phenomena identification and ranking table (PIRT). A PIRT is a structured, transparent, and auditable tool for eliciting expert advice on which phenomena dominate the uncertainty in the simulations.

DOE's Next Generation Nuclear Plant (NGNP) program generated several PIRTs relevant to NGNP safety and licensing. The documentation of these PIRT exercises outlines the nine steps to developing PIRTs (Ball and Fisher 2008), as summarized in Table 2-1.

Table 2-1. PIRT Steps (Ball and Fisher 2008)

Step	Action
1	Define the issue that is the driving need for the PIRT
2	Define the specific objectives for the PIRT
3	Define the hardware and the scenario for the PIRT
4	Define the evaluation criteria
5	Identify, compile, and review the current knowledge base
6	Identify plausible phenomena, that is, PIRT elements
7	Develop importance rankings of phenomena
8	Assess knowledge level for each phenomena
9	Document PIRT results

The PIRT exercise supports the prioritization of research and development efforts by identifying and narrowing the high-ranking phenomena that must be modeled in EMs. Furthermore, this set of phenomena will set the requirements for the qualification matrix to perform verification and validation (V&V). Finally, the PIRT process identifies gaps in the knowledge base for FHR technology.

Sections 3.2, 4.2, and 5.1 of this white paper provide a high-level, qualitative description of unique phenomena in FHRs. Because a key goal for FHR development is to use EMs, wherever possible, that have already been developed and applied for other reactor technologies (LWR, high-temperature gase reactors or HTGRs, and sodium-cooled fast reactors or SFR), some changes will be required to these EMs to model these different thermal hydraulic, neutronic, structural mechanics, and coupled/multiphysics phenomena (as described in Chapters 3, 4, 5, and 6, respectively). When the design of a baseline FHR matures into a detailed design, formal PIRTs can verify the completeness of this initial identification.

2.3 FHR Experimental Base Development

The FHR experimental program must be developed so it supports Element 2 of the EMDAP: *Develop Assessment Base* (Figure 2-1). The first step of Element 2 is to specify the objectives for the experimental assessment base. The subsequent chapters in this white paper outline the objectives of experiments needed to validate models for thermal hydraulics (Chapter 3), neutronics (Chapter 4), structural mechanics (Chapter 5), and coupled/multiphysics (Chapter 6). While this workshop identified FHR experimental needs, the fourth workshop focused on defining a development plan for these experiments to generate information needed to make key programmatic decisions during the FHR development and demonstration process.

Once the objectives of experiments have been defined, the second step in this element of the EMDAP is to perform scaling analysis to ensure that the experimental data are relevant and that the assessment base has sufficient range to envelope the specific event for the specific system. The approach to evaluating the applicability of experimental data depends on the type of EM involved.

For thermal hydraulic EMs, Regulatory Guide 1.203 (NRC 2005) recommends using a top-down scaling approach to derive non-dimensional groups governing similitude between experiments and applications, show that these non-dimensional groups scale the results between experimental facilities, and determine whether these experiments bound the event in non-dimensional space. These non-dimensional groups can be derived using the hierarchical two-tiered scaling (H2TS) approach that meets the requirements of severe accident scaling methodology (Zuber et al. 1998). This methodology has been applied to FHR thermal hydraulics to develop non-dimensional groups for the development of IETs to study loss of forced circulation (LOFC) and other transients (E. D. Blandford and Peterson 2009). Similitude in natural circulation heat transfer experiments can be ensured by simultaneously matching the Reynolds, Grashof, Froude, and Prandtl numbers in the experiment and application. Similitude for the advection and granular flow of buoyant pebbles can be ensured by simultaneously matching the Reynolds and Froude numbers, friction factors, and the pebble-to-coolant density ratio. The ability to match these key non-dimensional groups using simulant fluids helps simplify the process to develop knowledge base for SETs and IETs. Chapter 3 provides a more detailed discussion of SET and IET experiments to validate thermal hydraulic EMs for FHRs.

SETs are designed to study a specific phenomenon under closely controlled (and potentially idealized) boundary and initial conditions. Following a bottom-up scaling approach, SET experiments are typically highly instrumented and provide the basis to validate models for specific phenomena.

IETs are scaled experiments designed to reproduce the integral response of a system to multiple phenomena, with acceptably low and quantifiable distortions. A top-down scaling analysis leads to the identification of key system phenomena. IET experiments address the fact that, for coupled phenomena, the initial and boundary conditions might be significantly more complex than can be generated in the SET experiments, which validate the individual models used in codes. IET experiments provide a basis to validate system modeling codes to confirm that their SET-based phenomenological models adequately reproduce the integral system response.

Application of the H2TS process is intended to

- Provide a scaling rationale and similarity criterion between thermal hydraulic experiments and applications
- Provide a procedure for reviewing experimental facility designs
- Ensure prototypicality of experiments
- Quantify biases.

After verification to determine that the EM is developed with the necessary degree of quality assurance, its algorithms are stable and converge to the correct solution, and it is sufficiently numerically accurate, the EM can be validated (Oberkampf and Trucano 2007). A combination of separate effects tests, integral effects tests, and component tests provides data to quantify the predictive accuracy of the EM (INL 2010a). In addition, the H2TS process may be used to identify measurements needed during reactor startup testing to provide confirmatory validation of EMs prior to reactor power operation.

For neutronic EMs, Oak Ridge National Laboratory developed a means to assess the applicability of criticality benchmark experiments to a given application using representivity factors (Broadhead et al. 1999). The approach recommends the number of necessary critical experiments according to how well similitude is achieved. The methodology has been successfully applied to burnup credit analysis for spent fuel casks (Radulescu, Mueller, and Wagner 2008) and, using sensitivity and uncertainty analysis to guide the matching of phenomena, the approach can be extended to general validation efforts. Existing physical experiments can be leveraged if they are shown to be neutronically similar, to sufficiently quantify uncertainty, and to contain the necessary diagnostic measurements. The process is complementary to the traditional validation methodology, which requires matching geometry, fuel type, coolant type, and neutron flux spectra (Dean and Tayloe Jr. 2001).

For structural mechanics for reactors and their internals, requirements for design and licensing are governed by the American Society of Mechanical Engineers (ASME) Boiler and Pressure Vessel Code (ASME 2013). Little guidance is currently provided in the code for how to develop and experimentally validate EMs for high-temperature structures. As of January 2013, an ASME Task Group had been formed to establish standard material models for materials covered in Subsection NH (Class 1 Components, Elevated Temperature Service) of the code. The group also plans to present guidelines for analysis approaches. In addition, the task group plans to provide sufficient material information in the code so that independent designers would obtain similar results from fully inelastic modeling in the creep regime. Standard test models may be developed, but currently the designer must provide his own constitutive material models and code validation.

The ASME Subgroup Elevated Temperature Design is also developing a simplified limit load approach to screen components from the requirement for full creep/fatigue analyses. That is, a finite element limit load approach could be used in place of the difficult-to-implement elastic methods in the appendixes in Subsection NH.

The third step of the assessment base development is to verify that the assessment experimental database is sufficient and complete. Multiple sets of SET experimental data are preferred to provide a sufficient basis to quantify the uncertainty of the physics models and correlations used in the EMs. Similarly, counterpart IETs must be assessed on multiple scales to identify and quantify scaling distortions such as heat losses.

Once a sufficient and complete experimental database has been assembled, the final steps of the *Develop Assessment Base* element are 'to evaluate effects of IET distortion and SET scale-up capability' and 'determine experimental uncertainties.' Because FHR share substantially common phenomenology with LWRs and other advanced reactors, similar approaches to quantifying distortions and experimental uncertainties can be applied.

2.4 FHR Methods Program Development

The proposed philosophy for the FHR methods development program is to use, where possible, existing general-purpose transient analysis codes to support the development, design, and licensing for the FHTR and commercial prototype. Commonly, more than one general purpose code will exist, and the FHR methods development program encourages the development and application of more than one code, preferably by different research groups, to support comparisons of code predictions and enable effective benchmarking exercises to be developed and performed. The importance, for new system designs, of validating model predictions by comparing results from more than one modeling tool has been reemphasized by recent major problems with steam generator tube vibration and accelerated tube wear discovered at the San Onofre Nuclear Generating Station in California. In this case, predictions for steam velocities by the Mitsubishi code FIT-III were found to be three to four times higher than predicted by the NRC's ATHOS thermal hydraulic code, explaining the unexpected fluid-elastic instability problems in the steam generators (NRC 2012).

To use general-purpose codes to simulate FHR systems, the codes must be appropriately modified to incorporate the correct material properties and specific phenomenological correlations (such as for heat transfer coefficients), but further modifications should be limited only to cases where models are determined to be inadequate for FHR-specific phenomena.

Reg. Guide 1.203 (NRC 2005) discusses the use of general-purpose transient analysis codes in licensing safety analysis:

> "Very often, a general purpose transient analysis computer program (such as RELAP5, TRAC, or RETRAN) is developed to analyze a number of different events for a wide variety of plants. These codes can constitute the major portion of an EM for a particular plant and event … A certain amount of generic assessment may be performed for such codes as part of the generic code development. Applying portions of the EMDAP process to an existing general purpose transient analysis computer program is useful in determining its suitability for use as the basis for an EM and can identify deficiencies in models and assessment that should be addressed before the code is submitted for NRC review.
>
> The EMDAP starts with identification of the plant, event, and directly related phenomena. When applied to an EM that uses an existing general purpose transient analysis computer program, this process may indicate that the generic assessment does not include all of the appropriate geometry, phenomena, or necessary range of variables to demonstrate code adequacy for some of the proposed plant-specific event

> analyses ... Application of the EMDAP should be considered as a prerequisite before submitting a general purpose transient analysis computer program for review as the basis for EMs that may be used for a variety of plant and accident types. Evaluation models that use an approved general purpose transient analysis computer program that has been scrutinized or developed using the EMDAP process can efficiently identify the models and assessment that support the analysis of the specific plant and accident types for which the EM will be used."

The EMDAP is required to establish the technical foundation for expanding the applicability beyond that originally justified in the generic review of the general code for a specific plant, during a specific LBE, for a particular safety-related figure of merit.

Chapters 3, 4, 5, and 6 review existing general-purpose codes for their applicability to design and licensing of FHRs.

2.5 Graded Approach to EMDAP

Often, EMs used to analyze different LBEs for the same nuclear plant will share many similar elements of functionality. Therefore, performing a full EMDAP for each LBE is redundant. Conversely, the application of an existing EM or the development of a new EM for a first-of-a-kind system requires a partial or even a full EMDAP.

Section 5 of Reg. Guide 1.203 (NRC 2005)outlines the graded approach to applying the EMDAP. The guide specifies four criteria that determine the extent to which the EMDAP should apply:

1. Novelty of the revised EM compared to the currently acceptable model
2. Complexity of the event being analyzed
3. Degree of conservatism in the EM
4. Extent of any plant design or operational changes that would require reanalysis.

The next four subsections discuss the extent to which each of these criteria can be applied to the FHR EMDAP.

2.5.1 Novelty of EM

A significant effort will be required for the EMDAP in support of the first-of-a-kind FHR licensing process because no NRC-approved EMs exist for FHR transients. Therefore, the current pre-conceptual design phase for the FHR will focus on a set of characteristic DBEs and one or more beyond design basis event (BDBE) that capture the most important system transient response processes. These FHR-specific processes include the following steps:

1. Establish decay heat removal via natural circulation
2. Maintain decay heat removal in the event of overcooling
3. Establish sub-criticality via control system, and manage heat removal in the event of reactivity insertion

4. Establish sub-criticality based on temperature feedback, and manage heat removal in the BDBE of an anticipated transient without scram (ATWS).

Therefore, after a significant initial effort to develop the initial set of EMs for the characteristic sequences, less development should be required to develop EMs for the complete set of LBEs required for FHR licensing as long as the characteristic LBEs have been chosen appropriately. Furthermore, transitioning from licensing the FHTR to the commercial prototype should be simplified given their similarity and that an experience base will have been developed for FHR-specific phenomena after testing in the FHTR when the commercial prototype begins the licensing process.

2.5.2 Complexity of the Event

Simplifications in the application system yield corresponding simplifications in the EMDAP. In the case of the FHR EM development, a number of factors should significantly reduce the complexity of the system response and allow for a reduction of effort for each stage of the EMDAP.

The thermal hydraulics of FHRs are generally simpler than in LWRs under operating and transient conditions because the coolant remains a single-phase incompressible liquid. Furthermore, the figures of merit for FHR safety do not involve local, peak parameters in the reactor core but instead involve conditions outside the core, such as time at temperature and pressure for metallic structural components. FHR safety is not sensitive to local fuel temperatures during accident sequences, reducing the need for analysis and validation of models to predict precise local information in the core.

The neutronic analysis for FHRs introduces several complexities that diverge from the current experience base. The double heterogeneity of the fuel diverges from the LWR experience base but is consistent with much of the work currently being pursued for HTGRs. The pebble bed FHR designs also have some complexity associated with the uncertainty in core configuration because of continuous on-line refueling, mixing of pebble types at radial region interfaces, and equilibrium ^{6}Li generation. With respect to uncertainty in the core geometry, the impact would be mitigated for two reasons. First, because the peak local fuel temperature, which has the highest uncertainty based on geometric uncertainty, is not expected to be an important safety performance metric. Second, because on-line refueling maintains a low excess reactivity in the core, reducing the potential reactivity insertion.

2.5.3 Degree of Conservatism

FHRs have uniquely large thermal margins to fuel damage, which suggests that additional conservatism can be used in the analysis of transients that affect fuel temperature, even in the absence of a significant experience base. This conservatism in FHR design liberates the EMDAP from some stringency, thereby enabling some simplification.

2.5.4 Extent of Any Plant Design or Operational Changes That Would Require Reanalysis

This area would consider any design or operational changes made with an FHTR.

3 Thermal Hydraulic Modeling

Thermal hydraulics involves the key phenomena that control heat removal and addition in FHRs. The control of heat removal and addition is one of the six Top Level Design Criteria (TLDC) proposed for FHR safety assessment and licensing, as discussed in the first FHR workshop white paper on functional requirements and LBE identification. Convective heat transport in FHRs generally involves single-phase incompressible flow, although gas entrainment may occur at free surfaces, and helium bubbles may be deliberately injected into FHR coolant, or the coolant sprayed into a column to contact helium, to scavenge tritium. Because single- and two-phase flow also occurs in LWRs, FHR thermal hydraulics can be modeled using simulation tools that have been developed and applied to the design and licensing of LWRs, with appropriate code modifications to introduce FHR thermophysical properties and heat transfer correlations.

One DBE for FHRs that does not occur in LWRs is overcooling, which can potentially result in freezing of the coolant salt. The principal consequences of freezing are flow blockage, and when thawing occurs, expansion and potential damage to structures.

While LWR thermal hydraulic modeling codes are expected to be able to simulate the response of FHRs to most LBEs, the conclusion that LWR codes (such as RELAP5-3D) can be used for this purpose must be verified through a systematic process. The NGNP program (INL 2010a) developed such a systematic process, illustrated by the Figure 3-1 flow chart, which summarizes key factors and questions that should be answered to select modeling codes, such as the following:

“1. Has the software ever been used to analyze the phenomena or scenario that requires analysis, as identified in the Phenomena Identification and Ranking Table (PIRT)? By answering this question, the analyst may be introduced to references and other experts who have applied the software to similar phenomena or scenarios. Hence a body of useful information may be available.

2. Are the phenomena modeled properly, and does the model region of applicability correspond to the system phenomena or scenario envelope? These questions may be most easily answered by using the manuals and documentation required to describe the models and correlations, theory, scaling relationships and applications, developmental assessment reports, validations, etc.

3. Have validation studies been completed for the phenomena or scenario? If a body of validation results are not available, or if the validation results were not reasonable, as a minimum, then either the software should not be used or it should be validated to ensure that the calculated results are reliable rather than misleading.”

Only when acceptable answers are obtained for the questions listed above can the software under consideration be used with confidence for the required analysis.

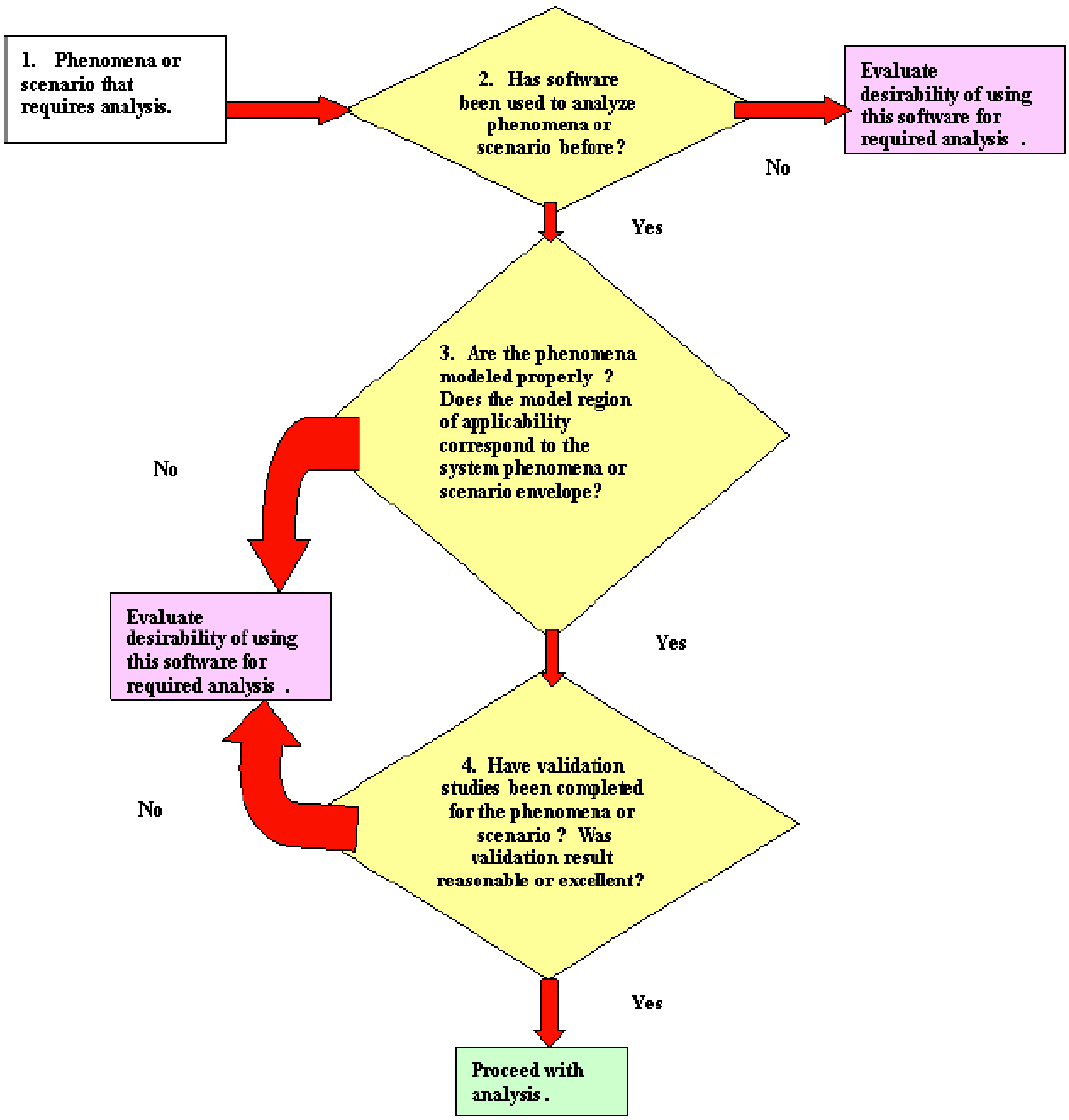

Figure 3-1. Evaluation of Applicability of Analysis Software (INL 2010a)

This chapter first highlights the most important figures of merit that must be captured when modeling thermal hydraulic phenomena for the FHR. While the thermal hydraulic phenomena in FHRs are largely a subset of those for LWRs, the FHR figures of merit are quite different than those typically used for LWRs. This brief discussion is followed by a list of key thermal hydraulic phenomena for the FHR technology. Then, the white paper presents an overview and a selection of codes that have been used for thermal hydraulic steady-state and accidental transient analyses for advanced nuclear reactor concepts.

While a very large number of codes have been recently developed for specific applications by national laboratories, universities, and nuclear vendors – as opposed to the limited number of widely used codes that were developed in the 1970s in the U.S. – for thermal hydraulics, the workshop experts recommended that the IRP focus on codes with a significant validation documentation basis from applications to LWRs, where the applicability to advanced reactor thermal hydraulic modeling has been demonstrated through extensive reports and publications. Thus, after identifying the subset of thermal hydraulic codes applicable to the FHR technology, the chapter discussion focuses on the current gaps in these modeling tools for application to FHRs and the subsequent experimental basis needed to identify FHR-specific phenomenology and to validate these codes.

3.1 Operating Modes, Characteristic LBEs, and Related Figures of Merit

Thermal hydraulic analysis of transients in FHRs will focus on a set of LBEs that are expected to potentially challenge the system's ability to meet TLDC. To aid the early FHR development process and guide pre-conceptual design, the first FHR workshop identified a subset of these LBEs, referred to as "characteristic LBEs," for the initial FHR development effort. This section provides an overview of the operating modes and characteristic LBEs for the FHR as detailed in Chapter 4 of the first FHR workshop white paper and principal figures of merit that arise from steady-state operation and thermal hydraulic transients in the FHR.

3.1.1 FHR Operating Modes and States

A conventional FHR is expected to have five general plant operating modes. These modes, illustrated in Figure 3-2, are ordered based on the overall demand on plant systems, which ranges from normal full-power operation to defueled maintenance conditions. Each mode of FHR plant operation is described in the Chapter 4 of the first FHR workshop white paper.

The set of operating states also includes a set of normal plant transient conditions under power operation that merit analysis to establish that the design can meet both the functional and safety requirements for these events. These transients include those for normal startup, shutdown, and load change. Figure 3-2 also shows the expected system transitions between shutdown and normal power operation. Evaluation of these normal transients will inform the FHR design process because such transients affect plant availability, but the evaluation will also form one component of the licensing basis for the reactor.

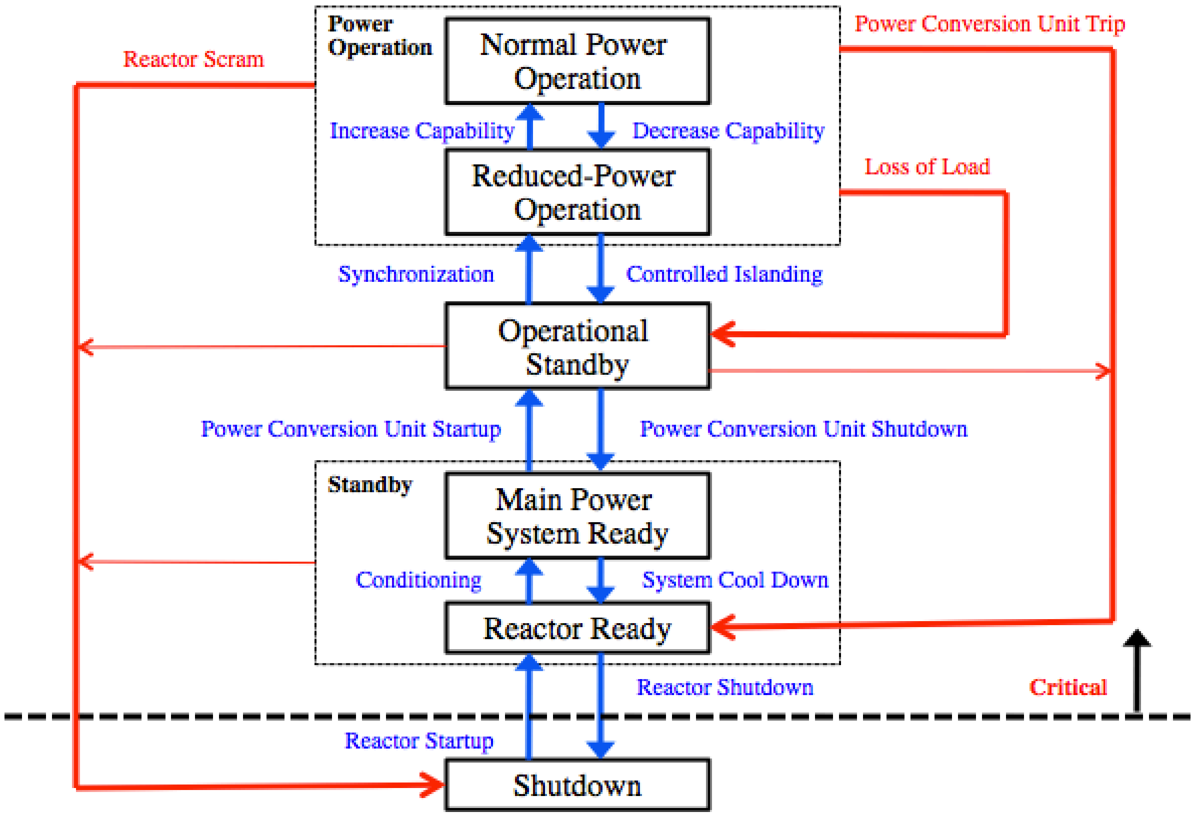

Figure 3-2. FHR Operation Modes from Shutdown to Normal Power Operation and the Plant Actions Required for Transition Between Them

3.1.2 Thermal Hydraulic LBEs

Chapter 4 of the first FHR workshop white paper postulated a set of bounding events for FHRs. These events put severe tests on reactor safety systems and are all considered to be events in the BDBE frequency range or lower. More details about the LBE selection approach are provided in the first FHR workshop white paper.

3.1.3 Principal Thermal Hydraulic Figures of Merit

Key figures of merit that arise from normal operation and key thermal hydraulic transients are as follows:

- **Peak fuel element temperature**, to avoid fuel failure and release of radionuclides (very unlikely to govern any FHR LBE because of the large thermal margin of FHR fuel)
- **Peak local power density**, which affects particle and element thermal stresses
- **Time at temperature for the fuel**, which influences radionuclides release
- **Peak bulk coolant outlet temperature**, which is a simple metric that is indirectly related to the structural integrity of the system
- **Time at temperature for metallic and ceramic structures**, for long-term creep deformation and degradation of structural materials

- **Peak thermal gradient induced in metallic and ceramic structures** (requires coupling with a structural mechanics code), resulting in coolant thermal shock, striping, and ratcheting
- **Minimum coolant temperature in the Direct Reactor Auxillary Cooling System (DRACS) loop**, to assess importance and duration of a potential overcooling transient, including freezing phenomena in the natural draft heat exchange (NDHX), reducing heat removal capacity of a safety-related component
- **Temperature difference across the DRACS,** which is one of the key parameters associated with passive decay heat removal through natural circulation
- **Time to establishment of natural circulation**, and how long it can be sustained.

These thermal hydraulics figures of merit should be considered to be preliminary, since ultimately the concern involves the potential for structural and fuel damage. As models for structural and fuel damage become more refined, it will be appropriate to update and prioritize the FHR thermal hydraulics principal figures of merit.

Any thermal hydraulic code used for steady-state and transient analysis of the FHR will be required to accurately predict the principal figures of merit, which depends on the capability of the code to properly account for thermal hydraulic phenomena in the system. To that effect, the following section details FHR thermal hydraulic modeling phenomenology.

3.2 FHR Thermal Hydraulic Modeling Phenomena

Fluoride salts are low-volatility fluids with high-volumetric heat capacity, melting temperatures, and boiling temperatures compared to other typical reactor coolants. The differences in thermal hydraulic phenomena in FHRs emerge from the differences in the thermophysical properties of the fluoride salts and the structural materials used with them, compared to other reactor coolants and their typical structural materials.

Table 3-1 compares the thermophysical properties of different reactor coolants and structural materials. Fluoride salts have very high volumetric heat capacities (ρC_p). The volumetric heat capacity of the primary coolant flibe exceeds even that of water; therefore, FHRs operate with lower primary coolant volumetric flow rates, pressure drops, and pumping power than LWRs, and much lower values than SFRs and HTGRs.

