

## FHR Code Benchmarking White Paper, Integrated Research Project -2, Workshop 1



## Fluoride-Salt-Cooled, High-Temperature Reactor Code Benchmarking White Paper

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



## Preamble

The University of California, Berkeley; Massachusetts Institute of Technology; University of Wisconsin, Madison; University of New Mexico; Georgia Institute of Technology; The Ohio State University; and Texas A&M University, are collaborating to conduct a series of code-to-code comparison and code validation exercises under two U.S. Department of Energy-sponsored Integrated Research Projects (IRPs) to develop the technical basis to design and license fluoride-salt-cooled, high-temperature reactors (FHRs).

The IRPs hosted a FHR Code Benchmarking expert workshop March 12-13, 2015, in Berkeley, California, to review code benchmarking needs for FHRs and to obtain advice from experts on best practices for code benchmarking. Experts from Oak Ridge National Laboratory, Idaho National Laboratory, the Shanghai Institute of Applied Physics, the Ulsan Institute of Science and Technology, and the IRP universities participated.

One of the key conclusions from the workshop was the recommendation to set up smaller working groups to develop plans and coordinate benchmarking activities in three code benchmarking areas: neutronics, thermal hydraulics, and materials chemistry, transport, and activation. Relatively frequent working group meetings were recommended, via videoconferencing or meetings co-located with technical meetings, as this is found to be the best practice in previous benchmarking exercises. The full IRP workshops, when held on an approximately annual basis, should include a day for breakout meetings by each of the working groups, in addition to a day for the full IRP meeting.

This report summarizes results from the workshop, and recommends future IRP activities.

# **Executive Summary**

Since the original concept of fluoride salt cooled, solid fueled high temperature reactors (FHRs) was first proposed in 2002 [1], substantial progress has been made in understanding the neutronics, thermal hydraulics, and materials issues posed by this technology. These studies have found that FHRs are likely to have high levels of intrinsic safety, enabled by the high volumetric heat capacity and intrinsically low pressure of fluoride salt coolants, and by the very large thermal margins, exceeding 700°C, to fuel damage during transients and accidents.

Given these attributes, in the United States significant effort has been made to develop the scientific and technical basis to design and license FHRs, including work to develop preconceptual FHR designs, as illustrated in Fig. P-1, to construct separate effect and integral effect test facilities to validate thermal hydraulics models, and to test FHR structural materials in static corrosion tests both in and out of reactors. In China, rapid parallel progress is underway in the Thorium Molten Salt Reactor (TMSR) program to construct and run salt loops and to design a 10-MWt FHR test reactor, the TMSR-SF1, as well as a 2-MWt, electrically heated TMSR-Simulator.



Fig. P-1. Four FHR preconceptual designs developed by ORNL and UC Berkeley

In 2012, the University of California, Berkeley; Massachusetts Institute of Technology; and University of Wisconsin, Madison, conducted a series of expert technical workshops to assess key areas important to the design and licensing of FHRs. These workshops identified major design options and subsystems for FHRs, identified and reviewed key FHR phenomenology, identified key licensing basis events, and recommended a range of general-purpose modeling codes that can be adapted to use for simulation of FHR neutronics, thermal hydraulics, and structural mechanics.

To be used in safety analysis reports for license applications to the U.S. Nuclear Regulatory Commission, simulation codes (referred to as "evaluation models, or EMs") must be validated by comparison with appropriate separate effect and integral system test data, and by benchmarks with other codes, as described in detail in the NRC Regulatory Guide 1.203 [2]. The Guide states,

"...an assessment should be made regarding the inherent capability of the EM to achieve the desired results relative to the figures of merit derived from the [General Design Criteria]. Some of this assessment is best made during the early phase of code development to minimize the need for later corrective actions. A key feature of the adequacy assessment is the ability of the EM or its component devices to predict appropriate experimental behavior. Once again, the focus should be on the ability to predict key phenomena, as described in the first principle. To a large degree, the calculational devices use collections of models and correlations that are empirical in nature. Therefore, it is important to ensure that they are used within the range of their assessment." (pg. 4)

This report lays out and prioritizes needs for EM assessment for FHRs, and recommends an approach to code benchmarking efforts during the 3 years of upcoming IRP research. The recommended approach involves forming three working groups, to establish and conduct EM benchmarking exercises in three key areas of FHR phenomenology: neutronic; thermal hydraulics; and materials corrosion, activation, tritium and transport (MATT).