The fact that low volumetric flow rates of fluoride salts can transport large amounts of heat has many implications for the design of FHRs. For example, this characteristic makes fluoride salts particularly effective in passive, buoyancy-driven natural circulation heat transfer. For future FHR reactors to be commercially attractive, it is critical that FHR designers leverage the favorable thermophysical properties of the fluoride salts to the maximum degree possible, while simultaneously mitigating the impacts of the non-favorable properties (primarily mitigating the effects of the high freezing temperature of the fluoride salts).

The following subsections review key thermal hydraulic phenomena that arise from the unique thermophysical properties of the fluoride salts and FHR structural materials.

Table 3-1. Thermophysical Properties* of LWR, HTGR, SFR, and FHR Coolants and Materials (Forsberg, Peterson, and Pickard 2003; Williams, Toth, and Clarno 2006)

Material	T_{melt}, °C	T_{boil}, °C	ρ, kg/m^3	C_p, kJ/kg°C	ρC_p, kJ/m^3°C	k, W/m°C	$\nu \cdot 10^6$, m^2/s
$^7Li_2BeF_4$ (flibe)	459	1,430	1,940	2.34	4,540	1.0	2.9
0.58 NaF-0.42 ZrF_4	500	1,290	3,140	1.14	3,583	0.49	1.6
Sodium	97.8	883	790	1.27	1,000	62	0.25
Lead	328	1,750	10,540	0.16	1,700	16	0.13
Helium (7.5 MPa)			3.8	5.2	20	0.29	11.0
Water (7.5 MPa)	0	100	732	5.5	4,040	0.56	0.13
Hastalloy C-276	~1350		8,890	0.43	3,820	9.8	
Graphite			1,700	1.90	3,230	200	

* Approximate physical properties at 700°C except the pressurized water data shown at 290°C for comparison. ρ is density, C_p specific heat, k thermal conductivity, and ν viscosity.

3.2.1 High Prandtl Number, Transparent Coolant

As seen in Table 3-1, the thermal conductivity of the baseline FHR primary coolant flibe is greater than water. However, flibe is also a highly viscous fluid, thus making it a high Prandtl (Pr) fluid (on the order of 12). Most previous nuclear experience is with moderate Pr (water/helium-) or low Pr (sodium-) cooled reactors.

The greater thermal conductivity of flibe creates the potential for achieving heat transfer coefficients comparable to those for water even though the viscosity of flibe is much higher. However, the fact that flibe also has a high volumetric heat capacity means that FHR convective heat transfer commonly occurs at Reynolds numbers that are barely turbulent or are in the transition regime even under forced circulation, and natural circulation heat transfer is almost always in the transition or laminar regime.

For this reason, unlike reactors using other coolants, FHR designs will almost certainly optimize to use enhanced heat transfer surfaces or small-diameter flow channels. Enhanced surfaces break up and regenerate boundary layers, so that thermal boundary layers are developing rather than fully developed. Enhanced surfaces, such as the twisted tubes shown in Figure 3-3 and the interrupted flow that occurs in pebble beds, are particularly effective in reducing boundary layer thicknesses and increasing heat transfer in transition regime and laminar flow. Equally as important, enhanced surfaces provide more predictable heat transfer coefficients in the transition and laminar flow regimes. Additional enhanced surface options include ribbed, dimpled, and knurled surfaces, which are commonly used in other technologies for augmenting heat transfer (Figure 3-4). Likewise, laminar flow in small-diameter channels can provide relatively high heat transfer coefficients from the reduced conduction length scale.

Convective heat transfer coefficients for enhanced surfaces can be measured experimentally for laminar, transition regime, and turbulent flows in geometrically scaled experiments using heat transfer oils like Dowtherm A, which have the same Prandtl numbers as the fluoride salts but at much lower temperatures (Bardet and Peterson 2008). Corrections must be made, however, to account for the effects of thermal radiation heat transfer because the fluoride salts can be transparent in the near-infrared and visible spectrums.

Figure 3-3. Twisted Tube Heat Exchangers, Which Provide Enhanced Heat Transfer on Both the Shell and Tube Sides[1]

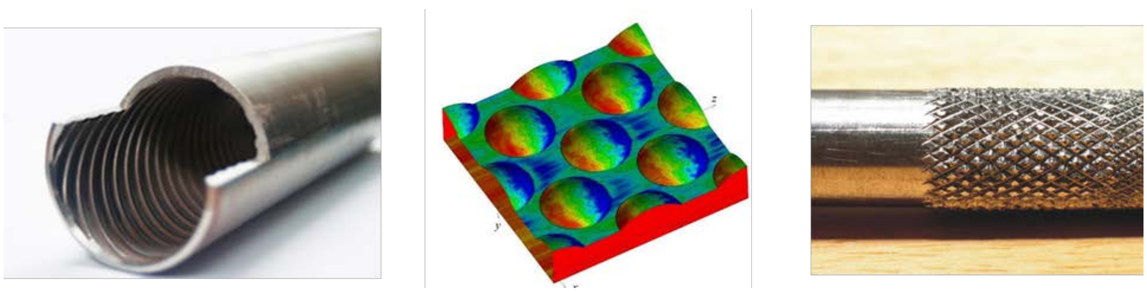

Figure 3-4. From Left to Right: Ribbed, Dimpled, and Knurled Surfaces for Other Heat Transfer Applications

FHRs operate at sufficiently high temperatures that thermal shock, striping, and ratcheting phenomena are potentially important in affecting the design and long-term reliability of metallic reactor structures. Graphite structures are highly resilient to thermal stresses arising from these phenomena, but FHR metallic structural materials (e.g., reactor vessel, the intermediate heat exchanger or IHX, and the dynamic heat exchanger or DHX) could potentially be damaged. The most important experience base for these phenomena exists with SFRs, which also operate at low pressure and thus have thin-walled metallic structures like FHRs do.

The major difference for transient thermal stresses in FHR and SFR structures involves the Prandtl number of the coolants. The liquid metal sodium has a thermal conductivity greater than that of metallic structural materials (Table 3-1) and thus transfers heat rapidly into structures during thermal transients, while the thermal conductivity of the fluoride salts is much lower than

[1] From http://www.kochheattransfer.com/products/twisted-tube-bundle-technology. Accessed February 21, 2013.

that of the metallic structures. This said, even though the salt thermal conductivities are low compared to sodium, the potential remains that transients can generate stresses exceeding elastic limits, causing inelastic deformation. Repeated multiple times, such transients may cause structural failures, and even if stresses remain within the elastic region, very large numbers of cycles can generate fatigue-induced failures.

Several design features of FHRs have the potential to mitigate against thermal transient-induced failures of metallic components. For example, the fact that FHRs will have relatively small downcomers with short fluid residence times reduces the potential for thermal ratcheting of the reactor vessel. The high Prandtl number of the fluoride salts likewise reduces the potential magnitude of thermal cycling and thermal stress caused by thermal striping. Likewise, the fact that the flow emerging from FHR cores and bypass pathways is collected and mixed inside graphite upper-core plenum structures reduces the potential for metallic structures to be driven with significant thermal cycling. While these attributes of FHRs are favorable, FHRs also operate at significantly higher steady-state temperatures than SFRs, so detailed understanding of thermal stresses and thermal stress cycling of FHR metallic structures with a high Prandtl number coolant is an important and unique element of FHR design and licensing.

3.2.2 Multi-Dimensional Porous Media Flow (for Pebble Bed FHRs)

Forced convection inside pebble beds results in high heat transfer coefficients, because flow around spheres involves tortuous paths, and new boundary layers form on each pebble. This section reviews a few key correlations, as an example of the heat transfer models needed in any thermal hydraulic code used for FHR modeling (Galvez 2011). Primary differences between models include how the fluid flow is characterized and at what temperature the properties are evaluated. Another difference arises from the use of superficial velocities in some correlations, as opposed to actual velocities in others, where the flow velocity is higher because of a constrained flow in a fraction of the total cross sectional area of the volume of the pebble bed.

Based on a literature review, the heat transfer coefficient is best approximated by the following relation suggested by Wakao and Kaguei (Wakao and Kaguei 1982):

$$h = \frac{k}{D_p}\left(2 + 1.1\,\mathrm{Re}^{0.62}\,\mathrm{Pr}^{0.33}\right) \tag{3-1}$$

for $5<\mathrm{Re}<100{,}000$ where the Reynolds number Re is based on superficial velocity, and thermophysical properties are calculated at the mean fluid bulk temperature. The pebble diameter is used as the length scale. The equation shown above includes two terms. The first constant term represents the heat conduction from a single pebble submerged in stagnant fluid. The second term is a function of the fluid flow through the pebble bed, thus indicating a dependence on flow conditions.

Another useful correlation was obtained by Whitaker (Whitaker 1972), primarily by performing experiments with gases in packed beds. However, the data also apply to fluids with similar thermophysical characteristics as liquid salts in the range of interest for the FHR:

$$h = \frac{k}{D_h}\left(0.5\,\mathrm{Re}^{1/2} + 0.2\,\mathrm{Re}^{2/3}\right)\mathrm{Pr}^{1/3}\left(\frac{\mu_b}{\mu_s}\right)^{0.14} \tag{3-2}$$

for 20<Re<10,000 where Re is based on pore velocity and thermophysical properties are evaluated at the bulk fluid temperature, except for the correction factor, which is evaluated at the mean surface temperature. The characteristic hydraulic diameter is used as the length scale.

Other correlations can be found in the literature for heat transfer coefficients in pebble beds. Experimental data will be needed to select correlations that best apply to various operating modes of the PB-FHR, and these data will also serve to validate thermal hydraulic models using these correlations.

Similar sets of correlations have been developed to relate friction factors, and thus pressure drop across pebble beds, to Reynolds number and the geometry of the bed. One of the important conclusions is that pressure drop is highly dependent on the pebble bed packing fraction and pebble diameter (Nield and Bejan 2006), which must therefore be carefully assessed in the thermal hydraulic modeling of FHRs.

For pebble beds, wall effects play a significant role in pebble packing. The Pebble Bed Modular Reactor (PBMR) had a dimpled pattern on the graphite blocks, to break up ordered packing of the pebbles at the walls and eliminate the channeling effect. These effects should be partly minimized with the use of smaller pebbles for a pebble bed-FHR (PB-FHR; 3-cm-diameter instead of 6-cm-diameter pebbles).

3.2.3 Effective Natural Circulation for Passive Decay Heat Removal

Natural circulation is the primary decay heat removal method for FHRs. Because the capability of natural circulation to remove heat is largely independent of the reactor core size, FHRs can be designed for passive safety even for large power levels. This effect is similar to LWRs, where passive heat removal can also be achieved with natural circulation. A study by the International Atomic Energy Agency reviewed experiments and the current state of the art in LWR natural circulation modeling (IAEA 2005).

Predicting natural circulation heat transfer can be relatively simple, because the buoyancy forces that drive the flow can be determined by integrating the coolant density around the loop. The temperature difference between the hot and cold sides of the loop can then be determined by balancing the buoyancy forces against the form and friction losses around the loop. In the turbulent regime, this can be written

$$\Delta\rho g \Delta H = \rho K \frac{U^2}{2} \quad \text{or} \quad \beta \Delta T g \Delta H = K \frac{U^2}{2} \tag{3-3}$$

where $\Delta\rho$ is the difference between the maximum and minimum fluid density in the loop, g the acceleration of gravity, ΔH the effective height of the loop, ρ the average density of the fluid in the loop, K the sum of form and friction loss coefficients around the loop, U the characteristic velocity of flow in the loop, β the thermal expansion coefficient, and ΔT the difference between the maximum and minimum temperature around the loop. The net heat transported by the loop is

$$\dot{q} = \left(\rho C_p\right) UA\Delta T \tag{3-4}$$

where *UA* is the volumetric flow rate of coolant and *A* is the characteristic flow area in the loop. The characteristic natural circulation loop height required to remove heat is then

$$\Delta H = \frac{K\dot{q}^2}{2g\beta\left(\rho C_p\right)^2 A^2 \Delta T^3} \tag{3-5}$$

The thermophysical property group $\beta\left(\rho C_p\right)^2$ emerges as an important parameter affecting the height of a natural circulation loop needed to transport heat by natural circulation. The ratio of this parameter for flibe, compared to sodium, is $\beta_{flibe}\left(\rho C_p\right)^2_{flibe} \Big/ \beta_{Na}\left(\rho C_p\right)^2_{Na}$ = 16.5. While the thermal expansion coefficient β of flibe is 20% lower than that of sodium, the much larger volumetric heat capacity of flibe makes it substantially more effective in natural circulation heat transfer.

While the steady-state flow rate in a simple natural circulation loop can be predicted easily, the flow distribution in an actual FHR will be more complex because of multiple natural circulation loops, including through the core, IHXs, DHXs, pebble injection stand pipes, and core bypass flow paths. Typical LWR thermal hydraulic modeling codes can solve for the transient flow distributions in multiple interconnected flow paths.

Additionally, more complex three-dimensional flow patterns and temperature distributions can emerge in reactor cores and the outlet plena of cores and heat exchangers. In experiments, local temperatures must be measured carefully using thermocouples to infer bulk average temperatures, and it is generally important to provide multiple thermocouples in locations where nonuniform temperatures could be expected. Three-dimensional computational fluid dynamics modeling of these regions may be valuable, to assess the effectiveness of mixing.

Finally, natural circulation flow systems may be subject to a variety of instabilities. Static instabilities can be explained by the steady-state version of the governing transport equations, while dynamic instabilities require the use of time-dependent conservation equations (IAEA 2005). It is commonly accepted that natural circulation is more inherently instable than forced circulation because of the nonlinear nature of the natural circulation phenomena that can result in oscillatory behavior. Note that two-phase flow natural circulation presents a significantly larger number of instability issues because of the dynamics of phase change and coupled neutronic and thermal hydraulic instabilities. Potential FHR instability modes can be divided into four categories based on the work of Vijayan and Nayak (IAEA 2005).

1. Stability of the rest state
2. Compound static instabilities
3. Dynamic instabilities
4. Compound dynamic instabilities.

Because of the infancy of the FHR design, each category of instabilities must be reviewed for applicability once a complete spectrum of initiating events has been identified.

3.2.4 Potential for Freezing (Overcooling Transients)

Mixtures of fluoride salts have high freezing temperatures, typically between 320°C and 500°C, which makes overcooling transients an important topic for design and safety analysis. The 8-MWth Molten Salt Reactor Experiment (MSRE), which operated from 1965 to 1969, experienced freezing in its air-cooled radiator, shown in Figure 3-5; the radiator was then thawed without damage. Operating experience with test loops, such as the MSR-FCL-2 forced-circulation materials test loop (McNeese 1976a), found that freezing could occur in coolers after the loop heating and forced circulation was shut down, because of heat transfer to structures around the cooler that were maintained at low temperature by the air flow. The loop could be rethawed without damage, as long as during reheating melted salt was not trapped between frozen plugs. Procedures developed for the MSR-FCL-2 test loop to maintain reduced-speed pump circulation for a period of time after the trip of the heaters was found to be effective in preventing freezing.

A wide variety of phenomena are important (1) to the transient behavior of natural circulation loops that can lead to salt freezing, (2) to methods to monitor for and prevent freezing (such as activating circulation pumps, electric heaters, or draining loop to drain tanks), (3) to predict effects in other parts of the reactor primary system caused by flow blockage from freezing, and (4) to mitigating and recovering from freezing events.

Figure 3-5. Air-Cooled Radiator in the 8-MWth MSRE in Operation. Bright yellow lines are electric heaters provided to prevent overcooling. Here they are operating because the enclosure has been opened to allow the photograph to be taken (Credit: ORNL).

Because volume changes caused by freezing and thawing will primarily affect the heat exchanger tubes, more needs to be done to determine the performance of (1) stability of flow in individual tubes in a tube bank against localized freezing, (2) the recovery from freezing of twisted tube heat exchangers, (3) pipe bursts during thawing, and (4) protection of the tubing.

3.2.5 Graphite Thermal Properties

To properly account for heat conduction in the fuel pebbles, any code that will be used for thermal hydraulic modeling of the FHR must include dose- and temperature-dependent graphite thermal properties. The conduction model will also depend on the exact composition of the pebble and more specifically the tristructural istropic (TRISO) coated particle and graphite matrix in the fuel region of the pebble (fuel design) and burnup of the fuel. If a homogenized model is to be used for the fuel region, validation will be needed to make sure that proper thermophysical properties of the assembly are being used.

3.2.6 Bypass Flow

The graphite reflector blocks in the FHR can shrink and swell as complex functions of irradiation and temperature. These changes can lead to the formation of gaps between the blocks through which coolant will flow. The nature of this bypass flow must be carefully studied to assess the impact on temperature profiles within the fuel blocks. Bypass flows can have significant effects on the coolant outlet temperature gradient. For fast transients, especially, detailed temperature profiles of the coolant should be taken into account for thermal stress calculations on metallic structures outside the core. Bypass flows through graphite blocks were an important issue for the PBMR, and the consequences of using flibe instead of helium as a coolant must be analyzed.

3.2.7 Radiative Heat Transfer

At high operating temperatures, radiative heat transfer to and from the cavity, as well as total heat transfer to and from the reactor vessel, must be calculated. Likewise, wavelength-dependent absorption data are needed for coolant salts to allow their radiative interactions with heat transfer surfaces to be assessed.

3.3 Current Thermal Hydraulic Modeling Capabilities

Numerous computer codes have been written to simulate the thermal hydraulic characteristics of reactor cores and the primary loop under steady-state and operational transient conditions as well as potential accidents. New versions of some of these codes can be expected to be developed, and efforts are now focused on adapting existing codes and developing new ones for the new generation of advanced LWRs as well as HTGRs. A similar capability is needed to properly model steady-state and transient thermal hydraulic phenomena for the FHR, with an initial focus on design codes that will allow for rapid prototyping of the FHR system. The main purposes of the continuing effort in the development of such computer codes have been improved computational effectiveness and improved ability to predict the response of the core and the primary loop. Therefore, efforts have continued to incorporate the recent models and methods of analysis in the areas of both hydrodynamics and heat transfer to the extent that their predictions are reasonably reliable.

Code users are therefore confronted with the need to develop criteria to choose the most appropriate version to handle a specified case. This is a two-pronged decision because it requires not only evaluating the models and methods used in each code but also comparing the results and experimental data to observe how well these data are predicted (Kazimi and Massoud 1980).

For confirmatory analysis, NRC prefers to use existing analytical tools to the extent feasible, with appropriate modifications for the intended purpose, which is also the preferred approach for the FHR IRP. For instance, for LWR safety analysis, the NRC traditionally uses its system-level MELCOR code, which is capable of performing thermal-fluid and accident analysis, including fission product transport and release. This code is planned to be modified for the NGNP (DOE 2008). Similar modifications may be required for the FHR.

Appendix A of this white paper reviews a subset of thermal hydraulic codes that have been successfully developed or adapted to model steady-state and transient phenomena for advanced reactor concepts sharing some important design characteristics with the FHR. These capabilities are summarized in Table 3-2, according to the list of key FHR thermal hydraulic phenomena reviewed in Section 3.2.

In Table 3-2, codes that have been used to model some key FHR phenomena but lack V&V (marked with x) have been differentiated from codes that have been used to model some key FHR phenomena, compared to other codes, but lack validation experimental basis (marked with xx), and codes that have been validated for modeling of key FHR phenomena, although with other reactor designs (marked with xxx). The *Regulatory Basis* category is specific to VIPRE-01 for the AP-1000, as an example of good practice with the NRC toward final design approval.

Table 3-2. Some Codes and Their Applicability to Key FHR Thermal Hydraulic Phenomena Modeling

Code	High Prandtl Number	Multidimensional Porous Media Flow	Effective Natural Circulation for Passive Decay Heat Removal	Potential for Freezing (Overcooling Transients)	Conduction in Fuel and Structures	Core Bypass Flow	Regulatory Basis
THERMIX		xxx			xxx		
COMMIX		xxx	xxx				
RELAP5-3D	xx	x	xx		x		
VIPRE-01			xxx				x
Computational Fluid Dynamics Codes	x	xx				x	

x: Code has been used but lacks V&V basis.
xx: Code has been used and compared to other codes but lacks validation experimental basis.
xxx: Code has been used and validated for other reactor designs sharing FHR phenomena.

3.4 Candidate FHR Thermal Hydraulic Codes

At this point on the development path of the FHR design, all thermal hydraulic analyses have been performed using the RELAP5 systems analysis code. This section describes the basis for thermal hydraulic modeling of the PB-FHR using RELAP5, along with the model itself and some results of thermal hydraulic transient analyses. As evidenced in Table 3-2, RELAP5-3D has the most capabilities needed to properly model FHR key thermal hydraulic phenomena. However, these models lack a complete V&V basis, and experimental work will be needed to fill these gaps.

One major outcome of the second FHR workshop was that other codes should be used to compare results of the FHR modeling effort. Any code will need to be altered to be fully applicable to the FHR, and RELAP5 may be the code eventually used for safety analysis. However, for pre-conceptual design studies and rapid prototyping of the FHR, commercially available Computational Fluid Dynamics codes such as Flownex, which has been partly verified and validated for HTGRs and the PBMR (see details in Appendix A), should also be used.

3.4.1 Knowledge Basis for Thermal Hydraulic Modeling of the PB-FHR with RELAP5

Although RELAP5 was originally developed for thermal hydraulic analysis of LWRs and related experimental systems during loss-of-coolant accidents and operational transients, the code has recently been improved to simulate candidate Generation IV designs cooled by gas, supercritical water, and lead-bismuth. Liquid salt coolants, and more specifically flibe, which is the primary coolant for the FHR, have also been implemented into the code (Davis 2005), which allows it to model thermal hydraulic steady-state and transient phenomena for the FHR. Thermophysical properties of flibe as implemented into RELAP5 have been benchmarked against available data for the salt (Sohal et al. 2010), and some of these properties are shown in Figure 3-6, for the range of temperatures at which the FHR is expected to operate.

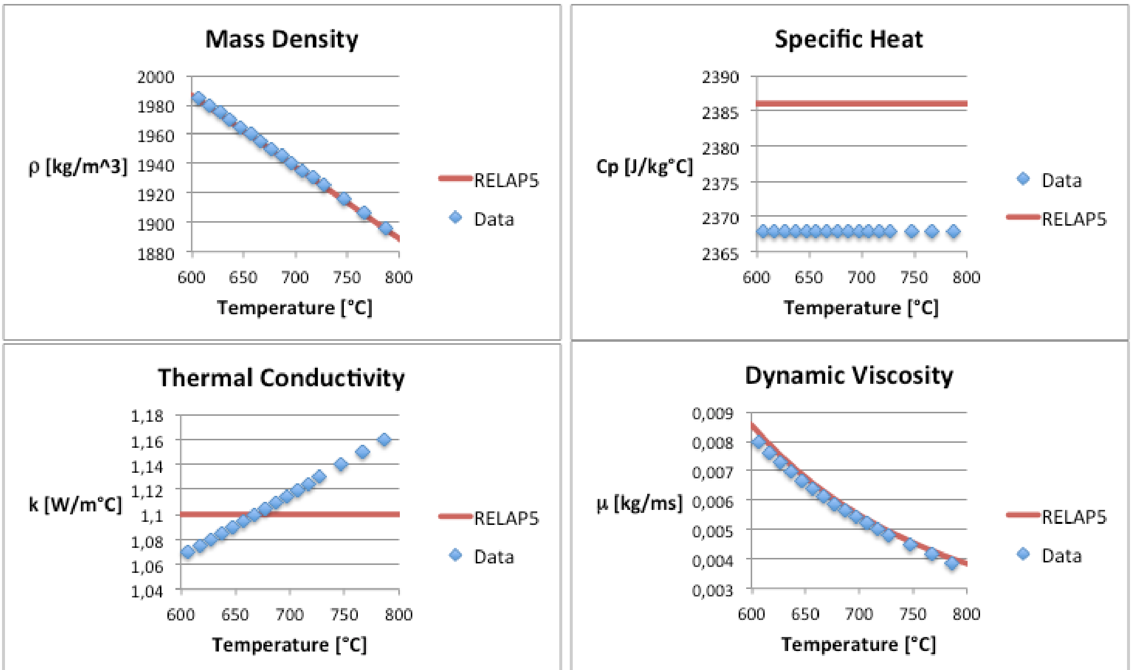

Figure 3-6. Benchmark of Flibe Thermophysical Properties in RELAP5 Versus Experimental Data

The results in Figure 3-6 show a satisfactory match between flibe thermophysical properties as implemented into RELAP5 and experimental data for some properties. However, RELAP5 uses a constant thermal conductivity, and the value used for the specific heat slightly differs from the value observed experimentally. Unless the code is changed to fix these discrepancies, distortions must be taken into account when using RELAP5 to model thermal hydraulic phenomena in the FHR. More specifically, deviations in the system response arising from these distortions should be carefully accounted for when studying steady-state and transient phenomena. These biases can be deterministically propagated in the code calculations and can therefore be precisely assessed. An additional effort should be conducted to implement secondary salt candidates thermophysical properties into RELAP5 [flinak has already been implemented (Davis 2005), but potential ZrF_4-based salts also need to be implemented].

Correlations for heat transfer and friction losses in the pebble-bed can also be manually implemented into the code, but a significant validation effort of these correlations is still required.

Because of its wide use in the nuclear industry for design and licensing of reactors, RELAP5 appears to be a good candidate for preliminary studies of the FHR steady-state and transient responses. However, additional efforts are needed to properly account for all phenomena described in Section 3.2 if RELAP5 is to be used as the system analysis code for thermal hydraulic behavior of the FHR.

3.4.2 Thermal Hydraulic Modeling of the PB-FHR in RELAP5

Figure 3-7 shows a PB-FHR plant nodalization diagram that has been used for modeling in RELAP5, with the major sub-systems indicated.

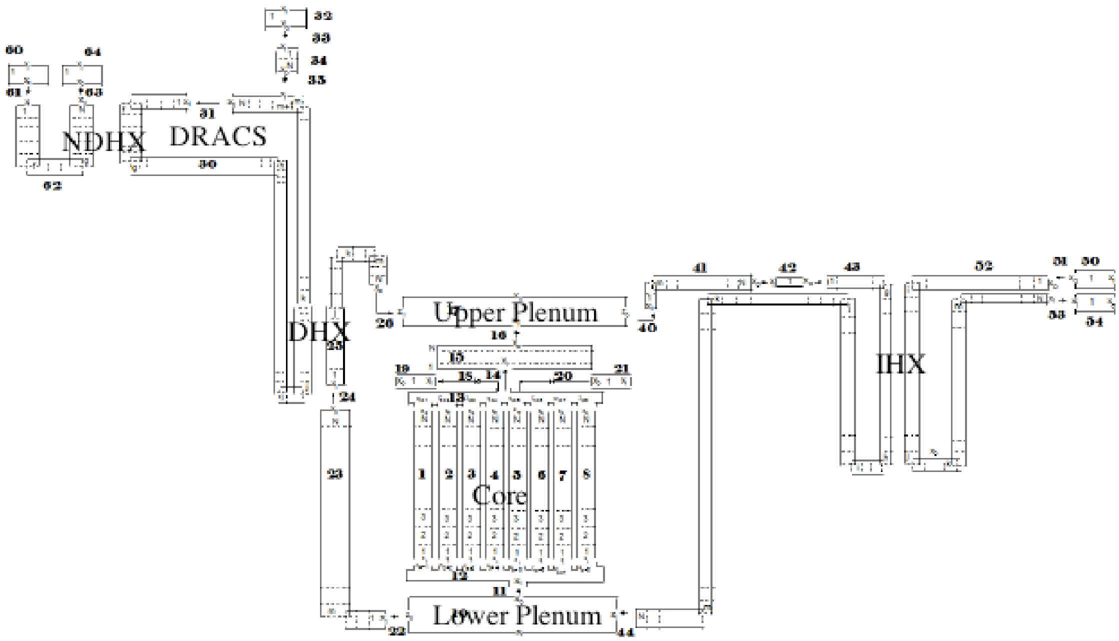

Figure 3-7. PB-FHR Plant Nodalization Diagram in RELAP5 (Galvez 2011)

The baseline design for this model is a 900-MWth pebble channel assembly PB-FHR core. Although the design is expected to significantly evolve during the development path of this project, this model serves as a first proof of principle regarding the capability to model the FHR using RELAP5.