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# **Acronyms and Abbreviations**

AHTR – Advanced High-Temperature Reactor ANL – Argonne National Laboratory ANS – American Nuclear Society ARE – Aircraft Reactor Experiment AOO – anticipated operational occurrences ASME – American Society of Mechanical Engineers ATWS – anticipated transient without scram BDBE – beyond design basis event BPV – Boiler and Pressure Vessel (Code) CFR – U.S. Code of Federal Regulations CFRC - carbon fiber-reinforced composite CTF – Component Test Facility DOE – U.S. Department of Energy DRACS - Direct Reactor Auxiliary Cooling System EAB – exclusion area boundary EDMG - Extensive Damage Mitigation Guidelines FHR – fluoride-salt-cooled, high-temperature reactor FHTR – FHR Test Reactor GDC – NRC General Design Criteria GT-MHR – Gas-Turbine Modular Helium-Cooled Reactor H2TS – hierarchical two-tier scaling (analysis) HTGR – high-temperature gas-cooled reactor HVAC - heating, ventilation, and air conditioning IRP - Integrated Research Project LBE – licensing basis events LMFBR - Liquid Metal Fast Breeder Reactor LMR – liquid metal reactor LOFC – loss of forced circulation LOHS – loss of heat sink LS-VHTR – Liquid Salt Very High-Temperature Reactor LWR – light-water reactor MSBR - Molten Salt Breeder Reactor MSR – molten salt reactor MSRE - Molten Salt Reactor Experiment NGNP - Next Generation Nuclear Plant NRC – U.S. Nuclear Regulatory Commission ORNL – Oak Ridge National Laboratory PASSC - Plant, Areas, Systems, Subsystems, and Components PB-AHTR – Pebble Bed Advanced High-Temperature Reactor PBMR - Pebble Bed Modular Reactor PCU – power conversion unit

PIRT – Phenomena Identification and Ranking Table

PRA – probabilistic risk assessment

PWR – pressurized-water reactor

SAMG – Severe Accident Management Guidelines

SAR – Safety Analysis Report

SDC – Safety Design Criteria

SFR - sodium-cooled fast reactor

Sm-AHTR - small modular Advanced High-Temperature Reactor

S-PRISM – Super-Power Reactor Innovative Small Module

SS – stainless steel

SSCs - systems, structures, and components

TEDE – total effective dose equivalent

TLRC – Top-Level Regulatory Criteria

TRISO – tristructural-isotropic

UCB – University of California, Berkeley

# **1** Introduction

This chapter serves as both an introduction to the structure and content of this whitepaper as well as an introduction to the current state of international fluoride salt cooled, solid fuel high temperature reactor (FHR) development. This white paper builds on the conclusions and results from the first FHR Integrated Research Project (IRP-1) funded at the University of California, Berkeley (UCB), the Massachusetts Institute of Technology (MIT), and the University of Wisconsin, Madison (UW), by the U.S. Department of Energy.

### **1.1 White Paper Outline**

This white paper covers a variety of topics important to the benchmarking of simulation codes for modeling FHRs. The purpose of Chapter Two is to describe current best practices for code benchmarking efforts. Key previous and current benchmarking efforts related to nuclear energy and reactor technology are reviewed in Section 2.1 and key best practices are distilled in Section 2.2. Section 2.3 defines the important problems to be addressed in the new IRP benchmarking campaign, to enable validation of these simulation codes for licensing new reactor technologies.

Chapter Three provides a review of key experimental facilities and data that can be used in benchmarking efforts FHR simulation. The facilities and data are separated into the three distinct technical areas in Sections 3.1 through 3.3. Also included in this chapter is Section 3.4, which is a discussion of the integration of data produced in the FHR benchmarking effort into the ORNL NE-KAMS data repository and management system.

Chapter Four provides a discussion of candidate benchmarking problems in the three technical areas. These candidate benchmarking problems represent possible exercises to be completed in this IRP based on the best practices and licensing goals from Chapter Two and the relevant experimental facilities and data from Chapter Three. This is a key outcome of this workshop.

Chapter Five is a recommendation of how to most effectively structure the new FHR IRP (IRP-2) to complete this benchmarking effort. Workshop participants recommended that three working groups, each focusing on one of the three technical areas, be formed and work on the benchmarking exercises in their area throughout the three years of IRP-2. Future workshop organization is discussed but detailed planning should be done after the three working groups are created.

### 1.2 Status of U.S. and International FHR Development Activities

FHRs have the long-term potential to economically and reliably produce large quantities of baseload and peaking power while employing full passive safety. Due to these characteristics, FHR research in the U.S. currently benefits from multiple DOE initiatives and funding that cover: <sup>7</sup>Li Cost, Tritium Management, Structural Ceramics, Safety and Licensing, and Fuel Cost and Qualification. In addition DOE as initiated an effort to consider building a new test reactor. Three point designs are underway with one of those designs being a Fluoride-salt-cooled High-

temperature Test Reactor. In 2011 the DOE funded one FHR related IRP comprised of MIT, UCB, and UW as IRP partner universities. In 2014 the DOE awarded funding for two new, separate FHR IRPs, one led again by MIT with the addition of the University of New Mexico, Albuquerque (UNM) and the other led by Georgia Tech (GT) and including Ohio State University and Texas A&M University. In addition to U.S. government support for university research, utilities and vendors (e.g. Southern Company, Westinghouse, Areva) have signaled interest in research activities related to FHRs in the U.S.

Furthermore, a large number of institutions outside the U.S. are conducting FHR related research. Countries with significant research projects are: Australia, China, the Czech Republic, England, France, India, Italy, Japan, Korea, and Russia as well as other EU member states that support FHR research as part of their MSR research and development strategies.

## 1.3 FHR IRP-1 Overview: Results from the First FHR IRP and Next Steps

The driving objective of IRP-1 was to develop a path forward to a commercially viable saltcooled solid-fuel high-temperature reactor with superior economic, safety, waste, nonproliferation, and physical security characteristics as compared to LWRs. This primary objective was broken down into three goals: (1) an economic goal of increasing plant revenue 50% to 100% relative to base-load nuclear power plants while keeping capital costs similar to LWRs; (2) an environmental goal of producing enabling technology for a zero-carbon nuclearrenewable electricity grid, with particular emphasis on dispatchable electricity capability that can avoid revenue collapse; and (3) a safety (and social) goal of no major fuel failures in the extreme case of a beyond-design-basis accident. The steps taken in IRP-1 in pursuit of these goals were the development of a commercial strategy and market applications for FHRs (MIT); the development of a commercial reactor point design (UCB); the development of FHTR goals, strategy, and design (MIT); and technology development by all IRP partner universities. IRP-1 has built a strong foundation for the viability and utility of FHRs in today's electricity market, but much is still to be done to fully develop the understanding and technology for FHR commercialization. The driving objective of IRP-2 is to continue the technology development from IRP-1 with a focus towards meeting licensing requirements that are necessary for eventual commercialization.

## 1.4 Key Results from IRP-1 Workshops: FHR Phenomenology, Licensing Basis Event Identification, and Applicable Modeling Codes

Although FHRs draw upon previous experience and technology development from light water reactor (LWR), sodium fast reactor (SFR), and high-temperature gas reactor (HTGR) technology development, one of the major findings of IRP-1 is to recommend that benchmarking, including both code-to-code comparisons and validation with experimental data, be performed to demonstrate that existing and new analysis codes can be applied to FHR safety analysis and design efforts.