Flibe is used as the primary coolant, while flinak – which has also been implemented into RELAP5 (Davis 2005) – is used as the secondary coolant. RELAP5 calculates friction losses across the pebble bed using Ergun's correlation, which is the most common correlation for porous media flow, while the model characterizes convective heat transfer between the coolant and the pebbles by the Wakao correlation (see in Section 3.2). The code derives the design of the IHX and the DHX from the heat exchanger design of the Molten Salt Breeder Reactor developed at Oak Ridge National Laboratory (ORNL) in the 1970s, while the code bases the design of the DRACS on a helical heat exchanger. Based on these designs, relevant heat transfer correlations are also implemented into RELAP5 (Galvez 2011).

Overcooling transients have not been considered in thermal hydraulic analyses of the FHR in RELAP5 so far, and at this point, the code is not able to properly model this phenomena. Similarly, the capacity to properly model bypass flow in the graphite reflectors has not been developed in RELAP5, because of the complexity of graphite blocks geometry changes under thermal transients as mentioned in Section 3.2.

Despite these limitations in the modeling capabilities of RELAP5 for the FHR, Galvez calculated preliminary results for the transient response of the system to a LOFC (Galvez 2011); these are presented below as an example of the capabilities expected from the thermal hydraulic modeling of the FHR.

3.4.3 Examples of Results Obtained with the RELAP5 Model of the PB-FHR

Galvez used the RELAP5 model of the PB-FHR to study the response of the reactor to a LOFC with scram, where the design relies on passive decay heat removal through coupled natural circulation in the primary loop and the DRACS loop (Galvez 2011). From the baseline design of the PB-FHR, the study optimized the DRACS dimensions to satisfy safety requirements regarding peak outlet coolant temperatures. Indeed, for every transient considered in the design of the FHR, thermal limits arise from metallic components used outside of the core (e.g., in the IHX), while the fuel elements have very high thermal margins.

The insertion of the shutdown control elements into the core is expected to bring the reactor power down very quickly. As a consequence, average fuel temperatures will come down rapidly as the power per pebble is reduced greatly from the full-power value; however, pebble fuel layer temperatures are always higher than coolant surface temperatures, because the reactor is still producing decay heat. The curve presented in Figure 3-8 is the primary safety indicator of the transient study. This figure seeks to demonstrate that the reactor core does not exceed thermal safety limits for fuel and metallic structures in contact with core outlet coolant.

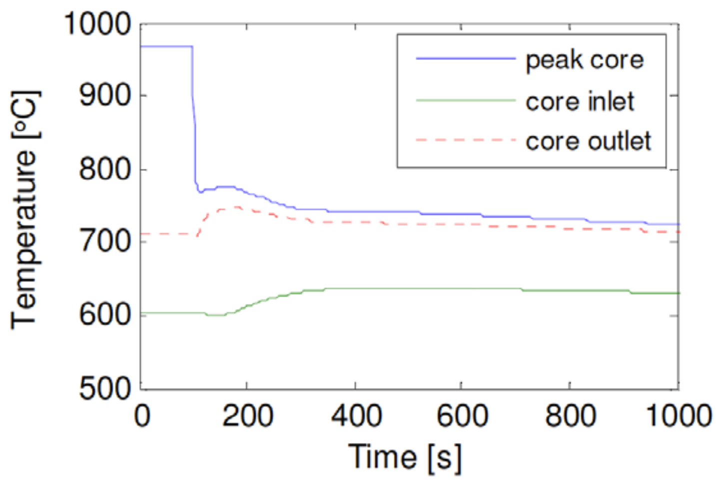

Figure 3-8. Peak Core Average Fuel Temperature Versus Inlet and Outlet Coolant Temperature (Galvez 2011)

Additional results are provided by Galvez (Galvez 2011).

3.4.4 Required Code Development and Additional Work

At this point, little validation work has been performed for the use of RELAP5 as the system analysis code for the FHR. Although the code has been extensively modified to model most of the key FHR thermal hydraulic phenomena (i.e., pebble bed core region), very little experimental data are available to confirm that these capabilities have been properly implemented. More importantly, it seems that some key phenomena for the FHR (overcooling transients, bypass flow, etc.) cannot be properly modeled at this point using RELAP5.

3.5 Existing and Required Experimental Basis for Thermal Hydraulic Modeling Validation

As highlighted in the previous sections, although preliminary thermal hydraulic modeling of the FHR has been performed using the RELAP5 systems analysis code, the code, in its current state, is not capable of capturing some of the key FHR thermal hydraulic phenomena. A list of V&V efforts needed to increase the reliability of any code to properly model thermal hydraulic phenomena for the FHR is presented here. One key point is that all V&V efforts should comply with quality assurance requirements, as developed in quality assurance information from the DOE Nuclear Energy University Programs[2] and the ASME (ASME 2008).

The experimental test program for the FHR will provide empirical data to validate models that predict plant reliability and safety (Bardet et al. 2008). The PIRT process provides the basis to identify the dominant phenomena that control the system response to a specific reliability- or safety-related transient. A PIRT-type exercise should be performed in the short term to that effect. Based on the current point design of the FHR, this exercise will help identify thermal hydraulic phenomena that must be modeled, and their priority, because of their importance for transient response of the FHR to LBEs and the lack of a reliable knowledge basis associated with these phenomena. This effort will also generate the experimental data needed to validate these models. The H2TS methodology, which informs IETs and SETs required for validation of thermal hydraulic models, is detailed in (Zuber et al. 1998) and explained in Section 2.3.

The thermal hydraulic transient phenomena associated with FHR response to LBEs evolve over relatively brief time periods of minutes to days. Here, the major constraint on experiments is not duration, but rather scale, because of the impracticality of performing IETs at the full-power level of the reactor. The major importance of power scaling was recognized early in the pre-conceptual design of the FHR. As described below, the thermophysical properties of liquid salts and the modularity of the FHR primary system and decay heat removal system designs allow the integral response to LBEs to be reproduced at a power level four orders of magnitude below the prototypical power with low distortion. The FHR design also adopts the approach of applying the CSAU methodology consistently across all transient system modeling.

Liquid salts are unique among candidate reactor coolants (water, helium, liquid metals) because simulant fluids can replicate salt fluid mechanics and heat transfer phenomena at reduced length scales and temperature, and with greatly reduced heater and pumping power. In the late 1990s, UCB demonstrated that water can be used as a simulant for replicating liquid salt fluid mechanics phenomena, noting that at approximately 40% geometric scale, room-temperature water experiments can match the Reynolds and Froude numbers associated with flibe (Cavanaugh and Peterson 1994). Subsequently, UCB identified a class of heat transfer oils that have the same Prandtl number as the major liquid salts and that can thus match Reynolds, Froude, Prandtl, and Grashof numbers simultaneously at approximately 50% geometric scale and heater power under 2% of prototypical (Bardet and Peterson 2008). While scaled oil experiments do not reproduce thermal radiation heat transfer from the salt-to-heat transfer surfaces, under most conditions this is a second-order effect that can be corrected in the system model (Bardet

[2] Available at https://inlportal.inl.gov/portal/server.pt/community/neup_home/600/quality_assurance. Accessed February 21, 2013.

and Peterson 2008). Figure 3-9 shows the Prandtl numbers of flibe and Dowtherm A, a commonly used heat transfer oil, over the range of expected operating temperatures of the FHR for flibe, and a scaled temperature range for Dowtherm A.

The availability of such simulant fluids significantly reduces the cost and difficulty of performing IETs required for system modeling code validation for reactor licensing, compared to working at prototypical temperatures and power levels with the actual coolant. These simulant fluids can also be used in SET experiments to develop heat transfer and pressure loss correlations for use in system modeling codes. The implications for IET and SET experiments are summarized in the next two subsections and detailed in Appendix B. One important challenge is the implementation of simulant fluid thermophysical properties into the modeling code that is validated. Dowtherm A has been implemented into RELAP5 using thermophysical properties provided by Dow (Dow Chemical Company 1997).

The following subsections outline an experimental program, including IETs and SETs.

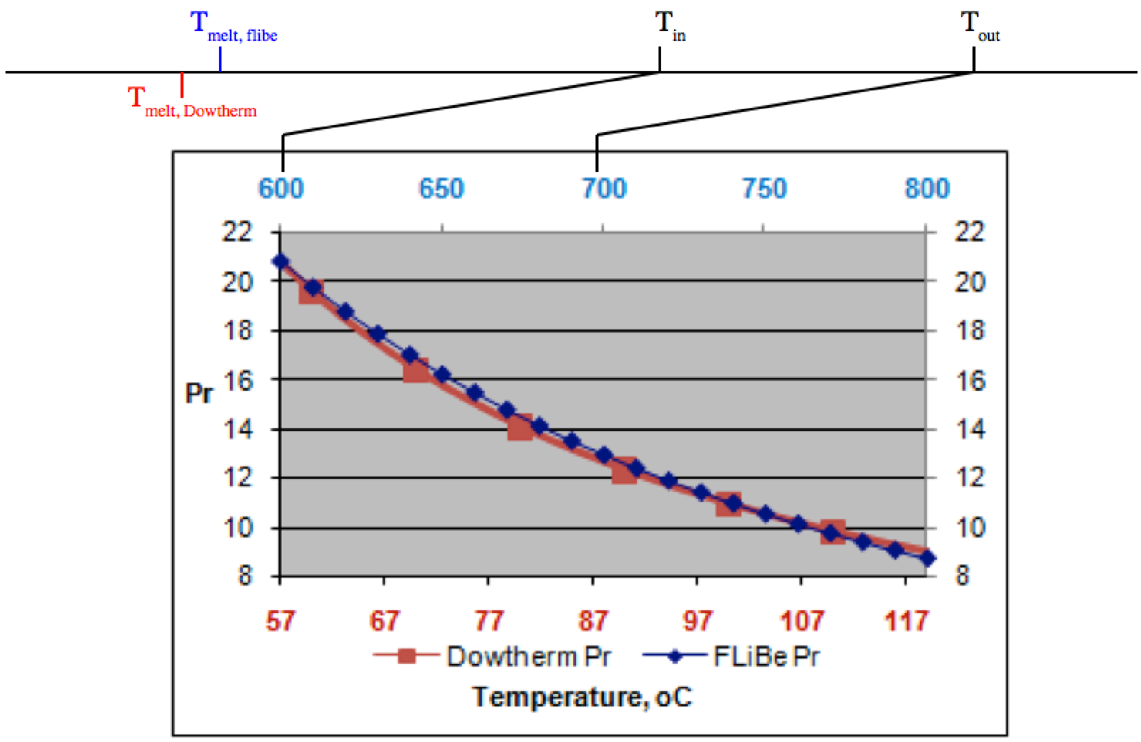

Figure 3-9. Prandtl Numbers of Flibe and Dowtherm A over the Range of Expected Operating Temperatures of the FHR for Flibe and a Scaled Temperature Range for Dowtherm A

3.5.1 IET Experiments

The liquid-salt-cooled FHR is distinguished from reactors that use other coolants because the FHR IETs can be performed with simulant fluids at greatly reduced power levels. Thus, the key IET experimental facilities needed to validate the FHR transient analysis codes are university-scale facilities built and operated during the viability phase of pre-conceptual design. These facilities are expected to continue to operate, as needed, during the performance phase of pre-conceptual design to provide new IET data as the detailed design and safety analysis are finalized.

Table 3-3 summarizes IETs needed to validate key FHR thermal hydraulic phenomena. Details about a subset of these IETs are provided in Appendix B.

Table 3-3. Existing and Projected IETs to Validate Key FHR Thermal Hydraulic Phenomena

Facility	High Prandtl Number	Multidimensional Porous Media Flow	Natural Circulation, 1Φ, Non-compressible	Freezing and Melting	Conduction in Fuel and Structures	Core Bypass Flow	Status
CIET	x	x	x		x		Operational
CIET 2	-		-			-	Under design/construction
PREX		x					Operational
APEX			q			q	
HTTF			q			q	
Ohio State DRACS Loop	-		-				Planned
ORNL Salt Loop	-		-	-		-	Under design/construction
Shanghai Institute of Applied Physics Salt Loop	-	-		-	-	-	Planned
Component Test Facility	-	-	-	-	-	-	Future roadmap
2-MW Test Reactor	-	-	-	-	-	-	Future roadmap
20-MW Test Reactor	-	-	-	-	-	-	future roadmap

x: Existing IET providing limited quality/scoping data
q: Existing IET providing quality data
-: Projected IET

3.5.2 SET Experiments

The FHR SET experiment program will cover FHR key thermal hydraulic phenomena for which high-quality, experimentally validated models are not yet already available. While detailed conceptual design phase PIRTs have not yet been developed, several dominant phenomena have already been identified in FHR modeling efforts where existing experimental data are insufficient.

Viability Phase

For the viability phase of pre-conceptual design, SET experiments will include studies of mixed convection heat transfer in pebble beds and in vertical channels using simulant fluids, where relevant experimental data do not exist in the range of Prandtl and Grashof numbers that occurs in the FHR.

Performance Phase

During the performance phase of pre-conceptual design, SET data will be collected for prototypical components with the prototypical heat transfer fluid in a FHR Component Test Facility. Adequate instrumentation should be used to collect heat transfer, pressure drop, and other SET data of interest. In particular, these data would address questions about the potential impact of thermal radiation on heat transfer to liquid salts.

Very limited data for infrared absorption are available for flibe and flinak (one of the candidate salts for the secondary coolant). Thus, the performance phase is also expected to have SET experiments to measure absorption in the primary, secondary, and DRACS salts.

Table 3-4 summarizes SETs needed to validate key FHR thermal hydraulic phenomena.

Table 3-4. SETs Required to Validate Key FHR Thermal Hydraulic Phenomena

Viability Phase		Performance Phase		
Heat transfer in pebble beds and vertical channels	Heat transfer in pebbles	Heat transfer at prototypical temperature	Pressure drop at prototypical temperature	Thermal radiation at prototypical temperature
x	-	x	x	x

-: Existing experimental basis
x: Additional required SETs

As progress is made in FHR development, a more and more substantial experimental database will become available to validate thermal hydraulic models of the FHR. A simultaneous effort should be made to refine code selection and implement new features in the codes to include proper modeling of all FHR key thermal hydraulic phenomena. Code-to-code comparison and formal benchmarking exercises can provide an efficient method to detect errors in the way codes model some phenomena. Eventually, code validation will be needed, including sensitivity analyses for relevant parameters and uncertainty calculations over a range of parameter values for all modes of operation of the FHR, down to BDBEs.

4 Neutronic Modeling

Neutronic modeling plays a central role in the design of FHRs. The neutronic analysis provides the heat source term for the primary coolant system. Furthermore, depletion analysis is required to determine the amount of energy that can be generated by the nuclear fuel – this is a key factor in the economic analysis of the PB-FHR system. Neutronics are likewise critical to the safety analysis. The neutronic modeling assesses effectiveness of the various power feedback mechanisms. The neutronics may need to be coupled to thermal hydraulics to simulate more complex transients such as ATWS.

This chapter discusses functionality requirements of neutronic methods and the phenomena that must be modeled accurately, evaluates candidate neutronic codes, and surveys the experimental base to validate these FHR neutronic codes.

4.1 Major LBEs and Figures of Merit

This white paper divides all neutronic simulation functionality into a subset of "capabilities." A set of neutronic codes can be employed to provide the different capabilities needed for an integrated EM. For example, detailed geometry and neutron physics need to be simulated faithfully when calculating reactivity feedback coefficients with a continuous-energy Monte Carlo neutron transport code. On the other hand, using this type of code for transient analysis makes generating power distributions challenging and results in long and expensive computation times when analyzing a transient with small time steps. Using more than one modeling method, and comparing results, also provides a method to benchmark calculations and to increase confidence in their accuracy.

The NRC has produced guides for the development of safety analysis reports for reactor licensing of commercial reactors (LWRs) and test reactors (mostly TRIGAs) in NUREG-0800 (NRC 1987) and NUREG-1537 (NRC 1996), respectively. Table 4-1 summarizes and organizes most of the required figures of merit into capabilities of neutronic modeling.

Table 4-1. Neutronic Values to be Determined By Neutronic Modeling, Organized by Capability

<table>
<tr><th>Capability</th><th colspan="3">Values Needed</th></tr>
<tr><td colspan="4">High-Fidelity Criticality Analysis (HFCA)</td></tr>
<tr><td rowspan="5">Power and flux distribution</td><td colspan="3">Radial</td></tr>
<tr><td colspan="3">Axial</td></tr>
<tr><td colspan="3">Nodal</td></tr>
<tr><td colspan="3">Non-separable aspects of power distribution</td></tr>
<tr><td colspan="3">Radiation damage to structural components</td></tr>
<tr><td rowspan="5">Reactivity coefficients</td><td>Fuel</td><td colspan="2">Doppler</td></tr>
<tr><td rowspan="3">Moderator</td><td>Graphite</td><td>Thermal scattering</td></tr>
<tr><td rowspan="2">Coolant</td><td>Thermal scattering</td></tr>
<tr><td>Void</td></tr>
<tr><td colspan="3">Power</td></tr>
<tr><td>Reactor kinetics</td><td colspan="3">Delayed neutron fraction</td></tr>
<tr><td rowspan="8">Reactivity control</td><td rowspan="2">Control elements worth</td><td colspan="2">Power</td></tr>
<tr><td colspan="2">Burnup</td></tr>
<tr><td rowspan="2">Minimum worths with single failure</td><td colspan="2">Power</td></tr>
<tr><td colspan="2">Burnup</td></tr>
<tr><td colspan="3">Burnable poison worth</td></tr>
<tr><td colspan="3">Soluble poison worth</td></tr>
<tr><td colspan="3">Xenon buildup worth</td></tr>
<tr><td colspan="3">Cold zero-power shutdown margin</td></tr>
<tr><td colspan="4">Depletion Analysis</td></tr>
<tr><td rowspan="3">Reactivity evolution</td><td colspan="3">Residence time (once-through)</td></tr>
<tr><td colspan="3">Equilibrium cycle length (fixed fuel)</td></tr>
<tr><td colspan="3">Average discharge burnup (pebble bed)</td></tr>
<tr><td rowspan="2">Power and flux distribution coupled to steady-state thermal hydraulics</td><td colspan="3">Nodal</td></tr>
<tr><td colspan="3">Burnup</td></tr>
<tr><td rowspan="2">Isotopic concentration evolution</td><td colspan="3">Nodal</td></tr>
<tr><td colspan="3">Burnup</td></tr>
<tr><td colspan="4">Transient Analysis</td></tr>
<tr><td rowspan="2">Power distribution coupled to transient thermal hydraulics</td><td colspan="3">Nodal</td></tr>
<tr><td colspan="3">Time variation</td></tr>
<tr><td rowspan="2">Short-lived fission product concentration evolution</td><td colspan="3">Nodal</td></tr>
<tr><td colspan="3">Time variation</td></tr>
<tr><td colspan="4">Sensitivity, Uncertainty, and Representivity Analysis</td></tr>
<tr><td>Similitude analysis</td><td colspan="3">Representivity factors</td></tr>
<tr><td rowspan="4">Uncertainty analysis</td><td colspan="3">Nuclear data</td></tr>
<tr><td colspan="3">Nuclide densities</td></tr>
<tr><td colspan="3">Geometry</td></tr>
<tr><td colspan="3">Modeling assumption</td></tr>
</table>

4.2 FHR Neutronic Modeling Phenomena

An important part of developing a model is determining the phenomena that must be incorporated in the simulation. This section summarizes key neutronic modeling features that will be needed for FHRs and notes potential gaps in EMs.

4.2.1 Generic Phenomena

This subsection discusses phenomena that must be modeled in each capability, including the double heterogeneity spatial self-shielding effect, flibe neutronics, FHR geometry, and internodal leakage.

Double Heterogeneity

The double heterogeneity self-shielding effect in nuclear systems with particle fuel is a key area of FHR neutronic phenomenology. Many methodologies have been developed and analyzed to account for this phenomenon, including the following:

1. Explicitly modeling fuel particles in continuous-energy Monte Carlo simulation
2. Generating an effective homogenized material for the active region of the fuel element
3. Developing a reactivity-equivalent physical transform (RPT).

Explicitly modeling the individual fuel particle kernels is the most straightforward way to account for the double heterogeneity effect, because this approach accurately models the physics of the system. However, this is also the most computationally intensive method to account for this phenomenon. Only general-purpose continuous-energy Monte Carlo codes have the capability to model the geometry and self-shielding faithfully, limiting the applicability of this methodology.

This double heterogeneity effect can also be accounted for by modeling the active region of a fuel element in a single node or cell with multigroup cross sections generated with a detailed unit cell model to preserve reaction rates (Goluoglu and Williams 2005). This methodology has been implemented in diffusion codes, deterministic neutron transport codes, and multigroup Monte Carlo neutron transport codes.

The RPT method models the fuel by collecting the fuel particles in a smaller RPT active region and then performing a volume-weighted material homogenization on the transformed active region and modeling the remaining region as an inert matrix (Kim, Taiwo, and Yang 2005). The RPT method accounts for the increased resonance self-shielding of the particle fuel by increasing the density of actinides locally in the RPT homogenized region. However, the extent to which this density must be increased must be calibrated against a high-fidelity simulation of the system that uses continuous energy and models fuel particles explicitly. This methodology has been implemented to study reactors with spherical, cylindrical, and plate fuel geometry. However, there is concern inthe neutronics community about the validity of using this methodology.

Note that this double heterogeneity effect is also present in HTGRs. The development programs for the NGNP and other HTGRs have already invested in advancing methods to account for this phenomenon. Therefore, the FHR program should borrow as much from the HTGR community as possible, especially with respect to neutronic methods.

Flibe Neutronics

Flibe was selected as the baseline coolant for FHRs because of its excellent properties as a coolant (heat capacity, required pumping power, and ability to establish natural circulation), relatively low neutron absorption probability (when using lithium depleted of ^{6}Li) and, therefore, its ability to provide negative temperature reactivity feedback. The reactor physics phenomena related to using flibe as a coolant in FHR systems include the flibe contribution to neutron slowing-down (moderation), reactivity feedbacks of coolant temperature change and voiding, the steady-state concentration of ^{6}Li in the coolant, and the larger nuclear data uncertainty of salt constituents compared to traditional moderators like water.

Negative temperature reactivity feedback at fuel-to-moderator volume ratios that offer nearly maximum discharge burnup is one of the primary reasons flibe was selected as the IRP baseline coolant. Flibe coolant heating and, hence, expansion has four primary reactivity effects:

1. Reduced moderation resulting in reactivity decrease (as the core must be designed to be undermoderated).
2. Reduced neutron loss to absorption in the flibe constituents - ^{6}Li, ^{7}Li, Be, and F, causing reactivity increase.
3. Enhanced neutron leakage probability from the core, reducing reactivity.
4. Spectrum hardening due to flibe moderator temperature increase resulting in reduced reactivity.

FHRs must be undermoderated to ensure negative coolant temperature reactivity feedback. The system is less sensitive to neutron poisons at low ratios of carbon to fuel heavy metal because of the larger fuel-to-flibe volume ratio and the harder the neutron spectrum.

^{6}Li is a strong thermal neutron poison in natural lithium. Even after residual ^{6}Li left from enrichment is burned out, it continues to be generated from (n,alpha) reactions in ^{9}Be and (n,2n) reactions in ^{7}Li. The relative rates of production and destruction of ^{6}Li depend on the neutron spectrum and therefore must be calculated for each new core design. Transmutation of ^{6}Li is more effective with softer neutron spectra and conversely, production of ^{6}Li is more effective with harder neutron spectra, so the equilibrium concentration of ^{6}Li depends on the neutron spectrum. The concentration of ^{6}Li is important to the neutronics of FHRs because the ratio of absorbers to moderators in the coolant determines the magnitude and possibly sign of the coolant reactivity feedback. Also, increasing the concentration of this neutron poison will impair the neutron economy, thereby reducing the attainable burnup.

There is significant uncertainty in the ^{7}Li capture cross sections because its capture daughters are short-lived and difficult to detect, and capture in elemental lithium is dominated by ^{6}Li. The depletion of FHR coolant shifts the sensitivity of neutron capture from ^{6}Li as in natural lithium to ^{7}Li, to the point that ^{7}Li becomes an important non-fission absorber and uncertainty in the cross section must be explicitly considered in the FHR core design. Additionally, no incoherent thermal scattering kernels currently exist for flibe or its constituents.

Geometry

Most neutronic codes have been developed to analyze LWRs, and sometimes they cannot accept geometries that deviate from cylindrical fuel elements on a square pitch. The two candidate FHR core designs are an annular core with expansion and converging cylindrical regions fully packed with annular spherical fuel pebbles and a hexagonal lattice of fuel assemblies with a layered plate fuel design consisting of two thin active fuel compacts surrounding an inert graphite matrix, both of which differ greatly in geometry from LWR fuel.

Similarly, methods developed specifically for HTGRs can often analyze fuel elements with solid cylindrical or solid spherical fuel compacts but often do not accept annular spherical or layered slab fuel compact geometry as shown in Figure 4-1.

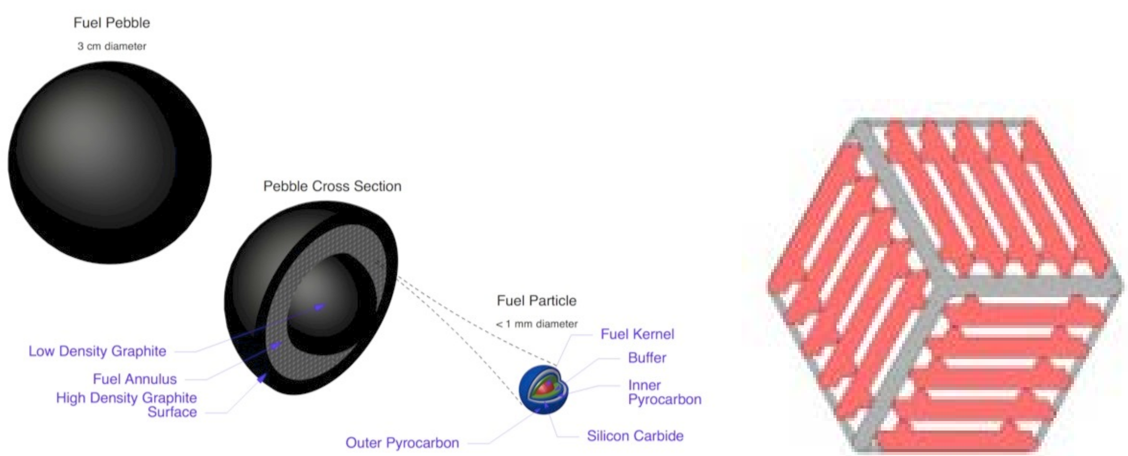

Figure 4-1. Geometry of Candidate FHR Fuel Elements: (left) Annular Fuel Pebble; (right) Layered Fuel Plate

Internodal Leakage

The NGNP methods development program (INL 2010a) identified internodal leakage (spectral interpenetration) as a core simulation requirement. Internodal leakage relates to the penetration of neutrons from surrounding regions into a region of interest. This phenomenon is exacerbated in HTGRs by the channels created by the neutronically transparent coolant, while in FHRs the channels are filled with a coolant that has moderating capability greater than the graphite in the fuel. Studies must be performed to assess how sensitive FHRs are to this effect.