# 2 Benchmarking Best Practices

Determining the best practices and overall strategy is the first step in beginning a new benchmarking campaign. This chapter reviews best practices for code benchmarking, obtained from previous benchmarking efforts, which are relevant to benchmarking for FHR simulation.

# 2.1 Related Benchmarking Efforts

A thorough literature review of previous benchmarking activities is key to understanding the fundamental steps of benchmarking and capturing the best practices for success. This section provides an overview of selected previous benchmarking efforts that are related to performing benchmarking studies for FHRs in some way and that were particularly informative of benchmarking best practices.

### 2.1.1 Evaluation of High Temperature Gas Cooled Reactor Performance: Benchmark Analysis Related to the PBMR-400, PBMM, GT-MHR, HTR-10 and the ASTRA Critical Facility

In 2013 the IAEA published a comprehensive review (e.g., TECDOC) that discusses a number of benchmarking exercises that have been performed in various IAEA member states (China, France, Germany, Indonesia, Japan, the Netherlands, the Republic of Korea, the Russian Federation, South Africa, Turkey, the United Kingdom and the United States of America) [3]. The benchmarking efforts followed procedures that may also be applicable for future FHR benchmarking exercises.

Relevant experiments were conducted and documented to understand thermal hydraulic and neutronic (also coupled) behavior of whole reactor systems or relevant parts of reactor systems. Later, or in some cases prior to the actual experiments, codes were developed to model the experimental results so that these codes could be validated with relevant experimental data. In addition, various code-to-code comparisons without the support of experimental data have also been performed to verify that the codes were giving consistent and reasonable results. These aspects of the process of verification and validation (V&V) are key elements of code benchmarking.

Since the IAEA is an international organization with various member states with national nuclear safety regulation agencies that can have differing safety requirements, these IAEA-sponsored benchmarks are not focused to fulfill the requirements of a particular national regulating body but instead try to create a broader understanding of reactor safety characteristics. For this reason, for a recent HTGR benchmarking project the IAEA specified the following fields that the project was intended to cover (IAEA 2013, p.12):

- The neutronic physics behavior of the HTGR core;
- Fuel performance and fission product behavior;
- The ability of the HTGR to dissipate decay heat by natural transport mechanisms;
- The design and evaluation of the HTGR-related heat utilization systems;

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- Evaluation of the HTGR performance: Benchmark analysis related to initial testing of the High Temperature Test Reactor (HTTR) and HTR-10.

These overall goals were defined in coordinated research projects related to the developments of the PBMR from the beginning of 2000 to now conducted at IAEA over a period of several years. Besides adding to the understanding of the safety characteristics of HTGRs, the coordinated research projected supported code development that may be useful for future reactor licensing efforts. The following objectives were provided by the projects' participants:

- Validation of analytical codes and performance models to actual operating conditions of HTGRs;
- Independent evaluation of benchmark problems for use in the Research and Development (R&D) and safety programs for the HTR-10, PBMR, GT-MHR and the ASTRA facilities;
- Investigation of analytical codes and models associated with the proposed GT-MHR and PBMR400 gas turbine plants; Investigation of code-to-experiment benchmarks associated with the three-shaft gas turbine micro model (PBMM).

The benchmarking efforts were documented in a 690-page report, along with numerous additional scientific reports and papers that describe the obtained results which are summarized in the document itself as following:

- Reactor physics benchmark analysis of the ASTRA critical facility with respect to development of the PBMR-400. These benchmarks include core height for criticality, control rod worth and related differential reactivity and interference coefficients, and investigation of critical parameters for differing heights of the pebble bed reactor.
- Code comparison benchmark problems of cell calculations (K<sub>inf</sub> and isotope content vs. burn up) and reactor physics of control rod worth and isothermal reactivity coefficients for the GT-MHR fuelled with plutonium.
- Code-to-experiment benchmark analysis related to the testing program of the HTR-10 plant including steady state temperature distribution with the reactor at full power, loss of primary coolant flow without scram, and control rod withdrawal without scram.
- Neutronics and thermal hydraulic code comparison benchmarks for the PBMR-400.
- Micro model investigation of steady state and transient operating conditions for a threeshaft gas turbine power conversion system.

As with many other IAEA reports, the TECDOC is freely available online<sup>1</sup> and may be used as a general guideline for similar benchmarking efforts related to a similar reactor system such as the FHR.

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<sup>&</sup>lt;sup>1</sup> http://www-pub.iaea.org/MTCD/Publications /PDF/TE-1694\_web.pdf

#### 2.1.2 CASL Benchmarking with WBN1: VERA-CS Validation Plan

The Consortium for Advanced Simulation of Light Water Reactors (CASL) is an Energy Innovation Hub established in 2010 by the U.S. Department of Energy to, "provide modern analysis tools that reliably model the effects of multiple processes occurring simultaneously inside reactor cores, thereby predicting core behavior and helping to improve operational/safety performance in light water reactors" [4]. Part of this overall mission is to develop a collection of methods and software (M&S) tools called the Virtual Environment for Reactor Applications (VERA) which also contains a core simulator component, VERA-CS. VERA-CS is meant to provide a model of pressurized water reactor (PWR) cores with a high degree of flexibility in its applications to parallel the capabilities of industry core simulators. Industry reactor core simulators are typically licensed by the U.S. NRC and as such go through a rigorous process of validation. Similar validation activities are thus considered necessary for VERA-CS to prove its credibility, and a detailed validation plan has been developed [5].

A critical piece in formulating the validation plan for VERA-CS was the development of a VERA-CS validation assessment matrix given in Figure 2-1. The VERA-CS validation assessment matrix compares the required capabilities, features, and application range of VERA-CS on the left of the matrix with proposed validation activities shown across the top of the matrix. In this way, all capabilities are covered directly or indirectly by a least one activity. Holes in this matrix can then be addressed in more detailed validation of individual physics capabilities elsewhere. The matrix represents an effort to cover all possible validation possibilities; in practice, due to budget and time limitations, the minimum set of validation activities to provide confidence in VERA-CS reliability and accuracy will be prioritized. In Figure 2-1, in general, the activities move from highest to lowest priority left to right for each component.

The Watts Bar Nuclear Plant in Spring City, Tennessee, owned by TVA, is a CASL core partner and was selected as CASL's "Physical Reactor" for the initial benchmarking exercises. Unit 1 was the most recent commercial nuclear power plant to come online and the completion Unit 2 will cause Unit 2 to take Unit 1's place in this designation. The startup of Watts Bar Nuclear Unit 2 will provide very high quality instrument and test data for startup with a clean core for VERA-CS validation exercises [5].

The clean startup data from Unit 2 is of course valuable for validation of VERA-CS, but is one experimental data set among many in the scope of LWR operations, including startup. For FHR modeling and simulation, a clean startup will necessarily be the first experimental data set of its kind and of any reactor operations data sets in the FHR design space as no FHR has been built to date. Understanding and adapting the validation plan for VERA-CS of Watts Bar Unit 2 is therefore very valuable for FHR validation plans, especially with the completion of the SINAP TMSR-SF1 test reactor in the relatively near future.

### 2.1.3 VHTR Benchmarking Efforts

Various VHTR benchmarking studies were conducted is the US in support of the Next Generation Nuclear Plant (NGNP) project (e.g. [6]–[8]). These documents may be of particular interest for future FHR benchmarking as they are (1) publicly available and (2) consider the licensing requirements of the NRC.

## 2.2 Key Lessons from Previous Efforts

Four key lessons were identified from previous benchmarking exercises:

- 1) Define purpose
- 2) Compose a mature benchmark
- 3) Secure funding
- 4) Motivate participation/participants.

These key lessons were identified as a result of an international benchmarking effort led by the IAEA and may not all be applicable to the benchmarking efforts within IRP-2. Nevertheless, it is believed that it is worthwhile to briefly discuss them here.