4.2.2 HFCA

The HFCA capability will be used as a benchmark against which to compare the lower-fidelity analyses tools. Therefore, the methodology used in the HFCA capability must model the physics as faithfully as possible. For example, in the pebble bed variants of FHRs the complicated fingering structure of pebble mixing at the interfaces between fuel-type regions must be represented faithfully to assess the uncertainties associated with using geometric simplifications.

To determine the reactivity worth of control elements, the HFCA must be capable of calculating the reactivity change with respect to a baseline case associated with insertion or removal of control elements, even in cases with complex geometry and/or unbalanced control element insertion or removal (to model accidents where control elements do not engage or are stuck).

4.2.3 Depletion Analysis

The importance and spectral dependence of ^{6}Li concentrations was discussed previously in this white paper. Because the burnup of the fuel affects the global neutron spectrum of FHRs, the steady-state ^{6}Li concentration feedback should be integrated into the FHR depletion analysis (Cisneros et al. 2012).

To accurately predict the spatial isotopic concentration evolutions in FHR depletion analysis, the depletion analysis capability must account for the temperature and coolant density feedback by interfacing with a steady-state thermal fluid analysis.

The pebble bed variant of the FHR utilizes pebble fuel that is continuously circulated through the core. Continuous refueling improves the fuel utilization compared to fixed-fuel designs that use periodic refueling, as shown in Table 4-2.

Table 4-2. Attainable Burnup in FHR Systems with Different Fuel Management Schemes

FHR Variant	**SmAHTR*** (Greene, Gehin, et al. 2010)	**AHTR** (Holcomb et al. 2012)	**PB-FHR** (Cisneros et al. 2012)
Refueling strategy	Once-through	Multi-batch	Continuously refueled
Batches	1	2	-
Uranium enrichment (wt%)	19.75	9	19.9
Attainable burnup (GWd/MT)	109-115	73	216
Normalized burnup (GWd/MT/wt%)	587	811	1085

*Sm-AHTR: small modular advanced high-temperature reactor

Utilizing continuously circulated pebble fuel introduces uncertainty in the analysis of the FHR. Stochastic variation in local pebble geometry is speculated to be one of the factors that contributed to significant overheating of some fuel pebbles in the German AVR pebble bed reactor and releases of ^{137}Cs, resulting in significant contamination of the primary circuit (Moormann 2008). Note that FHR pebbles operate at much lower peak temperatures than those in HTGRs, remaining hundreds of degrees below temperatures required to cause damage. Moreover, FHR cores operate with upflow, and the viscosity of fluoride salts decreases with increasing temperature, so that buoyancy and viscous forces enhance cooling in hot spots rather than degrade it as occurs in HTGRs.

While local fuel temperature is unlikely to be a concern, it remains important to be able to predict peak pebble powers (which affect peak thermal stresses in particles and pebbles) and the reactivity changes that may be caused by pebble circulation and bed porosity changes. While pebble cores operate with low excess reactivity, mechanisms that can change reactivity must be understood so that control and shutdown elements can be designed to have sufficient reactivity worth.

The probability distributions of residence times of pebbles and their trajectories can be estimated using granular flow simulations; however, the exact histories of specific pebbles cannot be modeled tractably. Neutronic and depletion analysis of these continuously refueled systems has assumed aggregate composition in the fuel kernels of the reactor in specific regions. This modeling assumption leads to uncertainty in the steady-state model of the core, which propagates to uncertainties in the reactor physics properties of the core (reactivity feedback coefficients, power and flux distribution, attainable discharge burnup, etc.).

Radial heterogeneity in the core can be maintained in an FHR by controlling the radial insertion location of pebbles. Radial pebble regions in the inlet of a fully packed pebble bed will be propagated with only moderate dispersion into the active region of the core; this phenomenon has been confirmed numerically and empirically in scaled experiments. Radial segregation enables the use of multiple fuel types, burnup zoning, or a graphite pebble reflector. Each fuel type's neutron moderation and residence time can be optimized independently by controlling the carbon to heavy metal (C/HM) ratio of the pebble fuel design and the number of times pebbles are recirculated, or burnup limits for the fuel. An outer graphite pebble reflector layer can reduce the radiation damage to the fixed graphite reflector, extending its lifetime. However, some radial pebble mixing at the interfaces between these radial regions can lead to a complicated fingering structure. This interface mixing introduces additional uncertainty for the peak power of individual pebbles and for the overall reactivity of the core.

4.2.4 Transient Analysis

The neutronic model in the transient analysis capability may need to be coupled to a transient thermal fluid model to account for the thermal fluid feedback mechanisms between neutronics and thermal hydraulics.

To faithfully model transients with spatial kinetics (ATWS, stability analysis), many neutron transport calculations must be performed because the time steps will be on the order of milliseconds at the start of these events. The NGNP methods program (INL 2010a) estimates these spatial kinetics neutron transport calculations must be completed with a computation time on the order of a single second.

More specifically, the ability to simulate the ATWS phenomenon is a key requirement for the safety analysis EM. ATWS is a low-frequency transient because it involves the failure of the reactor protection system in addition to a LOFC or a loss of heat sink. However, the NRC requires that these transients and their consequences be analyzed as part of the safety analysis report for licensing regardless of their frequency. One of the design goals of the FHTR and prototype FHR is to design the reliability of components and reduce the frequency of an unprotected transient by ensuring that it can be classified as a BDBE.

During an ATWS transient, the primary coolant temperature increases because heat removal is diminished while the reactor continues to generate fission power. The increase in the primary coolant temperature provides negative reactivity feedback. Because the fuel is at a higher temperature than the coolant, as its temperature drops it provides positive reactivity feedback. With these competing reactivity feedback mechanisms, the fission power drops to zero when the coolant temperature rises sufficiently for the coolant feedback to cancel the positive reactivity feedback from the reduced fuel temperature.

In LWRs, an ATWS vaporizes water in the core, removing moderator from the core and providing strong negative reactivity feedback but generating high pressure in the primary loop. The primary safety concern for ATWSs in FHRs involves heating metallic reactor structures, particularly the upper-core support structures, IHX, DHX, and reactor vessel, to temperatures where accelerated creep deformation and damage may occur.

The consequences of ATWSs in FHRs can be reduced if the average temperature of the fuel is minimized. Careful design of the core to provide a flow distribution that maximizes heat transfer effectiveness can help to reduce the coolant bulk temperature in high-worth regions of the core, using fuel geometries that enhance convective heat transfer and surface area, configuring the fuel elements so that the fuel layers are thin and are close to the surface of the elements, and selecting a sufficiently low power density can all contribute to minimizing the average fuel temperature.

4.2.5 Sensitivity, Uncertainty, and Representivity Analysis

Sensitivity, uncertainty, and representivity analysis plays an important role in the design and validation processes. Three primary functions have been identified: (1) quantify simulation uncertainties for important performance parameters to be incorporated into into design margins and acceptance criteria limits; (2) quantify the similitude for important neutronics-related phenomena between various configurations and point designs of the FHTR and FHR; and (3) identify nuclear data that are likely to cause the largest biases and should be interrogated with experiments. Probabilistic risk assessment and economics analyses must be applied to determine the performance parameters that most impact safety and economics, including (but not limited to) the following:

- Temperature reactivity coefficients. Must be negative to ensure operational stability.
- Normal and reserve shutdown worths. Must be sufficient to overcome effects like xenon poisoning (some conservatism is beneficial here) and negative power and temperature reactivity feedbacks.
- The ratio of fuel and coolant temperature reactivity coefficients is an important factor in determining the equilibrium temperatures during an ATWS.
- Pebble thermal conductivity determines the steady-state pebble temperatures, which affect the temperatures reached during an ATWS.
- The peak power density dictates the thermal gradient stresses within fuel and catalyzes fuel failure.
- The attainable discharge burnups and uranium loading determine the energy that can be extracted per pebble.
- The radiation damage rate of reflectors determines the necessary replacement interval.

The violation of any number of technical specification limits may hinder startup testing. It will be important to ensure that startup testing protocols contain only safety-related limits so that misprediction of unimportant figures of merit do not delay the startup process.

Sensitivity analysis determines how sensitive the important results are to simulation inputs and assumptions, enabling some phenomena or inputs to be discarded as secondary to impacting results. Also, knowing the uncertainty in those inputs, analysts can propagate them to result uncertainties, which serves as statistical estimates of simulation bias. Because uncertainties always have some degree of inaccuracy or ambiguity (i.e., uncertainty of the uncertainty), the utility of estimated result uncertainties is limited to order-of-magnitude estimates and relative rankings. If result uncertainties are limiting, design or licensing strategy changes may be necessary to minimize their impact.

When impact cannot be sufficiently minimized, these limiting uncertainties must be reduced by performing representative physical experiments. These experiments should be designed so that the specific phenomena of the limiting uncertainties are present, prominent, and measured—for example, if thermal scattering in carbon is a limiting uncertainty, an experiment must contain carbon, neutrons must scatter with carbon in a similar manner as in the design, and diagnostics must be performed for related quantities. By meeting these three criteria, the most important simulation biases can be directly reduced. Representivity factors are a quantitative means of determining the applicability of an experiment in reducing the simulation biases for a design.

Simulated results that are not related to safety or economics do not warrant sensitivity, uncertainty, and representivity analysis. For example, while it is essential that control rods have sufficient reactivity worth to shutdown the reactor, the exact control rod position that renders the system critical at startup has no impact on safety or economics. Simulations to predict critical control rod positions will be uncertain, but those positions will be determined empirically during startup testing. This approach of focusing only on safety- and economics-related simulation limitations and uncertainties and conducting unimportant validations during startup testing will be applied throughout the design process.

4.3 Candidate FHR Neutronic Codes

This section reviews a set of candidate neutronic codes for each neutronic capability identified in Table 4-1. The set of candidate codes evaluated was developed based on a literature of codes previously utilized to analyze FHR or HTGR systems.

4.3.1 Candidate Codes for HFCA

The following candidate neutron transport codes were evaluated for their ability to model the key phenomena with sufficient functionality to calculate the power and flux distribution in an FHR, the reactivity feedback coefficients, the delayed neutron fraction, and the worth of various control elements.

Monte Carlo N-Particle Code: MCNP5

MCNP5 is a continuous-energy general-purpose Monte Carlo neutral particle transport code that can assess the criticality of nuclear systems (X-5 Monte Carlo Team 2008). MCNP5's geometry engine defines arbitrary volumes between first-, second-, and third-degree surfaces or fourth-degree elliptical tori. Nuclear reaction rates (fission, capture, particle production, and neutron damage) can be estimated with flux tallies. Furthermore, MCNP is seen as a reliable, well understood code for performing high-fidelity neutron transport in the nuclear engineering community, so it is often utilized to produce reference values against which to benchmark results from new methods.

MCNP5 accounts for the double heterogeneity effect by modeling fuel particles explicitly of lattices of repeated structures and can stochastically translate the TRISO particles on a regular lattice (Brown and Martin 2004). As stated earlier, this approach is the most accurate and fundamental way to account for the double heterogeneity energy self-shielding.

MCNP5 can faithfully represent the geometry of both pebble and fixed-fuel variants of the FHR because of the flexibility of its geometry definition (Kelly and Ilas 2012). This flexibility enables MCNP5 to accurately account for azimuthal asymmetry in FHRs, as would be required for determining shutdown worth assuming a failure in one or more of the shutdown elements to insert.

Internodal leakage can be modeled accurately in MCNP5 because continuous-energy cross sections are used, the system geometry can be modeled faithfully, and the neutron transport model is not limited to discrete directions.

The capability to generate adjoint weighted kinetic parameters is implemented in version 1.60 of MCNP5 (Kiedrowski et al. 2010).

Studies have identified MCNP5's use of free-gas treatment for the scattering kernel of heavy metal isotopes like ^{238}U as a potential issue for modeling of particle fuels. This issue leads to biases of 600 pcm for k_{∞}, a 10% bias for the doppler reactivity coefficient, and a 4% bias in the ^{239}Pu inventory in an HTR-10 unit cell model (Becker et al. 2009).

As stated earlier, the neutronic phenomena in HTGRs are very similar to those in FHRs because these systems use low-enriched uranium coated-particle fuels and are graphite-moderated nuclear systems. Therefore, it is natural to use the accuracy at which MCNP5 simulates HTGR criticality experiments as a proxy for the accuracy that MCNP5 could provide for FHRs. Table 4-3 presents a comparison between experimental $k_{effective}$ and the results predicted by versions of MCNP in open literature. These validation studies show about a +1% Δk/k bias for the $k_{effective}$ predicted by the various versions of MCNP.

Table 4-3. MCNP Validation Calculations Against HTGR Criticality Experiments

Criticality Experiment	Experimental $k_{effective}$ Value	MCNP Version	Nuclear Data	MCNP Value
HTR-10[a] (Terry et al. 2006; Gehin et al. 2010)	1.000	MCNP5	ENDF-VII	1.0147 ± 20 pcm
HTTR[b] (Taiwo et al. 2005)	1.1363 ± 3.6%	MCNP4C	ENDF-VI	1.15714 ± 37 pcm
ASTRA[a]	1.000	MCNP5	ENDF-VI	1.0123

[a]initial criticality, [b]fully loaded core

Power and flux distributions can be generated with MCNP5 by tallying neutron flux (F4 tally) or tallying the energy deposition (F6 tally) throughout the core. Furthermore, radiation damage to components can be calculated by tallying the fast flux rate (F4 tally) or calculating the displacements per atom (DPA) using a flux-weighted average DPA cross section (F4 multiplier tally). Gas production rate in structural materials can be estimated by summing the reactions that generate protons, deuteron, tritons, ^{3}He nuclides, or alpha particles (F4 multiplier tallies) – this gas production is an import component to assessing the long-term mechanical integrity of metallic structures.

Reactivity feedback coefficients in FHRs can be calculated with MCNP5 by performing criticality calculations on a full-core FHR at different operating states (i.e., power-dependent temperature and density distributions).

Shutdown rod worth and shutdown margin can be calculated with MCNP5 by comparing results of criticality calculations with control elements in different positions.

The speed at which MCNP5 performs calculations can be scaled up by using multiple processors in parallel mode.

MCNP5, MCNPX, and MCNP6 are available for research applications free of charge through the Radiation Safety Information Computational Center (RSICC).

KENO-VI

KENO-VI is a Monte Carlo neutron transport criticality program developed for the SCALE (Standardized Computer Analyses for Licensing Evaluation) code developed at ORNL for criticality safety analyses. KENO-VI can perform neutron transport in either continuous-energy or multigroup mode. The volumes defined in KENO-VI are based on intersections of user-defined quadratic surfaces. Similar to MCNP5, reaction rates can be estimated using flux tallies.

KENO-VI can account for the double heterogeneity self-shielding effect by explicitly modeling fuel kernels in continuous-energy mode or using a double heterogeneity treatment to generate a homogenized treatment in multigroup mode for solid spherical or solid cylindrical geometries. However, the current double heterogeneity treatment cannot be utilized for either of the FHR fuel designs because KENO-VI is not set up to analyze unit cells with annular-spherical or layered slab geometries.

KENO-VI implements the SCALE generalized geometry package (SGGP), which can model any volume that can be bounded by quadratic surfaces. This geometry package enables KENO-VI to model either FHR variant. The fuel particles have been modeled on a simple cubic lattice using SGGP's repeated structure functionality. Furthermore, the flexibility of SGGP enables the user to model azimuthally asymmetric features.

Continuous-energy KENO-VI faithfully models neutron streaming between fuel elements and the interaction between the active core and the graphite reflectors.

The ^{238}U scattering model was corrected using $S(\alpha,\beta)$ tables in KENO-VI to account for resonance upscattering (ORNL 2011).

Validation studies have been performed on KENO-VI against criticality experiments. Selected results are presented in Table 4-4.

Table 4-4. KENO-VI Validation Calculations Against HTGR Criticality Experiments

Criticality Experiment	$k_{effective}$ Value	Double Heterogeneity Treatment	Nuclear Data	KENO-VI Value
HTR-10	1.000	Double heterogeneity homogenization	ENDF/B-VII	1.0153 ± 30 pcm
HTTR*	1.000	Continuous energy, explicit grain	ENDF/B-VII	1.0185 ± 30 pcm

* HTTR: High-Temperature Test Reactor

The flux and power distributions can be tallied using the KENO-VI Module for Activity-Reaction Rate Tabulation (KMART6) of the SCALE system. The neutron damage can be estimated by calculating the fast flux rate and the helium production in structural materials. KMART6 can collapse the flux into a thermal and a fast component that can be used to estimate the fast flux rate. The gas production rate can be estimated by tallying the activity of (n,p), (n,d), (n,t), (n,^{3}He), and (n,alpha) reactions. However, KENO-VI does not have the built-in capability to calculate DPA cross sections like MCNP5.

Reactivity feedback coefficients in FHRs can be calculated with KENO-VI by performing criticality calculations on a full-core FHR at different operating states (i.e., power-dependent temperature and density distributions).

Shutdown rod worth and shutdown margin can be calculated with KENO-VI by comparing results of criticality calculations with control elements inserted to different positions.

SCALE6.2, including KENO-VI, is available for research applications free of charge through the RSICC.

Serpent

Serpent is a three-dimensional continuous-energy Monte Carlo reactor physics code developed for burnup and lattice physics applications (Leppanan 2007).

Serpent can model the double heterogeneity energy self-shielding effect either explicitly or implicitly. The implicit method particle fuel model works by sampling new particles during the flight path and the tracking process. An alternative method models fuel particles explicitly; these particles can be modeled on a regular lattice, or their position can be defined explicitly in a separate input file (Leppanen and DeHart 2009). Additionally, the positions of pebbles can be defined explicitly to produce a doubly stochastic geometry definition. This methodology was developed to model the ASTRA criticality facility, where discrete element methods (DEM) were used to stochastically populate the pebble bed with a set of pebbles with 10 characteristic particle distributions. However, the DEM solution predicted a packed bed solution with more porosity (i.e., taller for the same number of fuel pebbles) than the experiment.

Serpent can model both variants of FHRs faithfully using the same methodology used to model the ASTRA facility. Using this doubly stochastic geometric definition, Serpent can explicitly model pebble mixing at fuel type interfaces. Serpent can model the AHTR fuel elements by bounding the plate cell volumes with planar surfaces.

Serpent can model azimuthal asymmetric geometries using its geometry engine. The ASTRA criticality facility model was azimuthally asymmetric.

Serpent models the internodal leakage intrinsically by using continuous-energy neutron transport.

Serpent calculates delayed neutron fraction and effective delayed neutron fraction by default.

Serpent calculates a heavy metal scattering cross section using the free-gas scattering by default; however Serpent can implement the Doppler Broadened Rejection Correction treatment proposed by Becker to accurately model upscattering off heavy nuclides in the epithermal region (Becker, Dagan, and Lohnert 2009).

Validation studies have been performed for Serpent against the ASTRA criticality experiment benchmark, as shown in Table 4-5.

Table 4-5. Serpent Validation Calculations Against the ASTRA Criticality Experiments (Suikkanen, Rintala, and Kyrki-Rajamäki 2010)

Criticality Experiment	$k_{effective}$ Value	Experimental Height, cm	Nuclear Data	SERPENT Value
ASTRA	1.000 ±3 60 pcm	179.36	ENDF/B-VII	1.01052 ± 8 pcm

A bias of about 1% in $k_{effective}$ was observed in these results relative to experimental measurements. Researchers conducted sensitivity analysis to identify the source of discrepancies between the experimental and numerical results. However, that study did not investigate the effects of the heavy nuclide scattering treatment (Suikkanen, Rintala, and Kyrki-Rajamäki 2010).

Serpent can calculate the power distribution using detectors to tally neutron flux and fission energy deposition. The gas production rate can be estimated by tallying the rate of (n,p), (n,d), (n,t), (n,^{3}He), and (n,alpha) reactions. However, Serpent does not have the built-in capability to calculate DPA cross sections like MCNP5, although this is relatively simple to add.

Reactivity feedback coefficients in FHRs can be calculated with Serpent by performing criticality calculations on a full-core FHR at different operating states (i.e., power-dependent temperature and density distributions).

Shutdown rod worth and shutdown margin can be calculated with Serpent by comparing results of criticality calculations with control elements inserted to different positions.

Serpent is available for research applications free of charge through the RSICC.

DRAGON

DRAGON is an open-source lattice neutron transport code developed at Ecole Polytechnique de Montreal (Marleau, Herbert, and Roy 2012). DRAGON has been investigated by the NGNP program to analyze the prismatic variant of NGNP and by Argonne National Laboratory to model the Liquid Salt Very High Temperature Reactor (LS-VHTR) (Kim, Taiwo, and Yang 2005). DRAGON can solve the integral transport equation with methods ranging from a simple collision probability method coupled with the interface current method to the full collision probability method.

DRAGON can model the double heterogeneity self-shielding effect with the Hebert double heterogeneity model (collision probability) or the Sanchez-Pomraning double heterogeneity (method of characteristics) model.

The lattice geometry cannot model the AHTR fuel design or the pebble fuel design. It also has trouble modeling the boundaries of a single prismatic fuel block.

DRAGON has some capabilities to determine the delayed neutron fraction.

Benchmarking against MCNP5 and WIMS8 suggested additional developmental work was required to analyze these high-temperature reactor systems.

Summary

Continuous-energy Monte Carlo codes can accurately model the double heterogeneity self-shielding effect and faithfully represent the geometries of the FHRs baseline designs, including azimuthal asymmetries. Methods have been developed to extract reactor kinetics parameters from these tools. Also, these codes are distributed freely from RSICC. However, they are computationally intensive. Validation studies show these Monte Carlo codes systematically overestimate $k_{effective}$ of criticality experiments by ~1% $\Delta k/k$. Further development is required to have confidence in the neutronic results from these codes for licensing safety analysis.

Lattice codes have trouble accurately representing the geometry of the FHR baseline design and accounting for the double heterogeneity self-shielding effect.

Table 4-6 summarizes the performance of these codes for HFCA.

Table 4-6. Code Performance for HFCA

Code	Double Heterogeneity	FHR Geometry	Azimuthal Heterogeneity	Internodal Leakage	Reactor Kinetics	Availability
Monte Carlo						
MCNP5	X	X	X	X	X	X
KENO-VI	X	X	X	X		X
Serpent	X	X	X	X	X	X
Deterministic						
DRAGON	X					X

4.3.2 Candidate Codes for Depletion Analysis

The following candidate neutronic depletion frameworks were evaluated for their ability to model the key phenomena with sufficient functionality to calculate the maximum attainable burnup, the burnup dependent power and flux distribution, and the isotopic concentration distribution evolution.

Oak Ridge Isotope Generation and Depletion Code: ORIGEN2.2

ORIGEN2.2 is a point-depletion and radioactive-decay code for analyzing nuclear fuel cycles. It solves the Bateman's equations using the matrix exponential technique for a specific problem.

Coupled MCNP5 and ORIGEN depletion analysis frameworks have been developed at UCB for both continuously refueled fuel management and multi-batch equilibrium fuel management scheme (Cisneros, Greenspan, and Peterson 2011).

Transport Rigor Implemented with Time-dependent Operation for Neutronic depletion: TRITON

TRITON couples one of the neutron transport drivers in SCALE to ORIGEN-S (a derivative of ORIGEN2.2 that has all of the same functionality and the expanded capability to utilize multigroup cross sections and updated data libraries) to perform depletion analysis. TRITON can use either Monte Carlo (KENO-V, KENO-VI) or deterministic (NEWT) modules for neutron transport.

TRITON currently cannot utilize the continuous-energy version to KENO-VI for neutron transport and cross section generation; this functionality is scheduled to be implemented in SCALE 6.2. Therefore, TRITON must generate multigroup cross sections for neutron transport, and this changes the way for which the double-heterogeneity effect is accounted. These codes cannot use the double heterogeneity treatment, which generates cross sections for particle fuel systems, because this treatment is not set up to work with annular spherical fuel geometry or layered slab fuel geometry. As of yet, there are no plans to update the double heterogeneity treatment in that manner. This double heterogeneity self-shielding effect can be simulated by modeling fuel particles explicitly and imposing a Dancoff factor with the latticecell function in SCALE. However, this Dancoff factor must be calibrated against a high-fidelity continuous-energy Monte Carlo simulation. The only other method available to impose this double heterogeneity energy self-shielding effect is to use the RPT method (Cisneros and Ilas 2012). The RPT dimension must also be calibrated against a high-fidelity neutron transport model. KENO-VI is arduous to utilize as a neutronic driver because it cannot perform calculations in parallel.

Because both TRITON and ORIGEN-S use neutron transport, they faithfully model the intermodal leakage.

Multi-batch depletion analysis has been implemented with TRITON with up to 14 batches. However, great effort was required to converge to the equilibrium fuel cycle. The baseline fuel management scheme only uses two fuel batches.

SCALE6.2, including TRITON, is available for research applications free of charge through the RSICC.

REBUS3/DIF3D

REBUS3 was developed to analyze fast reactor fuel cycles and can perform depletion analysis on systems with multi-batch fuel management schemes such as adjust the cycle length to impose a specific burnup, adjust the enrichment to impose a specific $k_{effective}$ at a particular point in burnup, adjust the poison concentration to maintain a $k_{effective}$ throughout the fuel cycle, or adjust the cycle length to impose a specific $k_{effective}$ at the end of the equilibrium cycle; this is similar to the functionality required to simulate the multi-batch fuel cycle of the AHTR (Cisneros and Ilas 2012).

DIF3D is a code package that solves steady-state neutron diffusion and transport calculations using either nodal or finite difference methods. DIF3D is also the neutron transport module for REBUS3 and is included in the distribution package. Cross sections used in the DIF3D nodal solver must be processed into multigroup cross sections for each node (fuel assembly). These nodal cross sections must be generated from a lattice code like WIMS8 or a Monte Carlo code like Serpent to incorporate the double heterogeneity energy self-shielding effects. At the nodal level all the element specific geometry is lost.

DIF3D and REBUS3 are available for research applications free of charge through the RSICC.

Serpent

Serpent can model the depletion of fuel particles and analzye burnup in an externally coupled system. This combination enables drivers to be developed to control multi-batch fuel management or continuously refueled depletion analysis.

PEBBED-THERMIX

PEBBED was developed to solve for the equilibrium state of continuously recirculated pebble bed HTGRs and perform neutronic analysis on this state. PEBBED has been coupled to THERMIX-KONVEX, a R-Z thermal hydraulic code developed for the German HTGR program (Gougar 2006). This coupling has been implemented for steady-state depletion analysis.

PEBBED is fed cross sections from COMBINE. COMBINE performs explicit neutron transport on the TRISO, pebble, and full-core radial wedge models using a 167-group energy structure to coalesce cross sections into few group cross sections. The Dancoff factors used in COMBINE are generated in PEBDAN to correct for the double heterogeneity self-shielding effect (Gougar 2010).

PEBBED can model systems having R-Z geometry. The pebble bed variant of the FHR can be modeled with this geometry definition. However, only a simplified model of the fixed-fuel variant of the FHR can be modeled with R-Z geometry. It is unclear whether COMBINE can generate cross sections for fuel elements with annular spherical geometry or layered slab geometry for the pebble bed and fixed-fuel FHR variants, respectively.

PEBBED uses a finite-difference diffusion solver for neutronics (Terry, Gougar, and Ougouag 2002; Gougar, Reitsma, and Joubert 2009). Energy-dependent radial leakage is treated in the core transport stage of the analysis (INL 2010b).

The equilibrium state is solved for directly in PEBBED. The Bateman equations are solved for using a Laplace transform for a simplified set of nuclides and their depletion chains. PEBBED can analyze once-through fuel cycles as well as continuously recirculated pebble fuel management schemes. PEBBED assumes the composition of each node is the average of the inlet and outlet composition and that pebbles only move axially once they are inserted into the core.

PEBBED is available to U.S. domestic research institutions free of charge through the Idaho National Laboratory.

Winfrith Improved Multigroup Scheme: WIMS

WIMS is a vendor-distributed code for reactor core analysis. It has been updated continuously, with WIMS10 released in 2008. It is flexible in the calculations that it can perform, as each calculation is specific to a module of the code. Modules can communicate and exchange data with interfaces, and expanding the code to include additional modules aids in its adaptability. It can be interfaced with other reactor physics codes, as it has been with REBUS/DIF3D (Kim, Taiwo, and Yang 2005).

The double heterogeneity self-shielding effect is treated by collision probabilities and the WIMS sub-group method. In this method at every level of heterogeneity, an artificial material is generated to give the same boundary-to-boundary transmission probability of the aggregate of each level's constituents (Newton 2002). This homogenized material replaces the heterogeneous geometry on the next level of heterogeneity moving from fine to coarse geometric detail. Variations of WIMS, WIMS8 and PANTHERMIX, were utilized to develop multigroup cross sections for the Organisation for Economic

Cooperation and Development (OECD) Nuclear Energy Agency's (NEA) PBMR268 benchmark problem (Reitsma et al. 2006). This process has been implemented for the PBMR geometry; however, it is not clear if significant developmental work would be required to integrate this methodology to annular spherical or layered slab fuel geometry though these geometries can be approximated well with one dimensional unit-cells like the PBMR fuel pebble.

The methodology for performing full-core flux solutions and burnup analysis proposed for the PBMR divides the core on two R-Z-θ meshes, a coarse mesh and a fine mesh (Newton 2002). WIMS can implement a variety of different flux solvers such as collision probability, Sn methods, and methods characteristic to Monte Carlo simulations. The whole core flux solution calculated for the fine mesh is coalesced onto a coarse mesh used for burnup analysis.

Version WIMSD has been coupled to the thermal fluid code COBRA for steady-state depletion analysis of the VVR-S research reactor, and results from this framework were validated against performance history of the VVR-S (Zare et al. 2010). A similar framework can be developed for an FHR system.

WIMS has a specific fuel management code for PBMRs by iteratively performing depletion analysis starting from fresh fuel. To account for the spectral changes, many iterations must be performed to approach the equilibrium state (Serco Assurance).

Because WIMS is a vendor-supplied code, its availability is subject to the cost of acquisiton.

WIMS was benchmarked against other neutronic codes for the analysis of pebble-type high-temperature reactors including single-pebble and full-core analyses with low-enriched uranium, plutonium fuel, and thorium/rranium-233 fueled systems (Hosking et al. 2006).

Purdue Advanced Reactor Core Simulator: PARCS

PARCS is a three-dimensional reactor core simulator that solves the steady-state and time-dependent neutron diffusion or SP3 transport equations to predict the dynamic response of the reactor to reactivity perturbations such as control rod movements, boron concentration, or changes in the temperature/fluid conditions in the reactor core (Downar et al. 2002).

PARCS represents full cores as a collection of homogenized nodes. The fine details of these nodes are coalesced into a set of multigroup cross sections. These cross sections must be generated externally using a high-fidelity code such as WIMS, TRITON, or Serpent (Xu et al. 2006; Reitsma et al. 2006).

PARCS can utilize either hexagonal lattices or R-Z-θ geometry, so it can simulate both FHR variants (Xu et al. 2006). The flux solution is solved on this mesh with either diffusion or SP3 methods using Coarse Mesh Finite Difference solver with Krylov linear Solver Bi-Conjugate Gradient Stabilized (Downar et al. 2002).

PARCS has been coupled to RELAP5 and TRACE for thermal hydraulics and DEPLETOR for depletion analysis as shown in Figure 4-2 (Xu et al. 2006). PARCS has been updated to integrate a multi-batch fuel cycle analysis capability to determine the equilibrium fuel cycle based on a maximum burnup convergence criteron or a maximum iteration convergence criterion (Downar, Xu, and Seker 2011).

PARCS version 2.8 is available for public distribution.

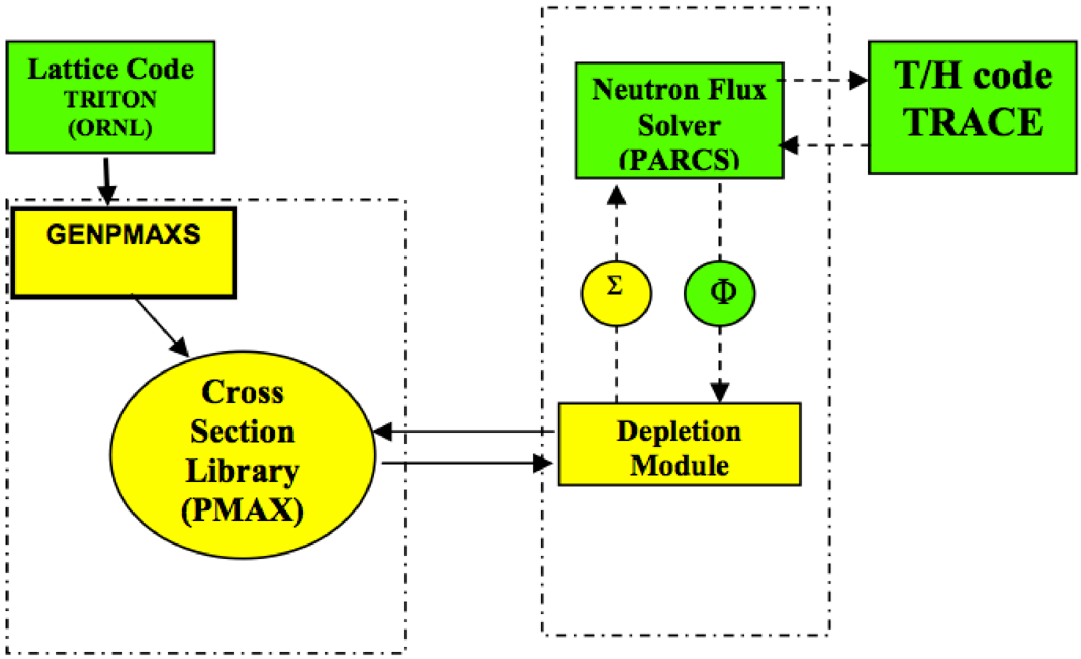

Figure 4-2. PARCS/TRACE Coupled-Code Analysis System

Summary

The equilibrium concentration of ^{6}Li is not a standard part of any existing depletion analysis software; however, it has been integrated into the equilibrium depletion analysis of the PB-FHR (see Appendix C). Depletion analysis drivers for FHRs must be able to analyze the ^{9}Be (n,alpha) and ^{6}Li removal cross sections to calculate the equilibrium concentration of ^{6}Li as needed.

Disconnecting the ORIGEN-S point depletion solver from the neutron transport cross section generation can accelerate the multi-batch depletion analysis. Alternatively, TRITON can be coupled to a version of ORIGEN externally. The make-up fuel can be depleted from beginning of cycle to end of cycle multiple times using the burnup and spatially dependent flux distribution and set of cross sections until the beginning of the equilibrium cycle composition converges. This method requires significantly less neutron transport. Furthermore, the methodology developed for equilibrium depletion analysis cannot be implemented at all without separating the cross section generation and point depletion analysis.

Table 4-7 summarizes the performance of these codes for depletion analysis.

Table 4-7. Code Performance for Depletion Analysis

Code	Double Heterogeneity	FHR Geometry	Internodal Leakage	Equilibrium ^{6}Li Concentration	Steady-State Thermal Fluid Coupling	Equilibrium Depletion*	Multibatch Depletion	Availability
Monte Carlo								
MCNP-ORIGEN	X	X	X	X		X	X	X
TRITON	X	X	X				X	X
Serpent	X	X*	X					X
Deterministic								
REBUS							X	X
PEBBED						X		
WIMS	X	X	X			X		
PARCS	X	X	X		X		X	X

*Pebble bed only

4.3.3 Candidate Codes for Transient Analysis

The following candidate codes were evaluated for their ability to model transients.

DIF3D

DIF3D was originally designed for fast reactor analysis; to account for specific thermal reactor phenomena and perform thermal reactor analysis on the prismatic VHTR, modifications had to be made (Lee et al. 2006). Included in these modifications were discontinuity factors to account for errors arising from nodal material homogenization and a module (NEUTRONXS) to account for burnup-dependent cross sections and self-shielding in the fuel. In the same analysis, long-lived and non-important fission products were lumped together in subsequent calculations to aid in computation time. However, important short-lived nuclides were tracked individually. A simplified thermal hydraulic feedback module was also constructed for DIF3D to account for thermal neutronic feedback in the core. As the FHR is also a thermal spectrum system, these modifications may also need to be implemented should DIF3D be used.

DIF3D has been coupled to thermal hydraulic codes but not for FHRs. Relevant characteristics (power density and flux) necessary for coupling can be generated with DIF3D for either the nodal mesh cells or with the region balance integrals.

Typical runtimes of DIF3D in test cases ranged on the order of seconds to minutes[3]. However, when paired with additional codes, such as REBUS, calculation times are much more variable.

PARCS

PARCS can perform for either steady-state and or time-dependent multigroup diffusion or transport calculations in cartesian, hexagonal, and cylindrical geometries. A number of spatial kinetics methods have been implemented to find solutions for these geometries, including both nodal or finite difference methods.

PARCS has the ability to perform steady-state and transient analyses, as well as depletion. Also, PARCS can track the evolution of various nuclide populations over time including short-lived fission products (Xe, Sm) in reactor transients.

PARCS has been directly coupled to TRACE for thermal hydraulic modeling. PARCS has also been coupled to RELAP5 to calculate thermal hydraulic and neutronic phenomena.

Runtime of PARCS varies with the complexity of the calculation, but an example two-group nodal diffusion for an LWR transient was calculated on the order of minutes (Downar et al. 2002). The amount of memory in the system can also be a limiting factor, with smaller problems taking ~1MB and larger problems requiring ~1GB.

WIMS/PANTHER

WIMS can perform calculations in a wide variety of geometries, including cartesian, spherical, and cylindrical coordinates, in one, two, or three dimensions. WIMS has been improved from previous versions to also include more complex geometry definition and has the ability to perform full-core analyses.

WIMS can account for double heterogeneity in the fuel with the PROCOL module using collision probability, but not on an assembly level, as it is limited in the lattice fidelity (Lee et al. 2006). In other analyses, the double heterogeneity effects in the fuel were accounted for in a two-step phase: first obtaining cross sections for a fuel unit cell, accounting for self-shielding, etc., and then expanding the cell to include other reactor parameters to the pin and assembly level.

WIMS also includes a Monte Carlo module, MONK, which can be used for internal code validation. In addition, it includes a depletion module, WBRNUP, which can treat all burnup problems. Cross sections can be generated with WIMS10 to perform a full-core analysis. Specifically, WIMS has been linked with the full-core code PANTHER to perform integrated thermal hydraulic and neutronic calculations (AEA Technology 1995). WIMS10 also features a module that can calculate the temperature profile in a fuel

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[3] Assessment available at http://www-rsicc.ornl.gov/codes/ccc/ccc7/ccc-784.html. Accessed February 21, 2013.

pin, based on the neutron source and the material properties of the fuel, cladding, and coolant materials.

WIMS can calculate most reactor physics parameters. In general, it can use a number of methods to solve for the $k_{effective}$, flux distribution, and reactor kinetic response. These three can be extended to calculations of reactivity coefficients, flux and power distributions, fission product inventory, changes in inventory with irradiation, burnable poison burnout, and reaction rates.

Summary

Table 4-8 summarizes the performance of the various candidate modeling systems for transient analysis.

Table 4-8. Code Performance for Transient Analysis

Code	**Double Heterogeneity**	**FHR Geometry**	**Internodal Leakage**	**Transient Thermal Fluid Coupling**	**Speed**	**Availability**
Diffusion						
DIF3D		X		X	X	X
PARCS		X		X	X	X
WIMS	X	X		X		

4.3.4 Candidate Codes for Sensitivity, Uncertainty, and Representivity Analysis

The following candidate tools for sensitivity, uncertainty, and representivity analysis were evaluated for their ability to simulate key phenomena with sufficient functionality to calculate sensitivities, uncertainties, and representivity factors of important neutronic results, both in an instantaneous and time-dependent manner.

MCNP5

MCNP5 contains a tool “pstudy” to perform direct perturbations using forward transport (X-5 Monte Carlo Team 2008). The Perl wrapper script automatically samples input file parameters (number densities, abundances, etc.) and executes MCNP5. The tool is somewhat limited in its scope, and a more thorough direct perturbation tool would likely be necessary if a direct approach to perturbation analysis is used. Also included is a tool “pert” to estimate the reactivity effect of perturbations using differential expansion of the transport operators. In this tool, perturbation of the fission source distribution is not considered, so it has limitations for criticality problems. Additionally, its implementation is awkward for producing energy-dependent sensitivities, which are required to propagate nuclear data uncertainties and to construct representivity factors. Both tools inherit the continuous-energy, double heterogeneous geometry, and three-dimensional transport abilities in MCNP.

MCNP6

MCNP6 is still under development but will contain a number of tools when it is released. The “kpert” tool is analogous to the “pert” tool in MCNP5, except that it uses iterated fission probability as a forward estimate of importance to weight results. While the effects of fission source distributions are implicitly considered, those of scattering are not. An adjoint-weighted tally tool “ksen” is also expected to be available with the full release of the code. Less is known about it, except that it is related to the “kpert” tool, it enhances consideration of thermal scattering perturbations, and it will be much more convenient for the construction of space- and energy-distributed sensitivities. The code will be available for research applications free of charge for universities through RSICC.

TSUNAMI

The SCALE suite contains a set of tools that can estimate instantaneous nuclear data sensitivities and uncertainties of neutronic responses using adjoint theory (ORNL 2011). The suite has no pareto-superior tool that can perform three-dimensional, continuous-energy transport for generalized responses for criticality and fixed-source problems. TSUNAMI-3D, for example, is three-dimensional, but uses multigroup cross sections and is limited to assessing the sensitivities and uncertainties of $k_{effective}$ in criticality problems. TSUNAMI-1D is one-dimensional and uses multigroup cross sections, but can be used for generalized responses, such as reaction rates and ratios of reaction rates. Neither TSUNAMI-1D nor TSUNAMI-3D are compatible with the double-heterogeneity abilities of SCALE. TSUNAMI-IP can construct a variety of representivity factors to quantify the similarity of nuclear systems. Work is being done to incorporate contribution theory (Rearden et al. 2010), which will allow for estimation of adjoint distributions using forward transport, but in its current state the tool can be thousands of times slower than a traditional forward/adjoint calculation. A new module SAMPLER, for direct perturbation methods, is likely to be included in the next release of SCALE.

Python Suite for Adjoint-Based Uncertainty Quantification with MCNP: PSABUQM

PSABUQM was developed to perform instantaneous adjoint-based sensitivity and uncertainty analysis for generalized responses of the depleted uranium-hybrid Laser Inertial Fusion Energy blanket (Seifried 2011). Fixed-source continuous-energy forward transport and multigroup adjoint transport is performed with MCNP6. Except for a slight enhancement to MCNP6 tally-tagging, all programming is outside of MCNP and automates the construction of adjoint bilinear functionals, sensitivity coefficients, and uncertainties for given responses. Great care is taken to propagate Monte Carlo counting uncertainties onto all results. The reliance on a 1,374-group cross section library for adjoint transport results in slow simulation times and introduces self-shielding errors. Additionally, the collision-based approach to constructing neutron source distributions brings large statistical uncertainties to source reaction sensitivity estimates. With some modification, it could be considered a general-purpose sensitivity and uncertainty analysis tool, but development of MCNP and SCALE tools will soon overtake PSABUQM in utility. Its availability for use in developing the FHR is not clear.

Summary

Currently, each tool described above possesses certain advantages and disadvantages in terms of ability, convenience, or fidelity. All tools are all limited to instantaneous analysis. Many tools exist for the somewhat slower direct sensitivity methods, in which uncertain inputs (spatial and spectral nuclear data) are directly perturbed one at a time. It is likely that some of these direct tools will be selected or custom-built and combined with the aforementioned tools for sensitivity, uncertainty, and representivity analysis.

Table 4-9 summarizes the performance of the various candidate codes for sensitivity, uncertainty, and representivity analysis.

Table 4-9. Code Performance for Sensitivity, Uncertainty and Representivity Quantification

Code	Double Heterogeneity	Innovative Fuel Design	Standard Perturbation Theory	Generalized Perturbation Theory	Time-Dependent	Sensitivity Distributions	Nuclear Data Uncertainties	Representivity	Availability
MCNP5	X	X	X						X
MCNP6	X	X	X			?	?	?	X
TSUNAMI			X		?	X	X	X	X
PSABUQM	X	X		X		X	X	X	?

4.4 Experimental Base for FHR Neutronic Model Assessment

The purpose of validation is to gauge the accuracy of the EM by comparison with physical experiments. Those experiments must be shown to share physical similarity with the design being simulated, to contain diagnostics to measure the phenomena of interest, to have been performed with sufficient quality assurance, and to have had an uncertainty analysis performed by those intimately familiar with the experiments.

4.4.1 Similitude Criteria

The traditional approach for determining the applicability of experiments for validating design simulations considers many aspects of each system (Dean and Tayloe Jr. 2001): the isotopic composition, physical form, temperature, relative atomic densities of the fissionable material, within-fuel moderator, interstitial moderator, reflector, and absorber, as well as the overall geometry and neutron spectra. Inevitably, some metrics do not match, so some degree of “expert opinion” or “regulatory guidance” is required to assign suitable ranges of disagreement, within which an experiment is deemed applicable.

A complementary (Broadhead et al. 1999) but more quantitative approach utilizes sensitivity and uncertainty analysis-guided representivity factors; compositions, atomic densities, geometries, and neutron spectra are all accounted for in sensitivity distributions. For each figure of merit ($k_{effective}$, reactivity coefficients, control rod worths, etc.), these factors can be calculated between the application and a suite of physical experiments to quantify the similarity of the systems and thus the similarity of the simulation biases. Two factors quantify the similarity of figures of merit sensitivities to nuclide-reaction pairs: the dot-product between sensitivity vectors (E) and the fractional overlap of sensitivity vectors (G). Figure of merit sensitivities to nuclear data uncertainty can be calculated between the designs (c_k) (ORNL 2011). Each experiment is then categorized as having excellent, adequate, or no similarity to the design. The number of experiments required for validation depends on the degree to which similitude is achieved with the design. Incorporating representivity factors in validation simplifies the process of gauging similarity and reduces the amount of qualitative judgment required to determine applicability.

4.4.2 Candidate Experimental Facilities

The best place to find well-defined, rigorously peer-reviewed benchmark experiments is within the International Criticality Safety Benchmark Evaluation Project (ICSBEP) and the International Reactor Physics Experiment Evaluation Project (IRPhEP) (Dean and Tayloe Jr. 2001). The ICSBEP handbook documents 533 evaluations with 4,552 critical, near critical, and subcritical configurations (NEA 2011a). The handbook provides an abundance of simulation materials, including neutron spectra and neutron balance information for all configurations and sensitivity distributions (generated with TSUNAMI) for 432 configurations. The IRPhEP handbook (NEA 2011b) documents 53 experiments performed at 31 experimental facilities, power reactors, and research reactors. Because IRPhEP experiments tend to be more complex than ICSBEP experiments, the simulation process is much more arduous and fewer peer-reviewed simulation materials (like input files or sensitivity distributions) are available. The strength of a validation exercise depends strongly on the degree of verification performed for the simulation materials.

For this white paper, the first step in the search for relevant validation benchmark experiments began with identifying HTGR facilities documented in the ICSBEP and IRPhEP, because such facilities share many neutronic characteristics with FHRs. This step identified the VHTRC, HTR-PROTEUS, HTTR, HTR-10, and ASTRA facilities, described in further details in Appendix D. The second step involved calculating representivity factors with respect to characteristic FHR unit cells for all experiments that had sensitivity distributions. This step identified critical experiments performed at the MARACAS facility and the Plutonium Recycle Critical Facility at the Pacific Northwest National Laboratory (PNNL). Note that this step was not exhaustive because only one tenth of the ICSBEP configurations and none of the IRPhEP experiments provided sensitivity profiles. Lastly, when sufficient validation gaps exist, future physical benchmarks can be designed and performed. Experiments may be performed at the LR-0 and AGN-201M facilities, and the new TMSR-SF experimental reactor at the Shanghai Institute of Applied Physics, described in further details in Appendix D, to validate the reactivity characteristics of flibe and its constituents. Additionally, archival documentation of experimental and research facilities can provide some degree of guidance for physical benchmarks. Appendix D describes each of these experiments and facilities in detail. Additionally, an FHR test reactor being pursued at SINAP may offer extremely valuable and relevant validation information.

4.4.3 Similitude Assessment

A preliminary analysis quantified the similitude of the 432 ICSBEP configurations with characteristic FHR unit cells that represent a large amount of the important physics. The unit cells consist of a single FHR pebble (fresh, spent, and at intermediate burnup), submersed in flibe coolant with a packing fraction of 60%. Future work will compare other ICSBEP configurations and the HTGR IRPhEP experiments with characteristic FHR full-core models.

The best agreement for a fresh pebble was achieved with configurations 18, 1, and 4 (c_k=0.66, E=0.78, G=0.5, respectively) of the LEU-COMP-THERM-049 benchmark performed at the MARACAS facility. The best for an intermediate burnup pebble was achieved with configuration 2s (c_k=0.65, G=0.2) of the MIX-COMP-THERM-002 benchmark performed at PNNL and configuration 3 of LEU-COMP-THERM-049 benchmark (E=0.53). The spent pebble achieves the best similitude with configurations 4s (c_k=0.64) and 2s (E=0.49, G=0.24) of the MIX-COMP-THERM-002 benchmark. Although classification is somewhat subjective, these experiments might be designated as “adequately similar” at best, meaning that only some degree of validation can be extracted and that additional experiments may be required.

4.4.4 Summary

The ICSBEP and IRPhEP handbooks document an abundance of criticality and reactor physics benchmark experiments. Very little validation is offered from those that provide sensitivity profiles. However, it is expected that the HTGR experiments will offer a large degree of coverage for the necessary physics, namely fuel and graphite reactivity coefficients, absorber reactivity worths, and power distributions. Future work will incorporate results from those experiments. Better understanding of flibe reactivity characteristics may or may not require benchmark studies to be conducted at the LR-0 and AGN-201M facilities.

5 Structural Mechanics Modeling

The most important operating limits for FHRs will ultimately be established primarily by structural limits, so the capability to model structural mechanics is key to the design and licensing of FHRs. Moreover, these structural evaluation models must be verified with experimental data, making it important to have effective methods for non-destructive and destructive examination. This work should also inform the selection of instruments and methods to perform on-line monitoring and in-service inspection during FHR plant operation. Testing of key components in molten salt test loops can be expected to play a major role in validating structural models, as will fuel irradiation tests and a variety of materials-related separate effects tests.

The purpose of this chapter is to identify and recommend candidate codes that can be used as evaluation models for the design and licensing of FHR plants. Here it is preferred to use codes that have already been applied to the design and licensing of other reactors. For FHR metallic structures, it is anticipated that previous experience with SFR structural modeling will be most relevant. For graphite and ceramic composite structures, as well as for coated particle fuels, codes applied in the modeling of HTGRs can be expected to be most relevant. Finally, for the modeling of FHR reactor building structures which use steel-concrete composite construction, codes applied in the design and licensing of the Westinghouse AP-1000 reactor building can be expected to be most relevant.

5.1 FHR Structural Mechanics Phenomena

The key operating limits for FHRs that affect their safety and economics (core power density and core inlet/outlet temperatures) are ultimately established by structural limits. But unlike other solid-fueled reactors, for FHRs these operating limits do not arise due to limits on peak fuel temperatures. Instead, FHR operating limits emerge from some combination of limits on thermal stress and thermal creep for metallic primary loop components, stresses induced by accumulated neutron dose to graphite reflector structures, and potentially from peak power levels in coated fuel particles as well. Additionally, operating limits must consider a range of potential equipment failures due to both internal and external events.

Because FHR operating limits are established primarily by structural limits, the capability to model short and long term structural response is critical to FHR design and licensing. Therefore a key objective for this second FHR white paper is to identify codes and methods to predict steady-state and transient temperatures and neutron irradiation of FHR structures, the resulting stresses, and any inelastic deformation and damage as well as time-dependent creep of FHR structures.

The design of high-temperature FHR primary loop structures is governed by ASME Boiler and Pressure Vessel (BPV) code (ASME 2013), which provides rules and limits on acceptable structural design methods and thus on the design approach for FHR high temperature structures. The DOE and NRC have supported recent efforts to update high-temperature design rules for nuclear reactors in the ASME BPV (INL 2010b).

The design of FHR reactor cavity and building structures is governed by American Concrete Institute (ACI), American National Standards Institute (ANSI), and American Society of Civil Engineering (ASCE) code requirements. Blandford et al. studied the design and modeling of modular reactor building structures to accommodate seismic and other externally imposed loads, including wind, tornado, and airplane crash (E. Blandford et al. 2009). In addition, the structural design of reactor buildings must consider a variety of internal loads, including gravity loads, thermal loads, and loads imposed by internal sources of pressure.

5.1.1 Time Dependent Structural Analysis in Metallic Components

The metallic structures in FHR primary and intermediate loop systems will operate at sufficiently high temperatures that time-dependent behavior must be considered in their design. The reactor vessels of FHRs will operate at steady state at the core inlet temperature (nominally around 600°C) and may reach higher temperatures during transients and accidents. Heat exchangers will operate in steady state at yet higher temperatures, up to the nominal core outlet temperature of 700°C, and can also reach higher temperatures during transients and accidents. Long-term creep phenomena at the steady-state operating temperatures, as well as accelerated creep when structures are heated to higher temperatures during transients and accidents, must be considered in the structure design and modeling. Additionally, thermal stresses arising from thermal transients, including thermal stripping and ratcheting, must also be considered.

The importance of high temperature design methods for reactors using fluoride salts were recognized early on, and were studied extensively for the Molten Salt Breeder Reactor Program (McNeese 1976b). They also overlap significantly with SFRs. The most recent gap analysis for SFRs at Sandia National Laboratory reached the following conclusions, based upon earlier gap studies by (Walters et al. 2011; Natesan et al. 2008). Thirteen major gaps were identified:

- Lack of materials property allowable data/curves for 60 year design life
- Lack of validated weldment design methodology
- Lack of reliable creep-fatigue design rules
- Lack of hold time creep-fatigue data
- Improved mechanistically based creep-fatigue life predictive tools are needed for reliable extrapolation of short term data to 60 y life
- Lack of understanding/validation of notch weakening effects
- Methodology for analyzing Type IV cracking in 9Cr-1Mo weldment (not applicable to FHRs)
- Lack of inelastic design procedures for piping
- Lack of validated thermal striping materials and design methodology
- Material degradation under irradiation
- Materials degradation under thermal aging

- Materials degradation in sodium environment (for FHRs the corresponding gap involves materials degradation in a salt environment)
- Degradation under sodium-water reaction (not applicable to FHRs)

Subsequent work to update the high temperature design rules of the ASME BPV code (ASME 2013) has addressed some of these gaps (Sims and Nestell 2012).

Heat exchangers are a key structure for FHRs that will experience high temperature operation and potentially significant thermal transients. A substantial base of early experience exists on methods to fabricate salt-to-air and other molten salt heat exchangers (Fraas 1989).

5.1.2 Radiation and Thermally Induced Stresses in Graphite and Composites

Like HTGRs, FHRs use graphite structures extensively within their reactor vessels. Because the graphite has lower density than the coolant flibe, the graphite structures are positively buoyant, which affects the design with respect to assembly and filling of the reactor with coolant and the need for the upper core support structures to transfer the upward vertical load from the graphite into the reactor vessel and reactor cavity structures. The near neutral buoyancy of the graphite also reduces the effects of horizontal acceleration during earthquakes. The high power density of FHRs, compared to HTGRs, results in FHR vessels being much smaller that HTGRs of similar power, but also results in the potential for higher neutron irradiation dose rates to graphite neutron reflector structures. The required replacement frequency for FHR graphite reflector structures will depend greatly upon the allowable maximum neutron dose limits, as well as on the potential use of neutron shielding (for example, the use of a radial layer graphite spheres to provide neutron shielding to the outer radial reflector in a FHR pebble bed).