The purpose of the benchmarking exercise may be defined thoroughly before the actual efforts begin to assure that the demands of all participants can be met. The purpose may be purely scientific or more pragmatic in a way that it identifies the biggest licensing issues that need to be addressed in order to receive the approval for construction from the associated licensing body. Resulting from these purposes it should be investigated whether or not challenges such as licensing issues can be addressed with currently available modeling tools or if new modeling tools need to be developed, and if that is the case, if these new modeling tools require additional experimental validation or if code-to-code comparisons with existing codes would be sufficient. Needless to say the uncertainties of all these efforts should be taken into account.

In a next step, a set of mature benchmarking exercises should be composed. Composing a mature benchmark that provides the right amount of data but does not limit the participants' ways of solving the exercises by assuming that certain tools will be used is an art form in itself. In reality, designing benchmarking exercises is a continuous process in which benchmarking participants give feedback and provide input to

- Correct errors
- Clarify
- Point out missing data
- Decode method specific data.

The benchmarking exercises should be kept as simple as possible to allow a wide range of participants to join the benchmarking efforts.

During the whole benchmarking efforts funding needs to be secured to allow continuous progress and provide certainty about the seriousness of the project.

Lastly the participation of benchmarking participants needs to be actively motivated. It was found that scientific publications greatly attract and motivate participation in benchmarking efforts.

																	tion Ac																
	Operating Power Plants						Critical Experiments										Post-Irradiation Exams						CE Monte Carlo										
Capabilities	Watts Bar	BEAVRS	Catawba	McGuire	Westinghouse 3-Loop	Krsko	B&W-Type	CE-Type	B&W	Helstrand	KRITZ	DIMPLE	VENUS	PEN/MB-01	RPI	SPERTIII	Strawbridge & Barry	axton	CREOLE	EPICURE	CAMELEON	crocus	AERI TCA	CSBEP	Catawba MOX LTAs	Three Mile Island	MALIBU	Robinson	Calvert Cliffs	Pin-by-Pin Fission Rates	ntra-Pin Distributions	Depleted Isotopics	Misc. Applications
PWR Types	>	-	0	2	>	×	-	0	-	I	×		>	=	<u>~</u>	S	S	S	0	<u> </u>	0	0		<u> </u>	0		2	<u>~</u>	0	<u> </u>			2
Westinghouse 4-Loop	x	x	x	x																					x					x			
Westinghouse 3-Loop	^	^	^	^	x								x												^			x		^			
Westinghouse 2-Loop				-	^	x							^															^		x			
Babcock & Wilcox (B&W)			-	-		^	x																			x				^			
Combustion Engineering (CE)				-	-		^	x							x											^			x				
Fuel Assembly Types								^							^														^				
17x17	x	x	x	x	x				x										x						x					x	x	x	
16x16	^	^	^	^	^	x			^										^						^					x	^	^	
16x16 CE	-			-		^		x	x						x															^			-
15x15	-				x			^	^						~												x	x					
15x15 15x15 B&W	-				^		x		~																	x	^	^					
	_			-			X		X																	X							-
14x14 CE	_			-				X							X														X				-
Mixed Oxide Fuel (MOX)			x								x		x					x	x	x					x		x						
Burnable Poison Types																																	
Pyrex	X	X	X	X	X	X			X	_			_							x										X			-
IFBA	X		X	X	X	X																			X					X			
WABA	x		X	X	X																				X					X			
Solid B4C-AL2O3					_		x	X																	X	X			x				
Gadolinia					_		x		x				X							х	х		x			X	x						
Erbia								X							X																		
Control Rod Types																																	
AIC	X	X	X	X	X	X	X		X					X				х		x	x					X				X			
B4C	X		X					X	X					X						x	x	x											
Hybrid	x		X																						X					X			
Gray	_						X														х					X				X			
Hafnium					X																												
Incore Instrument Types																																	
Moveable	X	X	X	X	X	X																			X					X			
Fixed	x						х	X	X																	X							
Radial Reflector Types																																	
Thin Baffle	X	X	X	X	X	X	X	X				X	X												X	X				X			
Thick (Heavy) Shroud																																	X
Physics Components																																	
Neutron Transport	x	X	X	X	X	X	х	X	X	X	X	X	X	X	X	X	х	х	х	х	х	х	х	X	X	X	X	X	X	X	X	X	X
Gamma Transport																																	X
Coolant Density Feedback	X	X	X	X	X	X	х	X			X								х				х		X	X	X	X	X	X			
Fuel Temperature Feedback	X	X	X	X	X	X	х	X			X								х				x		X	X	X	X	X	X	X		
Isotopic Depletion	x	X	X	X	X	X	х	X																	X	X	X	X	X		X	X	
Xenon Concentration	x	X	X	X	X	X	х	X																								X	
Shutdown Decay	x	X	X	X	X	X	X	X																	X	X	x	X	X				
Physics Results																																	
Reactivity	X	X	X	X	X	X	х	X	X		X	X	X	X	X	X	x	x	х	X	х	х	x	x	х					X	X	X	
Assembly Power Distribution	x	x	X	X	X	X	х	X																	х					x			
Pin Power Distribution									x		X	х	X	х	X			х	х	х	х									x	X	X	
Intra-Pin Power Distribution																															X		
Pin Burnup Distribution																									х	x	x	x	x		x		
Intra-Pin Burnup Distribution																													X		X		
Incore Instrumentation Response	x	x	x	X	X	x	х	x	x				x						х						x	x							
Excore Instrumentation Response			X	X	-							x	X																				x
Control Rod Worth	x	x	x	X	x	x	x	x	x									х		х	x	х			x					x			
Temperature Coefficient	x	x	x	X	X	x	x	x			x			x					x				x		X								