In general, it is expected that the same design and modeling methods used for HTGRs can be used for FHRs, and thus recent work by the NGNP program to develop methods for stress analysis for graphite structures can also be applied to FHRs (Mohanty and Majumdar 2011).

As shown in Figure 5-1, strains induced in nuclear graphite originate from four key sources, elastic strain (ε_e), steady-state creep strain (ε_{sc}), transient creep strain (ε_{pc}), thermal strain (ε_θ), and irradiation strain (ε_i). As discussed by Mohanty and Majumdar, simulation of the combined effects of these sources of strain normally involves the use of finite element methods.

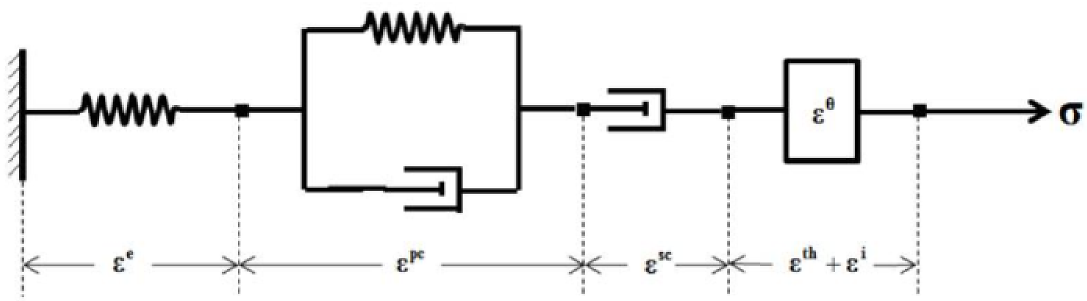

Figure 5-1. Maxwell-Kelvin Model of Graphite (Mohanty and Majumdar 2011)

5.1.3 Containment Response

The fluoride salts have very high chemical stability and very low volatility, and enable the design of reactor cores that have negative coolant void reactivity. Therefore one of the most noteworthy issues affecting the design of the FHR reactor cavity and containment structures is the lack of energetic phenomena that can generate significant pressures inside the reactor primary system and its containment. This raises questions about how to model FHR containment response, since it will be different from SFR, LWR, and HTGR containments.

In SFRs the energetic phenomena that must be considered and modeled in containment design (Schmidt et al. 2011) include sodium pool and spray/jet fires (AQUA-SF, NACOM, PULSAR, PYROS-1, SPHINCS), sodium/concrete interaction (RESORT, SORBET), sodium reactions inside steam generators (SWAMM-II), core disruptive accidents (SE2. SIMMER III/IV, VENUS-II), explosions and shocks (EUROPLEXUS, SPIKE, SWACS) and resulting containment response (CONTAIN-LMR/1B-Mod1). Similarly, LWR containments must be designed to accommodate a variety of energetic events, including blow-down from loss of coolant accidents, hydrogen deflagrations and explosions, and energetic releases from the interactions of molten core material with water (steam explosions), air (direct containment heating), and concrete (core-concrete interaction). For HTGRs the containment or confinement must be designed to accommodate pressures associated with blow-down during loss of coolant accidents.

While FHRs do not have stored energy sources capable of generating high pressures inside containment, three potential sources of pressurization must still be considered.

First, the gas inside the reactor cavity may be heated to higher temperatures during accidents, causing an increase in pressure. Particularly if the cavity is insulated so that the gas is already near the reactor operating temperature, this pressure increase would be modest and could be mitigated.

Second, there may be sources of water outside the reactor containment, including fire water systems and circulating water used for cooling of air, equipment, and possibly the reactor cavity liner system. These systems would be designed so that leaking water would be routed to a drain system away from the containment, but interactions of water with intermediate salt could still be possible. Experiments performed at ORNL indicated that the fluoride salts are sufficiently cool that steam explosions do not occur when they interact with water.

Finally, the power conversion system will use a working fluid at a pressure well above atmospheric, so a leak in the power conversion heat exchangers could cause pressurization of the intermediate loop. One functional requirement for the intermediate loop is to have pressure relief (likely a rupture disk) sized to prevent excessive pressurization of the intermediate heat exchanger.

5.2 Potential FHR Structural Mechanics Codes

The modeling of FHR structures and fuels can be performed at a range of different fidelities. The ASME B&PV code and the ASCE seismic and structural design codes provide simplified design rules and limits that can be used to establish initial design parameters and compliance with code requirements. However, it is expected that most FHR structures and fuels will also be modeled using finite element methods, to provide detailed predictions of distributions of stress and strain, and to predict the progression of time-dependent creep behavior and effects of irradiation. The application of these modeling tools to FHR structures and materials is reviewed below.

5.2.1 FHR Metallic Structures Codes

The design and licensing of FHR metallic structures shares many common issues with SFRs. A recent Sandia National Laboratory gap analysis for SFRs provides useful input on appropriate evaluation models (http://www.ansys.com). Most commonly, commercial finite element codes provide the most practical and appropriate modeling tool. The code ANSYS has been used extensively for this purpose. ANSYS is a generic reference to a suite of engineering simulation software tools developed and marketed by ANSYS Corp. Of particular note here are the structural mechanics and the explicit dynamics tools/codes. AUTODYN Explicit analysis tool (ANSYS suite) for modeling the non-linear dynamics of solids, fluids, gas and their interaction.

Other potential codes for FHR structural analysis that have been used outside the United States (Schmidt et al. 2011) include FINAS (Finite Element Nonlinear Structural Analysis System) (Anon. 1995); EUROPLEXUS, a general finite element software for non-linear dynamic analysis of fluid structure systems, jointly developed since 2000, by the CEA, the Joint Research Centre (EC) and SAMTECH (http://europlexus.jrc.ec.europa.eu/), (http://wwww.samtech.com/en/pss.php?ID=32&W=products).

5.2.2 FHR Graphite and Ceramic Composite Structures Codes

As summarized by Mohanty and Majumdar (Mohanty and Majumdar 2011), for graphite structures a variety of modeling tools exist to model steady-state and time-dependent behavior, including the time-dependent effects of neutron irradiation damage and creep deformation. The common practice is to use commercial finite element codes for some or all of the analysis.

A UK research group has developed a user defined subroutine for ABAQUS called MAN UMT for analysis of nuclear graphite under fast neutron irradiation and radiolytic oxidation to perform three dimensional, time integrated, non linear graphite stress analysis (Slater, Jones, and Davies 1999). Tsang and Marsden performed further development of the MAN UMT subroutine and presented additional results (Tsang and Marsden 2006).

JAERI in Japan developed a standalone finite element code called VIENUS (Iyoku, Ishihara, and Shirai 1991) for the analysis of stresses in HTTR graphite blocks. The input data for temperature was calculated using the ABAQUS code.

Lejeail and Cabrillat analyzed temperature and thermal stress distributions in HTGR graphite, using a finite element model based on the code Cast3M developed at CEA (Lejeail and Cabrillat 2005; Verpeaux, Charras, and Millard 1998).

Likewise, Wang and Wu have used a three dimensional finite element code named INET-GRA3D to analyze stress distributions in graphite components (Wang and Yu 2008).

Most recently, the INL has used the multi-physics finite element software COMSOL to conduct a fully-coupled thermal fluid and structural analysis for graphite structures (Bratton 2009).

5.2.3 FHR Fuel Codes

Various codes have been developed to model HTGR coated particles at the particle scale, such as the PARFUME code from INL (Miller et al. 2004). Other particle-scale simulation codes, some of which also model fuel element scale response, include ATLAS (France), PANAMA (Germany), RIGID SIC (Japan), COPA (Republic of Korea), GOLT (Russian Federation), and STRESS3 (UK) (IAEA 2012). At the fuel element scale, simplified one-dimensional models can be used to predict heat transfer, but commercial finite element codes provide the best capabilities to model multi-dimensional heat transfer and thermal stresses, similar to the modeling approaches discussed above for graphite structures.

5.2.4 FHR Reactor Building Structures Codes

Appropriate general-purpose finite element codes for analyzing reactor building structures include ANSYS, LS-DYNA, and ABAQUS. A current example of best practice in developing and validating reactor building structural models can be found in the NRC licensing documentation for the AP-1000 reactor shield building, which Westinghouse modeled using ANSYS.

6 Coupling and Multiphysics Modeling

Coupled and multiphysics modeling may be needed for some FHR steady-state and transient analyses. For example, because the distribution of fuel and coolant temperature affects the power distribution in the core, coupled neutronic and thermal hydraulic modeling may be required for some key transients such as start up from isothermal hot standby to full power, and ATWS. Similarly, the temperature and flow of the coolant will affect the steady-state and transient temperatures of structural components, creating the potential need for coupled thermal hydraulic and structural mechanics modeling. Finally, neutron fluence may induce long-term material degradation in the core, supporting the need for coupled neutronic and structural mechanics modeling capabilities. The degree and complexity of coupling required will depend on the phenomena and transients, and fully coupled modeling may be needed to simulate complex transients like an ATWS, as mentioned in Chapter 4. However, in the early design phase of the FHR, loose coupling or iterative modeling will most likely be sufficient. In that early phase, the need for more or less tight coupling can be assessed through small benchmarks and comparisons with other codes, as was done in the early stages of the PBMR-400 benchmark study.

Based on discussions from Chapters 3, 4, and 5, this chapter first highlights the most important figures of merit that must be exchanged between coupled codes for FHR modeling and addresses the potential need for more advanced multiphysics modeling, focusing on an unprotected LOFC transient as an example ATWS, which was identified as the most severe BDBE for the FHR in the first FHR workshop white paper on functional requirements and LBEs. Then, dividing the discussion into neutronic/thermal hydraulic, thermal hydraulic/structural mechanics, and neutronic/structural mechanics coupling, the chapter presents a selection of methods that have been used for steady-state and accidental transient analyses for advanced nuclear reactor concepts and provides recommendations for the FHR design development path, focusing on the subsequent experimental basis needed to validate the proposed coupling and multiphysics modeling tools.

6.1 Major LBEs and Related Figures of Merit

One key transient for the FHR, which involves neutronic, thermal hydraulic, and structural mechanics phenomena, is an ATWS. During this transient, multiple reactivity feedback mechanisms must be modeled to predict the peak coolant and structure temperatures reached before the fission power drops to zero. This type of transient results in the need to perform simultaneous, or at least tightly coupled, neutronic and thermal hydraulic modeling. The primary safety concern for an ATWS in FHRs involves heating metallic reactor structures, particularly the upper-core support structures, IHX, DHX, and reactor vessel, to temperatures that could cause accelerated creep deformation and damage. Therefore, coupled thermal hydraulic and structural mechanics phenomena must be modeled to ensure that these metallic structures, which provide a barrier to radionuclides and satisfy other Regulatory Design Criteria including control of the primary coolant inventory, are not compromised. The ATWS Section of NUREG-0800 (NRC 1987) specifies the following:

- "If fuel and clad damage were to occur following a failure to scram [which is unlikely to be applicable to FHRs due to very high fuel thermal margins], this condition should not interfere with continued effective core cooling;
- The calculated reactor coolant system transient pressure should be limited such that the maximum primary stress anywhere in the system boundary is less than that of the 'emergency conditions' as defined in the ASME Nuclear Power Plant Components Code, Section III [which is also unlikely to be applicable to FHRs, since the coolant is unlikely to even reach the boiling temperature; instead the principal issue is the temperatures and thermal stresses imposed on metallic reactor structures];
- Following a failure to scram, the containment pressure and temperature must be maintained at acceptably low levels based on [applicable] GDCs [NRC General Design Criteria]. The containment pressure and temperature limits are design-dependent; but […] those limits must ensure that containment design leakage rates are not exceeded when subjected to the calculated pressure and temperature conditions resulting from any ATWS event [which is also unlikely to be relevant to FHRs due to the lack of stored energy sources that can pressurize containment]."

Clearly, the performance issues for FHR ATWS differ greatly from those for LWRs. An ATWS may also be a significant transient for economics purposes, because it might limit the maximum allowable power density for the FHR commercial reactor.

The prediction of the reactivity insertion needed to raise the reactor power from isothermal, hot standby to full power also requires modeling of the coupling between thermal hydraulics, which determines how much the coolant and fuel temperatures increase, and neutronics, which determines the reactivity insertion required to overcome the negative reactivity feedback from increasing the power. The ability to predict the control element reactivity worth needed to reach full power is an important goal of FHR neutronic and thermal hydraulic modeling, and verifying the predicted control element worth will be an important component of reactor startup testing.

For steady-state modeling and other DBEs, tight coupling is not expected to be required. However, the same type of coupling should be used for all steady-state and transient analyses so that results are comparable.

Table 6-1 lists parameters that must be exchanged between coupled modeling codes to properly assess the system's behavior during steady-state operation and transients such as an ATWS. Parameters are exchanged from the code used for modeling phenomena in one column to the code used for modeling phenomena in one line. Chemistry control and radionuclide transport are important aspects of coupled modeling required for the FHR, and while they are only briefly mentioned in Table 6-1, they were major topics of discussion at the third FHR workshop.

Table 6-1. Parameters That Must be Exchanged between Coupled Modeling Codes to Assess the System's Behavior during Steady-State Operations and Transients (i.e., an ATWS)

From To	Neutronics	Thermal Hydraulics	Structural Mechanics	Chemistry
Neutronics	-	T_{fuel}, $T_{coolant}$, $T_{structures}$, pebbles packing fraction*, flow-induced pebbles re-zoning*	Geometry (pebble motion, control rod channels, etc.)	
Thermal hydraulics	Power distribution, DPA (conductivity)	-	Geometry (thermal expansion, etc.)	
Structural mechanics	DPA (damage)	T_{fuel}, $T_{structures}$, coolant velocity (flow-induced vibration)	-	Corrosion
Chemistry	Radionuclide source term	Radionuclide transport		-

* For PB-FHR

6.2 Neutronic/Thermal Hydraulic Coupling and Multiphysics Modeling

The neutronic model in the transient analysis capability must be coupled to a transient thermal fluids model to account for the temperature feedback mechanisms between neutronics and thermal hydraulics. The coupling system could be internal or external. The well known external method – or coupling method – is based on separate solving of neutronics and thermal hydraulics governing equations and external data exchange between codes used to solve these equations. In a sense, the only capability that must then be developed is an interface between existing – sometimes adapted – codes within a proper framework. On the other hand, the internal method – or multiphysics method – refers to the ability to solve simultaneously a system of equations that governs the behavior of more than one major distributed parameter. For core analyses, this approach usually means the simultaneous solution of neutron flux, heat transfer, and coolant transfer through the core, but fuel stress equations, photon transport, and other physics are also under consideration (INL 2010a). The ability to solve these equations simultaneously avoids the introduction of errors that often arise from solving the equations separately and coupling them explicitly via "split-operator" techniques.

Multiphysics codes can be used to investigate phenomena too complex for system codes, especially fast-evolving transients where neutronic and thermal hydraulic phenomena are tightly coupled, such as an ATWS.

6.2.1 Parameters Exchanged between Coupled Neutronic and Thermal Hydraulic Modeling Codes

Neutronic calculations rely on temperature-dependent cross section libraries. Therefore, fuel temperatures as calculated with a thermal hydraulic code must constantly be fed into the code used for neutronic calculations to use appropriate cross sections. More importantly during an ATWS, the response of the system strongly relies on competing temperature reactivity feedbacks between the fuel and the coolant. Therefore, both fuel and coolant temperatures as calculated with a thermal hydraulic code must constantly be fed into the code used for neutronic calculations to properly account for these temperature feedback effects. The temperature distribution in the moderator affects neutron spectrum in the core and must also be calculated by a thermal hydraulic code and serve as an input to neutronic calculations. Finally, in the PB-FHR, the reactivity of the core will strongly rely on packing fraction and burnup zoning of the pebble bed. Therefore, packing fraction and burnup zoning, resulting from thermal hydraulic phenomena (density of the coolant versus density of the fuel pebbles, flow-induced re-zoning, especially at the pebble bed free surface) must constantly be fed into the code used for neutronic calculations to properly calculate the core reactivity.

Conversely, temperatures as calculated with a thermal hydraulic code rely on power distribution in the core, calculated by a neutronic code. Therefore, power distribution as calculated with a neutronic code must constantly be fed into the code used for thermal hydraulic calculations to properly assess temperature distribution in the fuel and coolant. Additionally, because radiation damage degrades the heat transfer properties of fuel elements and structural materials (e.g., conductivity), thermal hydraulic analyses rely on proper neutron fluence calculations provided by neutronic codes.

6.2.2 Current Neutronic/Thermal Hydraulic Coupling Capabilities

Numerous coupling interfaces have been developed between neutronic and thermal hydraulic modeling codes, which always rely on the same exchange of parameters between the neutronic and thermal-hydraulic modeling tools. Such interfaces should be developed between neutronic and thermal hydraulic modeling codes selected for the FHR, after the issues raised in Chapters 3 and 4 have been resolved. While existing codes were presented in Chapters 3 and 4 and their applicability to the FHR was assessed, Appendix E reviews interfaces that have been used for coupled neutronic and thermal hydraulic modeling for advanced nuclear reactor concepts.

6.2.3 Current Neutronic/Thermal Hydraulic Multiphysics Capabilities

For complex, fast-evolving transients such as an ATWS, where neutronic and thermal hydraulic phenomena are tightly inter-dependent, multiphysics capabilities may be required to simultaneously solve neutron flux, heat transfer, and coolant transfer governing equations representing the core.

A multiphysics simulation tool named PRONGHORN has been developed for very high-temperature gas-cooled reactors (Park et al. 2009). The tool takes advantage of the Multiphysics Object-Oriented Simulation Environment (MOOSE) developed for the NGNP program and is capable of solving multidimensional thermal-fluid and neutronic problems implicitly in parallel. The initial development of PRONGHORN focused on the pebble bed core concept, but extensions required to simulate prismatic cores are underway. Current capabilities of PRONGHORN include solving steady-state coupled fluid flow-heat transfer problems and standard multigroup diffusion problems (fixed source, criticality, and time dependent). Both physics can be solved in multidimensional Cartesian coordinates and two-dimensional cylindrical (r-z) coordinates, with precursor and adiabatic thermal feedback models.

Results of PBMR400 benchmark problems (Reitsma et al. 2006) demonstrate the neutronic and multiphysics capability of PRONGHORN, and PRONGHORN results matched well with other codes, which is promising for future use of PRONGHORN in VHTR multiphysics modeling. However, because multiphysics tools are computationally intensive, it is still to be determined if such multiphysics capacities are needed for any neutronic and thermal hydraulic analyses for the FHR.

6.2.4 Validation of Coupled Neutronic/Thermal Hydraulic and Multiphysics Modeling

While considerable effort has been made in various countries and organizations on the development of coupled thermal hydraulic and neutronic codes, as illustrated by the few examples given in Appendix E, these code systems need to be properly validated for use with the FHR design.

For coupled neutronic and thermal hydraulic codes, the first step will be to validate the codes independently, following methodologies presented in Chapters 3 and 4. The coupled system, as well as any multiphysics tool used for FHR modeling, will eventually be validated through extensive experimental data collected in a test reactor.

As an intermediate step, benchmarks have been developed in international cooperation led by NEA/OECD that permit testing the neutronic/thermal hydraulic coupling and verifying the capability of the coupled codes to analyze complex transients with coupled core-plant interactions (Ivanov et al. 2007). However, these benchmarks have only been developed for LWRs (one boiling water reactor, one pressurized water reactor, and one VVER) and are therefore not readily applicable to use with the FHR technology.

6.3 Thermal Hydraulic/Structural Mechanics Coupled Modeling

One of the primary safety issues for ATWSs in FHRs involves heating metallic reactor structures, particularly the upper-core support structures, IHX, DHX, and reactor vessel, to temperatures that could cause accelerated creep deformation and damage. For steady-state, normal operation analysis, the main concern is the lifetime of these structures, which are exposed to high-temperature coolant. Modeling such factors requires coupling capabilities between thermal hydraulic and structural mechanics codes used for modeling the FHR.

6.3.1 Parameters Exchanged between Coupled Neutronic and Thermal Hydraulic Modeling Codes

Stuctural integrity of the reactor components relies on pressure and temperature of the coolant interacting with these components. This reliance is especially true for metallic components (e.g., the IHXs), which have the lowest thermal margins in the FHR and will likely be the first structures to experience damage or failure during accidents. Therefore, coolant temperature, flow, and heat transfer coefficients as calculated with a thermal hydraulic code must constantly be fed into the code used to model thermal conduction and stress in solid structures. Flow-induced vibrations, depending on flow velocities in the system, may also compromise structural integrity of the reactor components and must be accounted for. This approach also applies to steady-state operation modeling, to determine the lifetime of these components.

Conversely, fluid dynamics and heat transfer as calculated with a thermal hydraulic code rely on information about the geometry of the system, which may be calculated by a structural mechanics code. Therefore, geometry of all the reactor components, as calculated with a structural mechanics code, and perturbations to the as-built geometry caused by creep and thermal expansion – affecting the size of the downcomer and other support structures – must be provided to the code used for thermal hydraulic calculations to properly assess temperature and flow distributions in the coolant.

6.3.2 Current Thermal Hydraulic/Structural Mechanics Coupling Capabilities

Fluid-structure interaction occurs whenever a solid structure is in contact with a fluid. If the structure dynamic behavior can significantly be affected by the presence of the surrounding fluid, a coupled fluid-structure analysis is needed. Various numerical methods have been developed to model fluid-structure interaction problems. Most of these existing capabilities have focused on added mass effects caused by the presence of a fluid confined between two structures (Sigrist, Broc, and Lainé 2007). This approach is obviously insufficient for application to the FHR, where the main concern is the stress resulting from high temperature of the coolant more than pressure. Researchers in the fast reactor community have attempted to couple models of high-temperature reactors. However, additional thermal hydraulic and structural mechanics coupling capabilities may need to be developed to ensure that structural integrity of the system can be preserved in extreme events such as an ATWS, although it may only be necessary to exchange parameters from the thermal hydraulic module to the structural mechanics module, the key figures of merit being temperature and temperature gradients of the structural materials.

Multiphysics capabilities should not be required for thermal hydraulic and structural mechanics coupled analysis, as short time dependence between these phenomena is not as critical as the neutronic and thermal hydraulic phenomena inter-dependence.

6.3.3 Validation of Coupled Thermal Hydraulic/Structural Mechanics Modeling

Testing of key components in a FHR Component Test Facility can play a major role in validating coupled thermal hydraulic and structural mechanics models. However, the FHTR will provide the ultimate experimental basis for validation of the coupling capability.

6.4 Neutronic/Structural Mechanics Coupled Modeling

For steady-state as well as transient analysis of the FHR, interactions between neutronics and structural mechanics must be carefully studied to ensure that integrity of the reactor components is not compromised by irradiation stresses, and positive reactivity insertions are not caused by structural modifications in the core. One essential related issue is fuel performance, which was a key topic of discussion at the third FHR workshop on materials.

6.4.1 Parameters Exchanged between Coupled Neutronic and Thermal Hydraulic Modeling Codes

Stuctural integrity of the core components may be reduced by neutron irradiation. This change is especially true for components close to the center of the core, where neutron fluence is expected to be the highest. Therefore, neutron flux as calculated with a neutronic code must be provided to the code used for structural mechanics calculations to ensure structural integrity of the core components. Dimensional changes in graphite because of irradiation damage are also important in the FHR analysis, as they affect bypass flow through graphite blocks in the core.

Conversely, neutron fluxes as calculated with a neutronic code rely on the geometry of the system, calculated by a structural mechanics code. Therefore, geometry of all the core components, as calculated with a structural mechanics code, must constantly be fed into the code used for neutronic calculations to properly assess neuton flux and therefore reactivity in the core. The modeling capability should also make it possible to verify that structural degradation will not compromise free paths for control elements in the core. This approach is especially relevant after a potential seismic event, hence the need for a capability to properly model such events.

6.4.2 Current Neutronic/Structural Mechanics Coupling Capabilities

Coupling is not required between neutronic and structural mechanics analyses, as short time dependence between these phenomena is not as critical as the neutronic and thermal hydraulic phenomena inter-dependence. Therefore, no existing capability for coupling between neutronic and structural mechanics phenomena has been identified, and none should be required for analysis of the FHR.

6.4.3 Validation of Coupled Neutronic/Structural Mechanics Modeling

Fuel irradiation and graphite irradiation tests can be expected to play a major role in validating coupled neutronic and structural mechanics models. However, the FHTR will provide the ultimate experimental basis for validating the coupling capability.

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Appendix A Current Thermal Hydraulic Modeling Capabilities

A.1 THERMIX Code for the HTR-10 and Application to the PBMR

The HTR-10 is the first high temperature gas-cooled test module reactor built at Tsinghua University in China, with a pebble bed core and an output power of 10 MWth. The fuel elements of the HTR-10 are similar to the pebbles used in the baseline design for the PB-FHR.

The THERMIX calculation models were used in the transient analysis for the HTR-10. The basic code structure of THERMIX uses a two-dimensional cylindrical geometry and consists of the steady-state or transient heat conduction equation and a quasi-steady-state convection code (DIREKT) (Haque et al. 1983). These calculation models had been validated through a series of experiments carried out at the AVR-high temperature reactor and at the KFA-Julich in Germany (Kindt and Haque 1992).

The pebble-bed region is treated as a porous medium. In THERMIX, both the conduction in the pebbles and the radiation between the pebble surfaces are treated, while the 2-D helium flow in the bed is treated by DIREKT. These two models are coupled by the heat transfer from the pebble surface to the helium coolant. For the core region, 2-D temperature profiles for fuel and moderator temperatures of the pebbles are calculated. To this end, a 1-D calculation for the temperature profile inside the pebbles is used, taking into account that the pebbles have a fuel-free (graphite) zone in the outer shell. Besides the power profile, the temperature and heat transfer coefficient at the outer surface of the reactor, determined by the reactor cavity cooling system, are used as boundary conditions for the THERMIX model. The boundary conditions for the DIREKT model are the helium inlet pressure, temperature, and mass flow.

For validation purposes, calculation results of normal operation, an LOFC transient, and a control rod withdrawal transient without scram were compared with experimental data obtained in the HTR-10. The code was also applied to the 400-MWth PBMR design, including the analysis of three different LOFC transients. Absent any experimental data for the PBMR, theses results were compared to the results of the existing TINTE code system.

It was found that the code system is capable of modeling both small (HTR-10) and large (PBMR) pebble-bed reactors and therefore provides a flexible tool for safety analysis and core optimization of future reactor designs (Boer et al. 2010).

A.2 COMMIX Code for S-PRISM

S-PRISM, also called PRISM (Power Reactor Innovative Small Module), is a SFR design by General Electric Hitachi Nuclear Energy. Thermal hydraulic analyses of the S-PRISM core were performed using the COMMIX code. COMMIX-I is a three-dimensional, transient, single-phase, component computer code for thermal hydraulic analysis of both continuum (reactor plenum, etc.) and quasi-continuum (rod-bundle, etc.) applications. The porous medium formulation with volume porosity, surface permeability, distributed resistance and distributed heat source is employed in the COMMIX computer codes. The concept of surface permeability is a new feature added in the present porous medium formulation. It greatly facilitates the modeling of the anisotropic characteristics of a medium containing solid objects such as fuel rods in a reactor fuel assembly. The porous medium approach with volume porosity, surface permeability, and distributed resistance and distributed heat source (or sink) is employed for rod-bundle thermal hydraulic analysis. It was found to provide a greater range of applicability and an improved accuracy compared to conventional subchannel analysis (Domanus, Shah, and Sha 1980). The ability to model porous media makes the COMMIX code a candidate for FHR thermal hydraulic modeling.

Several sets of numerical results were obtained from the single-phase versions of the COMMIX code and successfully compared with experimental data, for phenomena including natural circulation (used for passive decay heat removal in S-PRISM), planar blockage, loss of piping integrity, etc.