Figure 2-1. VERA-CS Validation Assessment Matrix [5]

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## 2.3 Benchmarking Goal Considerations

It is important to establish the goals of benchmarking in general, for the benchmarking of the FHR proposed by this white paper, and how to balance these goals with the best practices developed above to optimize the outcome using the limited time and resources available to the IRP-2. Regulations and licensing concerns are significant challenges during the commercialization of any reactor, and are therefore significant goals of IRP-2 efforts.

U.S. NRC Regulatory Guide 1.203 provides guidance on requirements for transient and accident analysis models [2]. Specifically, the Evaluation Models Development and Assessment Plan (EMDAP) is a systematic process for developing evaluation models for the analysis of transient and accident behavior of reactors. The EMDAP suggests using existing general-purpose codes to support development, design, and licensing of reactor technologies. Development and application of more than one code, preferably by different research groups, is also encouraged. The EMDAP provides good rationale for performing benchmarking studies for FHR technology, and will be used to guide the benchmarking efforts. This should simplify licensing challenges in the future.

The earlier FHR IRP-1 has put considerable effort into developing experimental programs in neutronics, thermal hydraulics, and materials [9], [10]. These resources will be utilized to help select models for benchmarking applications, as well as the forming of benchmarking exercises that will be the most useful in pursuing licensing and fulfilling NRC regulations for the FHR. An important tool identified in these previous efforts are Phenomena Identification and Ranking Tables (PIRTs). PIRTs are a valuable tool that should be developed prior to benchmarking exercises, given a mature experimental facility that is meant to provide experimental validation data. As the facility changes and evolves to meet additional needs, an additional PIRT exercises may need to be performed to verify that the facility is well-suited to address the phenomena of interest. Face-to-face contact is needed for PIRT development, although video-conferencing can be used to supplement this process. PIRTs should start with internal discussions, then outside experts can be invited in when the initial plan has been drafted.

A second resource that may prove valuable will be the DOE/NRC Advanced Reactor Design Criteria [11]. These criteria are still under development, but should provide a more flexible and technology neutral framework for FHR licensing than the current, LWR-centric General Design Criteria. Efforts on this front will be monitored and utilized as they are established.