A.3 RELAP5-3D for the LS-VHTR

The LS-VHTR represents a unique merging of design features from other reactor systems. The reactor core is similar to that used in graphite-moderated helium cooled reactor systems, such as Fort St. Vrain and the Gas-Turbine Modular High-Temperature Reactor. The LS-VHTR uses the same coated particle fuel, cylindrical fuel compacts, and hexagonal graphite fuel assemblies as these reactors. The liquid salt coolant allows for efficient heat transfer and is based on experience gained from the earlier Molten Salt Reactor program. Because the liquid salt coolant operates at low pressure, the vessel enclosure system and facility design are similar to pool-type sodium reactors. The passive decay heat removal system is based on the PRISM design developed by General Electric. A lot of these design features are common to the FHR, which makes this a good example for code benchmarking for the thermal hydraulic modeling of the FHR.

A one-dimensional model of the LS-VHTR was developed using the RELAP5-3D computer program. The program was originally developed for thermal hydraulic analysis of light water reactors and related experimental systems during loss-of-coolant accidents and operational transients. The code has recently been improved to simulate candidate Generation IV designs cooled by gas, supercritical water, and lead-bismuth. Liquid salt coolants have also been implemented into the code, which allows it to simulate the LS-VHTR. The primary coolant was assumed to be flibe, which is also used as the primary coolant for the FHR. The thermal calculations from the one-dimensional model of a fuel block were benchmarked against a multidimensional finite element ABAQUS model. The fuel centerline temperatures calculated by RELAP5-3D were within 0.6 and 2.2 °C, respectively, of the values calculated by ABAQUS (Davis and Hawkes 2006). Thus, the RELAP5-3D one-dimensional annular model can accurately predict fuel centerline temperatures.

This is a promising preliminary result, which calls for further benchmarking and validation of the RELAP5-3D code for use in FHR thermal hydraulic modeling.

A.4 RELAP5-3D for SmAHTR

SmAHTR is a 125 MWt, integral primary system FHR concept developed by a multidisciplinary team of reactor systems specialists and nuclear technologists at Oak Ridge National Laboratory in 2010. A pre-conceptual design review was issued in December, 2010 (Greene, Gehin, et al. 2010).

RELAP5-3D/ATHENA, Version 2.4.2, was used to perform thermal hydraulic evaluations of the SmAHTR concept. RELAP5-3D includes properties for four salts: flibe, flinak, $NaBF_4$-NaF, and NaF-ZrF_4. For the pre-conceptual design analysis, flibe was used for the primary coolant and flinak for the secondary coolant of both the primary heat exchanger and the DRACS. Analyses were made to assess thermal hydraulic behavior of the reactor in steady-state operation, and the capability to rely on natural convection for passive decay heat removal using the DRACS during a LOFC with scram transient.

A.5 VIPRE-01 Code for the AP1000

The AP1000 is a two-loop pressurized water reactor sold by Westinghouse Electric Company. In December 2005, the NRC approved the final design certification for the AP1000. As the first Gen III+ reactor to receive final design approval from the NRC, the AP1000 is a good example of current thermal hydraulic modeling best practices. Furthermore, it shares with the FHR the concept of passive decay heat removal, raising interest regarding the methods that should be used for the thermal hydraulic design and modeling of the FHR.

Westinghouse performed the AP1000 core safety analysis of transient events using the VIPRE-01 computer code and the WRB-2M critical heat flux correlation.

VIPRE-01 is a subchannel, thermal hydraulic computer code used to analyze the reactor core of a reactor system. Battelle Pacific Northwest Laboratories, under the sponsorship of EPRI, developed VIPRE-01 and submitted it to the NRC for generic review in 1984. The NRC approved VIPRE-01 for application to pressurized water reactors (PWRs) in 1985, with the condition that each VIPRE-01 user submit documentation describing the proposed use for the code, other computer codes with which it will interact, the source of each input variable, and the selected correlations and their justification. WCAP-14565-P-A, issued in October 1999, documents the applicant’s use of VIPRE-01 for Westinghouse-designed PWRs. The staff approved this topical report in 1999. The staff has determined that use of VIPRE-01 for the AP1000 core thermal hydraulic analysis is acceptable because the AP1000 is a Westinghouse-designed PWR for which the VIPRE-01 modeling is qualified, as described in WCAP-14565-P-A (Westinghouse Electric Company).

Although Westinghouse focused its analyses on departure from nucleate boiling, which is not expected to occur in the one-phase flow FHR system, this procedure with the NRC is an example of good practice which should be replicated during the development of the FHR, in order to comply with the NRC requirements when a license application is submitted for the FHR.

A.6 CFD Codes

The design and analysis of fluid flow and heat transfer in complex closed-loop systems like nuclear reactors require the use of a variety of analysis techniques and simulation tools. These range from one-dimensional pipe network codes, to very advanced three-dimensional Computational Fluid Dynamics (CFD) codes. Three-dimensional CFD codes are useful for accurate geometrical and physical modeling of individual system components, but are not practical for analyzing complete integrated systems due to the excessive computational resources required and the time it takes to solve. On the other hand, while one-dimensional tools cannot resolve the detailed flow field within components, they allow efficient analysis of complete systems.

As part of the NGNP program, CFD has been considered as a tool to analyze, for instance, bypass flow between prismatic graphite blocks in the core (Johnson and Schultz 2010). This type of use of CFD codes can complement lumped-volume system analysis codes like RELAP. Flow conditions differences between helium for the NGNP and flibe for the FHR may affect the need to use CFD. Sensitivity of the system response to bypass flow is one of the main elements that will dictate the need for use of CFD codes. Therefore, preliminary sensitivity analyses should be key steps to assessing the need for CFD codes for FHR thermal hydraulic modeling.

One of these codes, Flownex Nuclear, has been developed to perform thermal-fluid analyses on a high-temperature gas-cooled reactor coupled to a direct, recuperated Brayton cycle in an implicit way. Since it is the first software product of its kind, a diverse number of verification and validation methods have been used to qualify the software. At PBMR, Flownex Nuclear was used to predict mass flows, heat transfer and pressures in the reactor core and the Brayton cycle during expected operational modes and states, as well as under accident conditions. It was used for both steady-state and transient simulations (Van Ravenswaay et al. 2006). In order to ensure the accuracy of these simulations a rigorous V&V process has been implemented. The validation phase included:

- Mass flow balancing behavior of a compressible gas in a complex pipe network;
- Transient pressure behavior using three inter-connected pressure vessels at different initial pressures;
- Performance of a closed three-shaft, recuperative Brayton cycle.

The code was also applied to the 400-MWth PBMR design, including the analysis of three different LOFC transients. Absent any experimental data for the PBMR, theses results were successfully compared to the results of the existing TINTE code system

(Dudley et al. 2008) and THERMIX/DIREKT code system (Rousseau, Du Toit, and Landman 2006). One remaining effort to properly model the FHR with Flownex will be the implementation of freezing and thawing phenomena, which are specific to this system.

Appendix B Thermal Hydraulics Validation Integral Effects Tests

The two IET facilities required for the FHR program are the Compact Integral Effects Test (CIET) facility, and for the pebble-fueled variant of the FHR the Pebble Recirculation Experiment (PREX). CIET is a scaled integral heat transfer loop, using oil as a simulant fluid. PREX is a scaled experiment to replicate pebble recirculation phenomena, using water as a simulant fluid. During the Performance phase, additional IET data for heat transfer and pebble recirculation under prototypical conditions will be collected.

The baseline design for CIET uses a 10kW, 10V DC power supply, already existing at UCB. Due to the scaling for heat transfer oils as simulant fluids, CIET is effectively equivalent to a 0.63MW IET facility using the prototypical liquid salt under prototypical conditions. The CIET facility has 50% height scaling compared to the prototypical FHR. Because the FHR primary system height is expected to be half that of a conventional LWR or Modular Helium Reactor (MHR), and because CIET is half that height, the CIET facility with its DRACS loops can fit inside a 10-m high laboratory. A CIET Component Test Bay using simulant oil has actually been built in the thermal hydraulics laboratory at UCB, and is currently being used to collect data on natural circulation for passive decay heat removal. Figure B-1 shows pictures of this facility. The CIET facility, a two-loop experiment aimed at validating models of the LOFC with scram transient, using coupled natural circulation loops, is scheduled to start running in August, 2013, using the same Dowtherm A oil. A preliminary diagram of this facility is shown on Figure B-2.

The difficulty of performing IET experiments is much lower when one can work with a near room-temperature fluid at reduced power and length scales. The simplification of the experiment design, and reduction in cost, are the unique attributes of liquid salt coolants that make it possible for a major IET facility to be built and operated during the Viability phase of R&D.

For the pebble-fueled variant of the FHR, pebble recirculation is the second key process that requires experimental validation. The availability of water as a simulant fluid that can match Reynolds and Froude numbers allows experimental validation of pebble recirculation model predictions to be made during the Viability phase. This experiment also includes a pebble injection system. Figure B-3 shows a photo of the PREX 3.1 experiment that is geometrically scaled to match a slab of the annular PB-FHR core. The test section is instrumented with manometers to measure the pressure field in a pebble bed. Therefore, this experiment has already been used to validate a RELAP5-3D model of porous media flow distribution, one of the key areas of pebble fuled FHR thermal hydraulics phenomena. It has been demonstrated that when implementing Beaver's

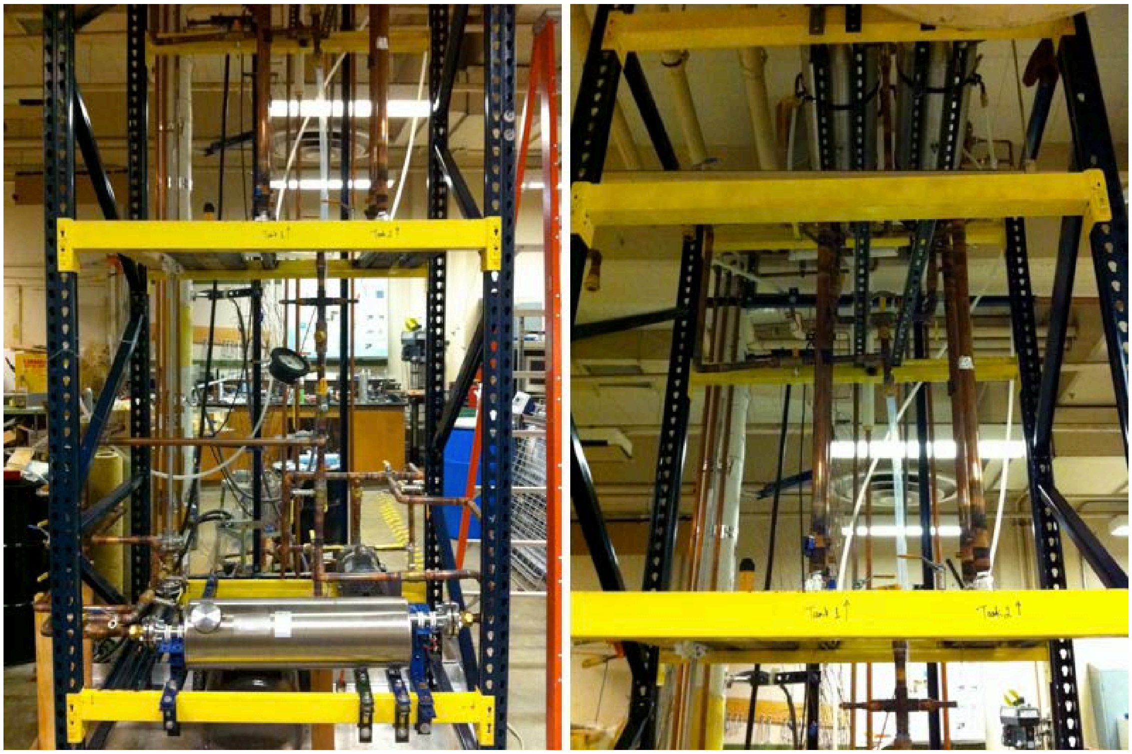

Figure B-1. The CIET Component Test Bay in the Thermal Hydraulics Laboratory at UCB

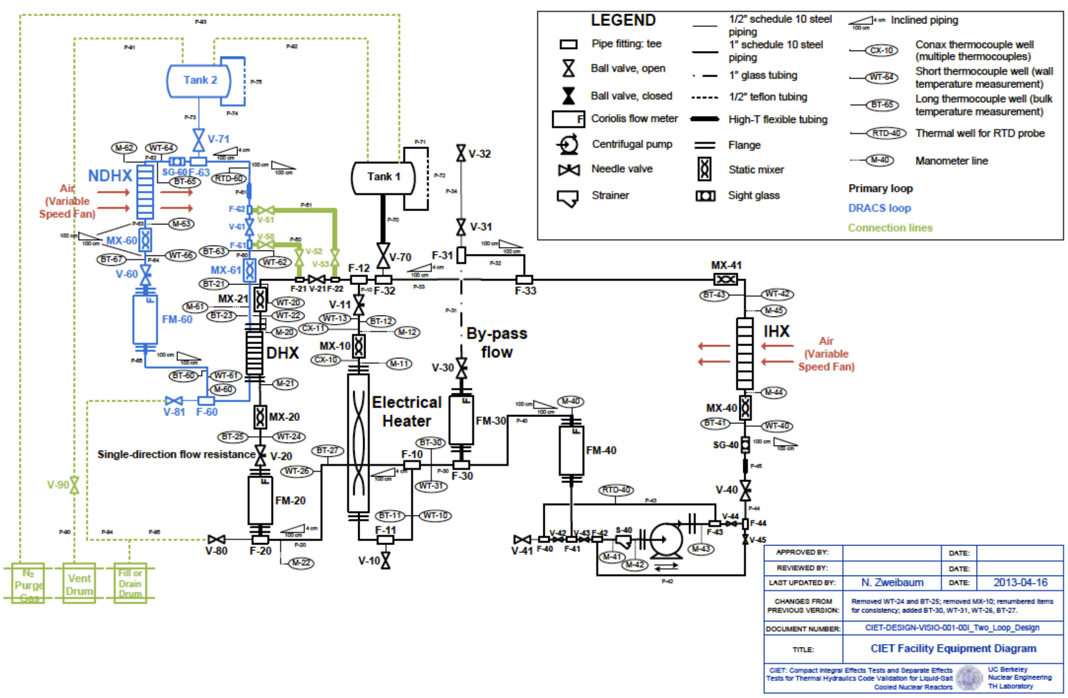

Figure B-2. Preliminary Diagram of the CIET Facility for Simulating the LOFC with Scram and Other FHR Transients

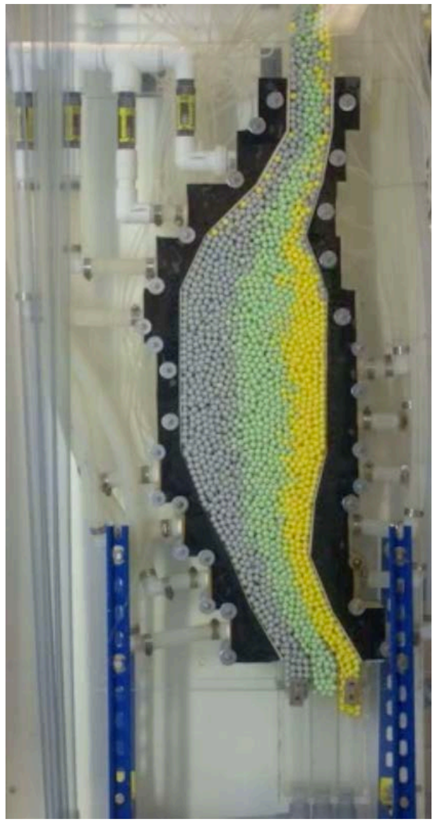

Figure B-3. PREX 3.1 Test Section in its Tank
Pebbles are injected through the white piping at the left side of the test section into separate hoppers at the bottom of the bed. Flow can be directed axially through the pebble injection ports or through the faces in the lower sections of the inner (right) and outer (left) reflectors. Outlet flow can be controlled through either the top in the discharge cone or through the faces on the upper section of the outside reflector (Laufer, Bickel, and Peterson 2010).

correlation – one of the standard correlations for porous media flow modeling – into the RELAP5-3D model of PREX 3.1, the model properly accounts for axial flow distribution in the turbulent regime. However, significant distortions arise from modeling cross-flow and laminar regime flows, which becomes an issue when modeling natural circulation through the core during natural circulation decay heat removal (Zweibaum 2011). This serves as an example of the importance of experimental data collection to validate thermal hydraulic models, and shows the limits of the RELAP5-3D code to properly model thermal hydraulic phenomena for the FHR without implementation of improved models into the code.

Additional scaled IET facilities exist outside of UCB, which can be used to further validate thermal hydraulics models for the FHR, or at least serve as examples of best practices for model validation.

The Advanced Plant Experiment (APEX) at Oregon State University (OSU) was designed and constructed on the basis of the H2TS Methodology (Zuber et al. 1998). It was the most accurate geometric representation of a Westinghouse AP600 nuclear steam supply system. The OSU APEX test facility has served to develop an essential component of the IET database used to assess the AP600 and AP1000 thermal hydraulic safety analysis computer codes(Reyes and Hochreiter 1998). Although the AP600 was a LWR design, it was relying on natural circulation for passive decay heat removal, which is one of the key thermal hydraulic phenomena for the FHR. Therefore, an important knowledge basis can be obtained with experimental data collected in that facility.

The OSU High Temperature Test Facility (HTTF) is another IET facility that is currently being constructed on the OSU campus. The HTTF facility is a 1/4 geometric length scale, 1/2 time scale, representation of the Modular High Temperature Gas-Cooled Reactor (MHTGR) design. The facility will operate at prototypical temperature using helium as the working fluid at reduced pressure. HTTF will be used to simulate the following phenomena:

- Core conduction and radiation heat transfer;
- Vessel radiation heat transfer;
- Core temperature profiles;
- Air-ingress by lock-exchange
- Air-ingress by molecular diffusion
- Air natural circulation.

The facility will be used to generate validation data for the NGNP thermal hydraulics methods development (Schultz et al. 2010). As such, and because the MHTGR design shares some key phenomena with the FHR (high temperature, TRISO fuel, natural circulation, etc.), experimental data from the HTTF facility should also serve as a good knowledge basis for validation of FHR thermal hydraulic models.

However, as of today, no existing or projected IET facility has the capability of testing overcooling transients and bypass flow across the core in FHR. Experimental data for both of these phenomena will be required in order to complete the validation matrix for FHR thermal hydraulic modeling.

Appendix C Current Neutronics Modeling Capabilities

Before recommending a set of neutronics codes to develop for design, safety analysis and licensing of FHRs, it is important to review the past efforts to analyze neutron transport in FHR systems. This section reviews the neutronic and depletion analysis of FHR systems, including what framework was developed to analyze the FHR, what methodology was utilized, what codes were coupled, the general details of the specific FHR system that was investigated and what figures of merit were calculated.

C.1 Burnup Equilibrium Analysis Utility for PB-AHTR

Burnup equilibrium analysis utility (BEAU) was used to perform parametric design studies on the fuel design of the PB-AHTR and the preliminary design work on a pebble-bed FHTR. The PB-AHTR is a fluoride salt-cooled 900MWth reactor that uses low-enriched uranium (LEU) fuel compacted into annular spherical fuel elements that are buoyant in the coolant with low-density inert graphite cores and nominal density inert graphite shells. The baseline design is a fully-packed annular pebble bed that utilizes a graphite pebble reflector surrounding the active pebbles to reduce the neutron radiation damage rate to the outer graphite reflector. The FHTR is a 10-20 MWth test reactor that uses similar buoyant annular spherical fuel elements. However, the FHTR is a simple cylindrical homogeneous pebble bed with a free surface on the bottom.

BEAU searches for the maximum attainable burnup in a continuously refueled nuclear system. It generates a set of spatially and burnup dependent one-group cross sections for burnup states throughout a full-core reactor. The user defined makeup fuel charge is depleted with the cross sections generated in each burnup state under constant flux sequentially from the lowest burnup state to the highest burnup state so that the expected burnup and power distribution is calculated based on this depletion analysis. The fuel cycle parameters (burnup and fission neutron source) are perturbed iteratively to impose a target aggregate $k_{effective}$ and full-core power; see Figure C-1. A special FHR-specific module (AUtomatic Salt Composition Equilibrator, AUSC-E) has been implemented to adjust the equilibrium ^{6}Li concentration based on the system and burnup specific neutron spectrum in the coolant for every estimate of the equilibrium composition. BEAU uses MCNP5 to estimate the $k_{effective}$, generate the one-group cross sections for depletion, and map the full-core flux distribution and uses ORIGEN to perform the point-depletion analysis. The MCNP5 model of the fuel elements models each fuel kernel explicitly on a simple cubic lattice but homogenizes the TRISO layers together with the graphite matrix.

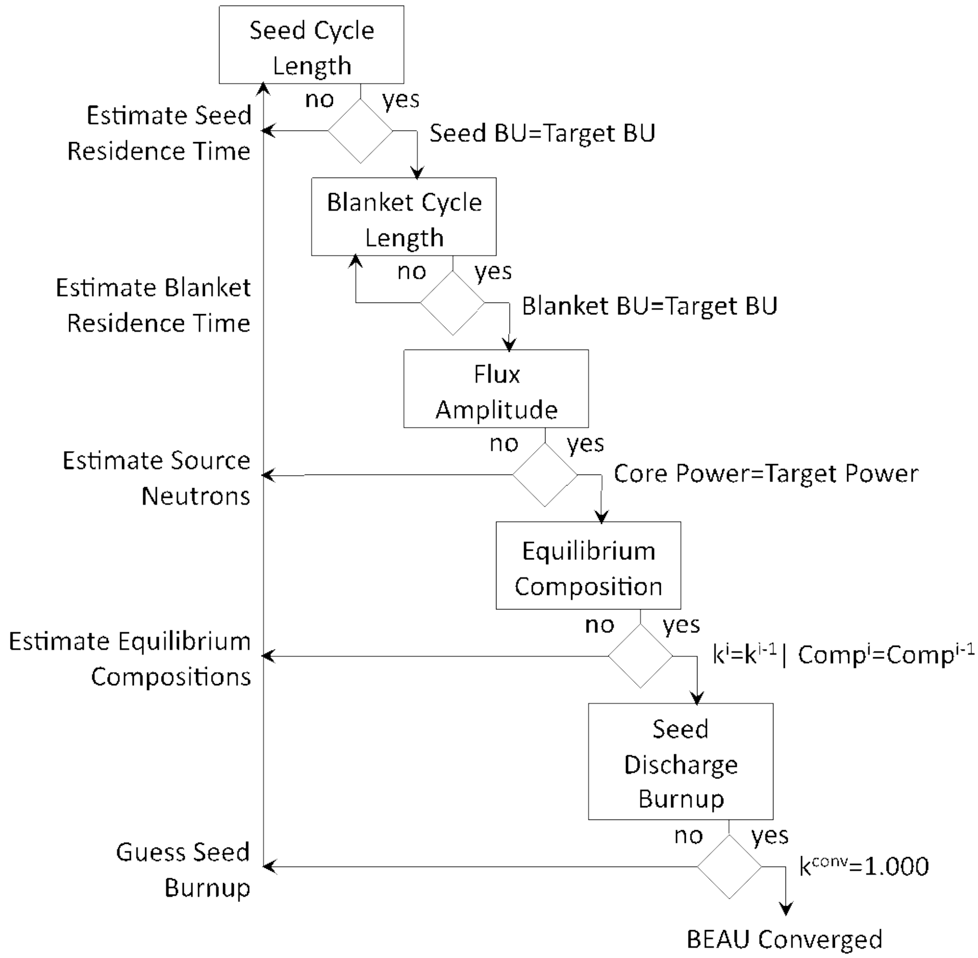

Figure C-1. BEAU Equilibrium Depletion Methodology Algorithm

In these parametric studies, BEAU calculated the maximum attainable burnup and identified the equilibrium state of the core. Once this equilibrium state was identified other parameters could be calculated such at temperature reactivity feedback coefficients, radiation damage rates to structural components, and shutdown margin.

C.2 SCALE Equilibrium Analysis Utility for AHTR

SCALE Equilibrium Analysis Utility (SEAU) was developed to benchmark an analytical method for fixed-fuel FHR designs to extrapolate single-batch depletion analysis results to determine the maximum attainable burnup in a multi-batch fuel management scheme, the non-linear reactivity model (NLRM). The AHTR studied here is a fluoride-salt cooled, 3400-MWth reactor that uses coated-particle fuel compacted into layered plate fuel grouped into fuel assemblies with 18 fuel plates each (see Figure 4-1) (Holcomb et al. 2012). The fuel assemblies are arranged in a hexagonal lattice with no axial heterogeneity. To make the depletion analysis tractable the fuel geometry was simplified using the RPT method. This methodology was benchmarked against depletion analysis with multigroup explicit grain Monte Carlo model of the AHTR using TRITON with KENO-VI as the neutron transport code and a continuous energy Monte Carlo model of the AHTR using VESTA with MCNP5 coupled to ORIGEN2.2.

SEAU searches for the maximum attainable burnup in a multi-batch fixed fuel core design. SEAU implements a two-tiered solver to explicitly define the maximum burnup equilibrium cycle (Cisneros and Ilas 2012). The first tier is a search for the equilibrium fuel cycle that simultaneously determines the beginning of equilibrium cycle (BOEC) composition. The second tier searches for the maximum discharge burnup by systematically sampling the end of equilibrium cycle (EOEC) $k_{effective}$ as a function of burnup until a burnup is identified that meets the maximum burnup condition of zero excess reactivity at EOEC. This iterative equilibrium analysis search methodology is presented in Figure C-2. SEAU calls SCALE's coupled neutron transport and point depletion analysis utility, TRITON. TRITON uses the KENO-VI code for 238 multigroup neutron transport and the ORIGEN-S code to deplete the fuel.

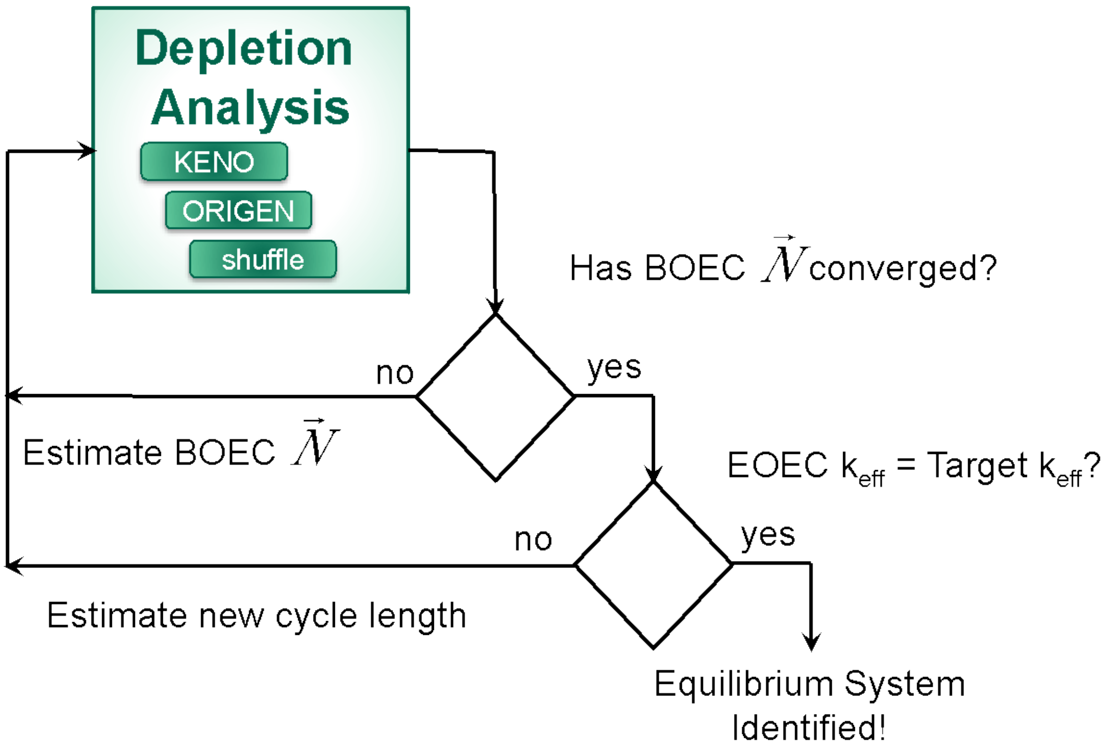

Figure C-2. Algorithm for the Iterative Equilibrium Depletion Search

NLRM was used to perform a parametric study on the fuel design and fuel management scheme of the AHTR. The first step in the NLRM is to generate an mth order polynomial to match the numerical reactivity evolution of the system assuming full-core model with a single batch fuel management scheme. The NLRM expands the linear reactivity model to include higher order terms to increase the applicability beyond those of the LRM; see equation (C-1) (Driscoll, Downar, and Pilat 1990).

$$
\begin{aligned}
\rho(b) &= y^o + y'b + \ldots + y^{(m)}b^m \\
\rho_{EOEC} &= \frac{1}{n}\sum_{i=1}^{n}\rho(b_i^{EOEC}) \\
\rho_{EOEC} &= \frac{1}{n}\sum_{i=1}^{n}\rho\left(\frac{ib_{discharge}}{n}\right) \\
\rho_{EOEC} &= \frac{1}{n}\sum_{i=1}^{n} y^o + y'\left(\frac{ib_{discharge}}{n}\right) + \ldots + y^{(m)}\left(\frac{ib_{discharge}}{n}\right)^m \\
\rho_{EOEC} &= y^o + \frac{y'b_{discharge}}{n^2}\sum_{i=1}^{n} i + \ldots + \frac{y^{(m)}b_{discharge}^m}{n^{m+1}}\sum_{i=1}^{n} i^m \\
0 &= y^o + \frac{y'b_{\max}}{n^2}\sum_{i=1}^{n} i + \ldots + \frac{y^{(m)}b_{\max}^m}{n^{m+1}}\sum_{i=1}^{n} i^m
\end{aligned}
\tag{C-1}
$$

NLRM was used to estimate the maximum attainable burnup in a multi-batch fuel management scheme. Furthermore, it was also utilized to estimate the BOEC reactivity of the AHTR under different decay cooling assumptions to determine whether criticality could be reestablished after “pseudo-online” refueling outage.

C.3 TRITON Depletion Analysis for SmAHTR

SmAHTR is a 125-MWth FHR that uses coated-particle LEU fuel compacted into either cylindrical, annular or plate type fuel compacts (Greene, Holcomb, et al. 2010). These fuel elements are completely immersed in the coolant flowing through 19 fuel channels.

The TRITON depletion sequence was used to perform depletion analysis for the SmAHTR. As stated earlier TRITON couples a transport solver within the SCALE family of codes, KENO-VI, to the point depletion code ORIGEN-S. The baseline cylindrical fuel compact variant modeled as a homogeneous material. This “double-heterogeneous” treatment generates multigroup resonance self-shielding cross sections and preserves the mass of fuel in this homogeneous material.

This framework was utilized to estimate the maximum attainable burnup of the SmAHTR, calculate the excess reactivity at beginning of life, and predict the temperature feedback coefficients for the fuel and the coolant (Ilas, Gehin, and Greene 2010).

C.4 Laser Inertial Fusion Energy (LIFE) Nuclear Control (LNC) for Fusion Fission Hybrid LIFE

The hybrid LIFE blanket (Moses et al. 2010) consists of a spherical laser deuterium-tritium fusion chamber surrounded by a subcritical fission blanket, which multiplies thermal power and breeds tritium for the fusion reaction. The blanket contains a beryllium multiplier layer, a fertile or fissile TRISO pebble fuel layer, and a graphite outer reflector and is cooled by flibe throughout (Kramer et al. 2009). In order to achieve the largest discharge burnup (Fratoni, Kramer, and Latkowski 2010), the fueling scheme is once-through. Therefore, when using fertile fuel, operation is broken into a breeding phase, during which fissile material is bred, a power phase, during which there is sufficient fissile material to maintain full nominal thermal power and net breeding of tritium, and an incineration phase, where remaining heavy metals are transmuted by the fusion neutron source. The lithium enrichment of flibe is the primary control mechanism for subcritical multiplication and tritium breeding rates. The non-equilibrium operation requires temporal resolution of thermal power and tritium production as well as the lithium enrichment necessary to achieve them. The LIFE group built the simulation tool LNC to orchestrate the transport, depletion, and control aspects of operation. Effectively, it is a wrapper program that adds a lithium control layer to the existing transport and depletion abilities of Monteburns, which itself couples neutron transport in MCNP5 with depletion in ORIGEN2.2. The coupling of transport, depletion, and control steps are addressed with an operator split—MCNP5 performs quasi-steady-state transport, ORIGEN2.2 depletes inventories with a constant neutron flux, and LNC adjusts the lithium composition at discrete points in operation (Kramer 2010). Double-heterogeneity of the TRISO pebble fuel is modeled by modeling fuel particles explicitly on regular lattices with MCNP5. This was shown to have a large effect on reaction rates. Pebbles and TRISOs are “chopped” at cell interfaces. Temporal neutron and gamma heating, decay heat, tritium breeding and decay, and structural material DPAs are all simulated within LNC. Spatial dependence of neutron flux and power, reactivity coefficients, and integration with fuel-performance modeling were also studied.

C.5 WIMS8/DIF3D/REBUS for LS-VHTR

The LS-VHTR is an early FHR design based primarily on the Gas Turbine MHR (GT-MHR). The LS-VHTR used cylindrical fuel compacts arranged in the GT-MHR fuel block design but cooled with liquid fluoride salt (Kim, Taiwo, and Yang 2005). Because of the increased heat capacity of flibe, the coolant channels were reduced in diameter from 1.584 to 0.953 cm and the number of active fuel blocks was increased from 102 to 265, increasing the full-core power to 2400 from 600 MWth in the GT-MHR.

An assembly level unit cell was the primary model used for single-batch depletion analysis using REBUS for depletion analysis and WIMS8 for lattice physics. The cross sections used in WIMS8 were generated with its PROCOL module that accounts for the double heterogeneity energy self-shielding effect. These depletion results were extrapolated to determine the maximum discharge burnup in multi-batch fuel management schemes using the linear reactivity model. Additional neutronics studies were performed including: uranium enrichment studies, power density studies, and coolant void reactivity feedback analysis.

C.6 SCALE for the Liquid-Salt-Cooled Pebble Bed Reactor (LSPBR)

Just as the LS-VHTR was based on the design of the GT-MHR, the LSPBR design closely resembles a PBMR with the helium replaced with liquid salt. The LSPBR is a 2500 MWth reactor that utilizes coated particle fuel compacted into solid spherical fuel elements (De Zwaan et al. 2007).

Three frameworks were developed to study the static design of this reactor – a neutronics only model, a coupled steady state analysis capability, and a coupled transient analysis capability.

The neutronics only capability was utilized to perform a salt selection study. This component of the study used the CSAS sequence in SCALE that generated cross sections with BONAMI and NITAWL and performed neutron transport with the Monte Carlo code KENO. The Dancoff factor used in the resonance shielding calculations was derived analytically. This capability was utilized to assess the advantages and disadvantages of using different liquid salts as coolants with respect to neutron economy and coolant void reactivity feedback. Additionally, SCALE was co-opted to generate 2-group cross sections for the deterministic code EVENT.

Steady state and transient calculations were analyzed in this study by coupling the deterministic code EVENT to THERMIX and HEAT respectively. As stated in Chapter 3, the THERMIX thermal fluids code had been previously used to analyze the PBMR. HEAT was coupled with EVENT to model natural convection phenomena in a LOFC transient. This framework was utilized to determine the temperature evolution of the LSPBR during a LOFC transient operating at different power levels. More details about this coupling framework are provided in Chapter 6.

C.7 Summary

Most of FHR neutronics methods developmental work has focused on developing the depletion analysis capability. However, these fuel cycle models have not been integrated with a steady state thermal fluids codes.

There has been one study that coupled a deterministic FHR neutronics model to a thermal fluids code for temperature feedback at steady state analysis and establishment of decay heat removal in a LOFC accident (De Zwaan et al. 2007).

These studies have confirmed the FHR strategy of co-opting existing general-purpose codes. Also, it is promising to see that are no show stoppers have been identified in terms of modeling the neutronics of FHR reactors. A summary of the FHR neutronics methods development studies are presented in Table C-1.

Table C-1. Summary of FHR Neutronics Methods Development Programs

Code	Reactor	Institute	Year
BEAU	PB-FHR	UC Berkeley	2012
SEAU	AHTR	ORNL	2012
TRITON	SmAHTR	ONRL	2010
LNC	LIFE	LLNL	2011
WIMS8/DIF3D/REBUS	LS-VHTR	ANL	2005
SCALE, EVENT	LSPBR	Delft University	2007

Appendix D Neutronics Validation Experiments

VHTRC-GCR-EXP-001 is a draft IRPhEP benchmark that documents experiments that took place in the VHTRC facility in Japan from 1985-1988. The facility was an open-air graphite-moderated critical assembly made up of prismatic particle-coated uranium-dioxide fuel enriched to 2 and 4 weight percent. Control rods consisted of cadmium and stainless steel. Critical configurations were measured at temperature intervals from room temperature up to 200°C. The purpose of the VHTRC facility was to provide validation and an experience base for the HTTR facility.

HTR-PROTEUS-GCR-EXP-001 is a draft IRPhEP benchmark that documents criticality, reactivity coefficient, shutdown worth, kinetics, water ingress, and flux distribution experiments performed at the zero-power PROTEUS facility at PSI, Switzerland between 1992 and 1996. The regular dodecagon core was defined by graphite moderating slabs and cooled with helium. Fuel and moderator pebbles were arranged in two types of regular lattices and a stochastic lattice with packing fractions of 74.05%, 60.46%, and 62%, respectively. Around 9400 uranium kernels enriched to 16.7 weight percent and with 500μm OD were randomly distributed in fuel pebbles. 13 critical configurations varied the ratio of fuel to moderator pebbles, the number of pebbles, and the packing arrangement.

The HTTR-GCR-RESR-001 IRPhEP benchmark documents start-up reactor physics tests at the zero-power HTTR facility in Japan that took place during 1998-1999. The critical configuration, axial flux distribution, reactivity worths, and isothermal temperature reactivity coefficients were measured in the helium-cooled, graphite-moderated, prismatic particle-coated fueled reactor. Uranium-dioxide enrichements varied from 3.4 to 9.9 weight percent and control rods consisted of boron carbide enclosed in alloy 800H. The HTTR-GCR-RESR-002 IRPhEP benchmark documents start-up reactor physics tests for the HTTR facility with an alternate annular loading scheme, which took place 1998-1999. The critical configuration, axial flux distribution, and reactivity worths were measured. The HTTR-GCR-RESR-003 IRPhEP benchmark documents zero-power high-temperature tests that took place 1999-2000. In this experiment, iso-thermal reactivity coefficients were measured between 150°C and 470°C.

The HTR10-GCR-RESR-001 IRPhEP benchmark documents the initial criticality of the HTR-10 facility in China in 2000. Modeled after the AVR, the facility is a 10 MWth helium-cooled, pebble-bed (6cm OD) with graphite moderators and graphite dummy pebbles. Fuel pebbles contained 500μm OD uranium dioxide kernels enriched to 17 weight percent. Pebbles were packed into a regular lattice of 61% packing fraction. Thermal hydraulic and neutronic experiments performed at this facility and the HTTR are the subject of an IAEA international coordinated research project in which the simulation results from ten international groups are compared (IAEA 2003).

The ASTRA-GCR-EXP-001 IRPhEP benchmark is a link to the IEU-COMP-THERM-008 ICSBEP criticality safety benchmarks performed at the ASTRA facility in Russia during 2003-2004. The facility consists of a room-temperature helium-cooled randomly packed bed of 6cm OD graphite pebbles, each containing 2.44g of uranium dioxide in 511μm coated particle kernels, enriched to 21 atom percent. Inner and outer octagonal reflectors were also made of graphite. Five critical configurations were made with different numbers of fuel pebbles and boron-carbide control rod positions. The motivation for these benchmarks was for validation of transport simulations for helium-cooled graphite-moderated high-temperature reactors.

The LEU-COMP-THERM-049 ICSBEP experiment took place in France during 1983-1987 and measured criticality for polyethylene-moderated uranium-dioxide powder at a maximum 5 weight percent. Configurations varied by hydrogen-to-uranium atom ratios (H/U) and the arrangements of various enrichments of fissile materials and a borated stainless steel mock control rod. Configurations 1-4 possessed an H/U of 2 and materials in configuration 18 had an H/U of 2 and 3.

MIX-COMP-THERM-002 experiment, performed between 1975 and 1976 at PNNL, contained zirconium-clad MOX fuel rods arranged in a rectangular array, submerged in water coolant/moderator. Critical configurations consisted of different numbers of fuel rods in varying physical arrangements.

The LR-0 is a 5 kWth reactor facility in the Czech Republic that first went critical in 1982 and has performed international benchmark experiments in the past. The U.S. DOE is highly interested in collaborating with the facility to perform flibe reactivity experiments for FHR validation. Experts are still making recommendations for experiments, so the details are not finalized and the timescale is uncertain.

Texas A&M University houses the 5 Wth AGN-201M nuclear reactor facility built in 1957. It contains an experiment port for inserting reactivity samples. Dr. Radek Skoda is designing a pile-oscillator device for determining reactivity worth of samples. Work is currently being done to determine if such an experiment would be beneficial.

Through the IRPhEP, 160 reports and other archival information are available for the AVR, a German 15 MWe helium-cooled pebble-bed reactor that was built in the late 1960’s and operated for 21 years. While the archive doubtlessly contains an abundance of useful information, it is not clear how much can be used for validation. IRPHE-HT-ARCH-01 is an archive of numerous documents for experiments relevant to HTR designs, including CESAR, OTT, Gulf, MARIUS, KAHTER, and other facilities. IRPHE-DRAGON-DPR is an archive of similar documentation for the DRAGON reactor.

The Chinese Academy of Sciences is designing and constructing a 2-MWth, pebble-fueled, fixed-lattice, flibe-cooled experimental reactor, called the Thorium Molten Salt Reactor-Solid Fuel (TMSR-SF). This reactor will provide high-quality sub-critical, zero-power critical, and low-power critical neutronic test data.

Archival reports can be found for the MSRE, an epithermal molten fluoride-salt reactor fueled with ^{239}Pu, ^{235}U, and ^{233}U that operated from 1965 to 1969. Among other tests, criticality, reactivity worth, temperature reactivity coefficient, and dynamic tests were performed at zero power (Prince et al. 1968). The degree of quality assurance and uncertainty estimation employed during the experiments is not clear.

Appendix E Current Neutronics/Thermal Hydraulics Coupling Capabilities

E.1 DALTON-THERMIX Coupling for the HTR-10

The DALTON-THERMIX code system has been developed for safety analysis and core optimization of pebble-bed reactors. The code system consists of the three-dimensional diffusion code DALTON, which is coupled to the existing thermal hydraulic code THERMIX. These codes are linked to a database procedure for the generation of neutron cross sections using SCALE-5 (Boer et al. 2010).

Before the thermal hydraulic and neutronic calculations are started, a neutron cross-section library is created as a function of the fuel and moderator temperatures and the xenon concentration. These cross-sections are also dependent on the local fast and thermal buckling. For the simulation of the HTR-10 transients, both a point-kinetics model with externally calculated reactivity coefficients and a 2-D model in DALTON with space and temperature-dependent neutron cross-sections have been used. The procedure uses several modules of the SCALE-5 code system in order to take into account the double heterogeneity of the fuel.

The DALTON code can solve the 3-D multigroup diffusion equations on structured grids (x-y-z or r-z-θ coordinates). Spatial discretization is performed using a second-order accurate finite volume method. A 2-D (r-z) model is used in the DALTON code to calculate a 2-D zone-averaged power profile using neutron cross-sections that have been obtained through linear interpolation using the local temperature and xenon concentration. In the case that the point-kinetics equations are used, a fixed power distribution is scaled to the calculated total power.

The use of the THERMIX code is discussed in Appendix A. The power profile calculated by DALTON is used in THERMIX to calculate the temperature profile in the reactor at the new time point.

For validation purposes, calculation results of normal operation, a LOFC transient, and a control rod withdrawal transient without scram have been compared with experimental data obtained in the HTR-10. The code system has been applied to the 400-MWth PBMR design, including the analysis of three different LOFC transients. These results were verified by a comparison with the results of the existing TINTE code system. It was found that the code system is capable of modeling both small (HTR-10) and large (PBMR) pebble-bed reactors and therefore provides a flexible tool for safety analysis and core optimization of future reactor designs, including, potentially, the FHR.

E.2 PARCS-AGREE Coupling for Pebble-Bed Gas-Cooled High Temperature Reactors

The PARCS-AGREE code system has been developed at University of Michigan for safety analysis and core optimization of pebble-bed gas-cooled high temperature reactors.

Future collaboration is expected between University of Michigan and the FHR IRP to adapt this code system to the coupled neutronics and thermal hydraulics modeling of the FHR.

PARCS is a US NRC-approved three-dimensional reactor core simulator which solves the steady-state and time-dependent, multigroup neutron diffusion and SP3 transport equations in orthogonal and non-orthogonal geometries (Downar, Xu, and Seker 2011). AGREE is a 3-D thermal hydraulics code that solves the energy, mass and momentum balance equations for both steady-state and time-dependent analyses. The presence of the heat source in the solid medium results in a considerable temperature gradient. Therfore, agree solves separate energy equations for each medium (Seker and Downar 2009). The coupling scheme between these two codes is presented in Figure E-1.

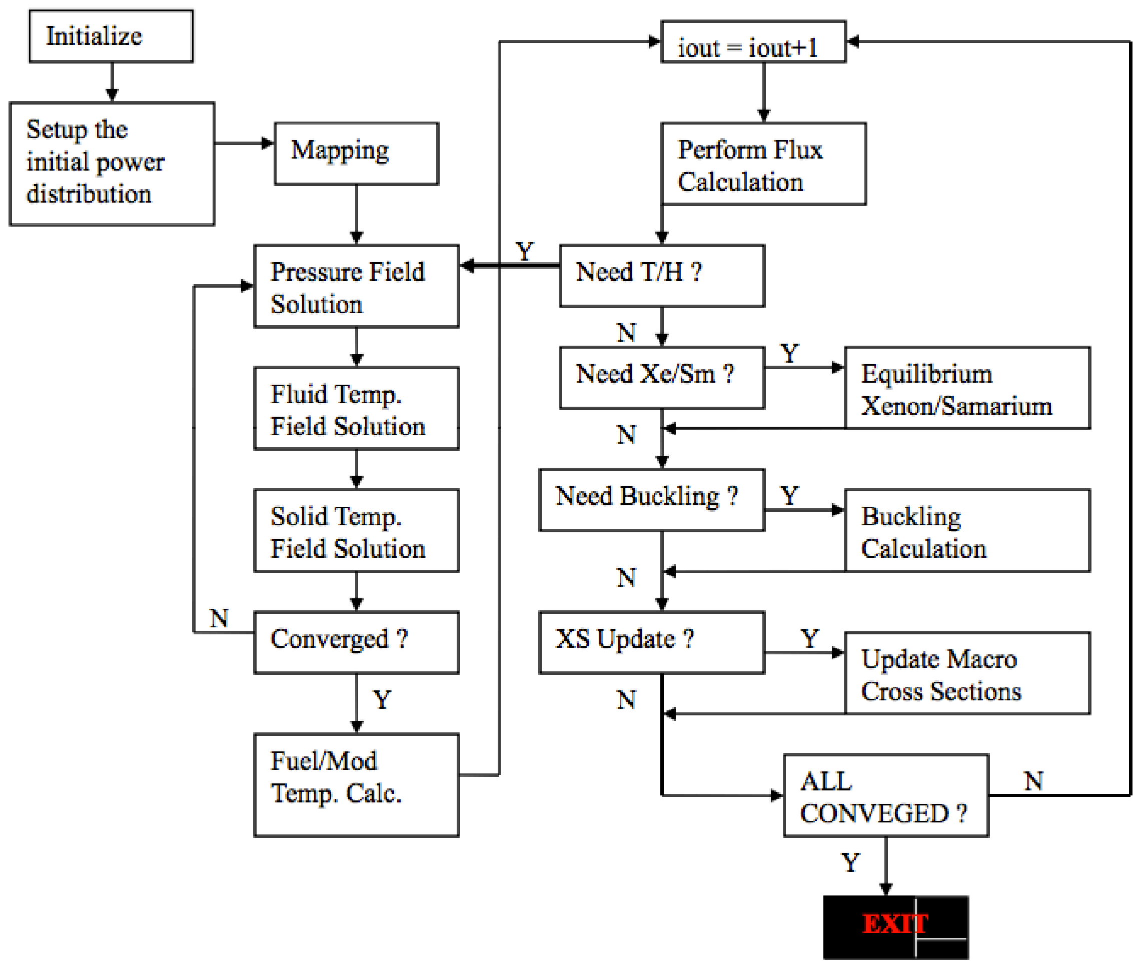

Figure E-1. PARCS-AGREE Coupled Calculation Flow Chart (Seker and Downar 2009)

E.3 EVENT-THERMIX Coupling for the LSPBR

To date, there has only been one study that coupled a deterministic FHR neutronics model to a thermal fluids code for temperature feedback at steady-state analysis and establishment of decay heat removal in a LOFC accident. Coupled neutronics and thermal hydraulic calculations were performed to obtain the steady-state power distribution and the corresponding fuel temperature distribution. Calculations were performed to investigate the decay heat removal capability in a protected LOFC accident (De Zwaan et al. 2007).

To examine the behavior of the LSPBR during normal operation, steady-state calculations were performed with a coupled neutronics and thermo-hydraulics code system. The 3-D neutron transport code EVENT was coupled with a modified version of the THERMIX code. Two-group temperature-dependent cross-sections were generated with the SCALE code system. The steady-state solution of a core configuration is found by iteratively transferring the power distribution from EVENT to THERMIX and returning the temperature distribution to EVENT (Figure E-2). With THERMIX, temperature profiles in the fuel and the coolant, the velocity field of the coolant and the pressure field are calculated. The pressure drop over the reactor and heat fluxes can also be calculated. The neutronics code EVENT is able to calculate the neutron flux density and k_{eff} in the LSPBR core by solving an eigenvalue problem for the particular reactor shape.

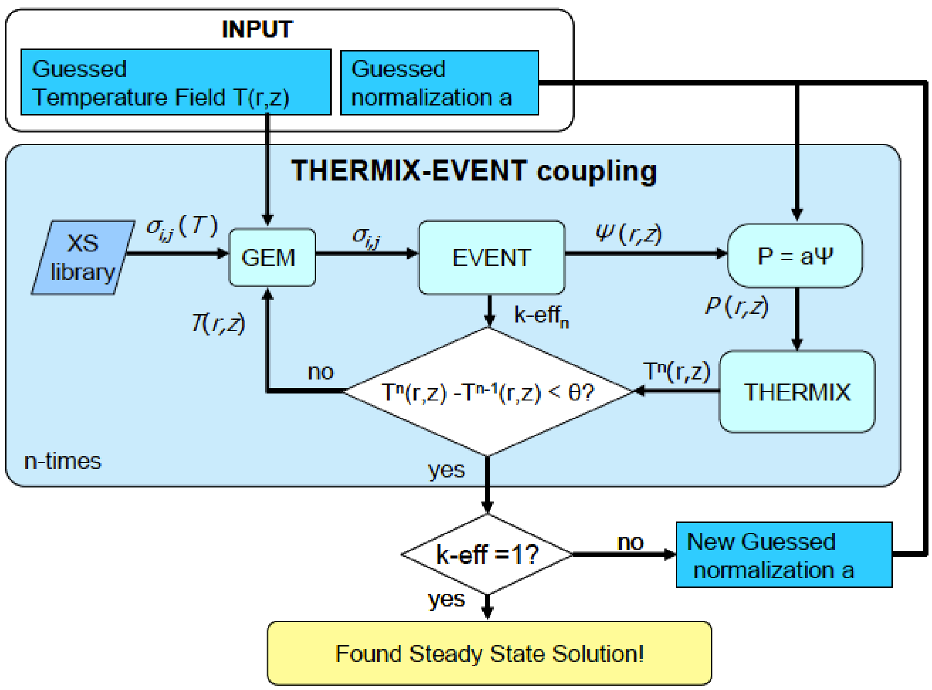

Figure E-2. Scheme of Coupled THERMIX and EVENT Calculation to Find Steady State Solution

Although THERMIX is a standard code to handle thermal hydraulics calculations of gas-cooled pebble-bed reactors, it is not suitable for decay heat removal calculations in the LSPBR. In THERMIX the interaction between the solid material and the coolant is programmed between two numeric fields, the convection field and the solid material field, as shown in Figure E-3.

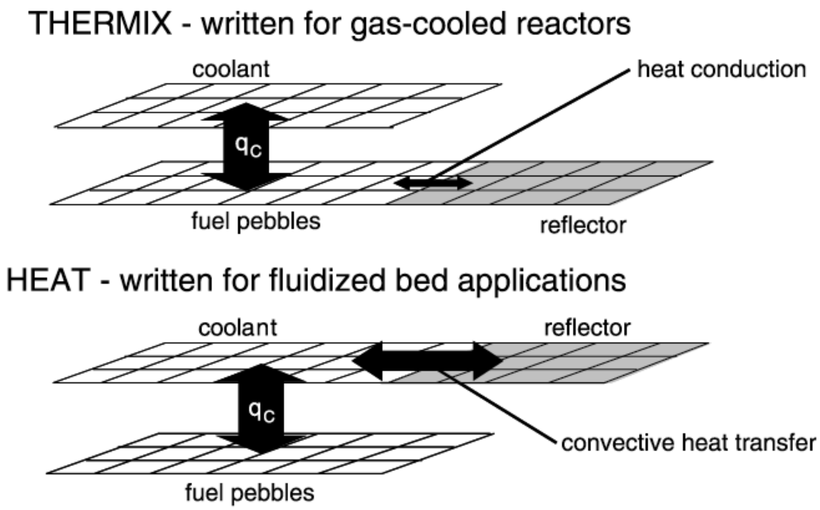

Figure E-3. Difference Between the Thermal Hydraulics Code THERMIX and HEAT

In both codes there is interaction between the convection grid and the solid grid through heat sources and sinks in the core. In THERMIX the heat transfer to the reflector is modeled by conduction from the core to the reflector, while in HEAT the heat is transported from the coolant to the reflector by convection heat transfer (De Zwaan et al. 2007).

Heat can be transferred from the center mesh of the core to the outside mesh of the core by natural convection but from there it must be transferred out of the core by conduction (in the solid material calculation). In the LSPBR, the convective heat transfer from the coolant to the reflector is the main heat transport mechanism in decay heat removal problems, as is the case between the coolant and heat exchangers in the FHR. Therefore, to examine the temperature distribution during a LOFC with scram, the decay heat calculations were performed with the code HEAT (Lathouwers and Bellan 2001). The code HEAT can solve time-dependent natural circulation problems in packed beds and was originally written for fluidized beds in chemical applications (Lathouwers and Bellan 2001), but has been modified for several other applications, like the decay heat removal in the fluidized bed nuclear reactor (Agung et al. 2006). The code HEAT has the benefit that the convective coolant field is connected to the solid reflector field (as shown in Figure E-3) so that convective heat transfer between the coolant and the reflector is taken into account. The solid conduction heat transfer between the pebble bed and the reflector is neglected in this code.

Because the LSPBR shares the fundamental phenomenology of passive decay heat removal through natural circulation, which is not the case for gas-cooled high temperature reactors, this code system seems to be more readily applicable to the FHR design.