FHR commercialization is the ultimate goal of the IRP-2; the guiding purpose of this effort is to solve the key problems that vendors will face before they can build an FHR. Therefore, IRP-2 partner universities should focus on research and development of FHR technology, not bringing the design to market. The path forward for the IRP is to bring FHR technology and understanding to a point where vendors can pick up the efforts and continue with developing the commercial technology.

# **3** Relevant Experimental Facilities and Data

A key component of benchmarking is the validation of codes and models against relevant experimental data. There are several sources of experimental data in the FHR space, including several facilities that have been or are currently operational. These experimental facilities and data will be essential for performing validation of evaluation models for FHRs.

# 3.1 Neutronics Experimental Facilities and Data

Neutronics simulation will play a major role within IRP-2. Four major areas of interest for neutronics simulations have so far been identified and may be investigated on in the IRP. The four areas are briefly introduced below (in no particular order) and are explained in more detail throughout this chapter:



Because no FHR has been operated in the past to provide experimental neutronics data, IRP-2 will use experimental results from neutronics experiments performed to study the behavior of other types of reactors that share similarities with FHRs.

## 3.1.1 MIT Reactor (MITR)

The MITR is a heavy-water reflected, light-water cooled and moderated nuclear test reactor that utilizes flat, plate-type, finned, aluminum-clad fuel elements, as shown in Figs. 3-1 and 3-2 [12].



Figure 3-1. Drawing of the MITR



Figure 3-2: MITR Fuel Elements

The average core power density is about 70 kW per liter. The maximum fast and thermal neutron flux available to experimenters are  $1.2 \times 10^{14}$  and  $6 \times 10^{13}$  neutrons/cm<sup>2</sup>-s, respectively. Experimental facilities available at the MIT research reactor include two medical irradiation

rooms, beam ports, automatic transfer facilities (pneumatic tubes), and graphite-reflector irradiation facilities. In addition, several in-core experimental facilities (ICSAs) are available. It generally operates 24/7, except for planned outages for maintenance. The MITR encompasses a number of inherent (i.e., passive) safety features, including negative reactivity temperature coefficients of both the fuel and moderator; a negative void coefficient of reactivity; the location of the core within two concentric tanks; the use of anti-siphon valves to isolate the core from the effect of breaks in the coolant piping; a core-tank design that promotes natural circulation in the event of a loss-of-flow accident; and the presence of a full containment. These features make it an exceptionally safe facility.

Several neutronic codes are presently used by MIT students: CITATION, REBUS-PC/DIF3D, MCNP5, and MCODE and may be available for code-to-code comparison or even validation of small scale experiments in the reactor. These codes could for instance be used to better understand the behavior of material important for FHRs under irradiation. Recent experiments by Sun et al., shown in Fig. 3-3, provides an example how the MITR can provide data to validate activation models for materials like iron-chromium-nickel wire [13].



Figure 3-3: Example of Wire Irradiation Experiment Conducted by Sun et al. in the MITR

Of particular interest for future FHR deployment are experiments related to the production, transport, and control of tritium in the FHR flibe coolant, as tritium control is identified to be of prime importance reactivity control in FHRs.

Figure 3-4 provides an overview of the neutron spectrum in a FHR, the MITR and the lithium cross section.



Figure 3-4: Comparison of the Neutron Spectrum in the MITR and typical FHR to Illustrate Tritium Production

Validation of codes that predict tritium production in the MITR may be used to provide confidence in FHR tritium source estimation. Figure 3-5 shows an experimental setup designed for this purpose. Flibe would be inserted into the setup shown below and resulting tritium may be monitored as shown.



Figure 3-5: Planned Configuration for Tritium Measurements

### 3.1.2 X-Ray Pebble Recirculation Experiment (X-PREX) at UCB

X-PREX seeks to demonstrate the viability of pebble fuel handling and reactivity control for FHRs. The research results also improve the understanding of pebble motion in helium-cooled reactors, as well as the general, fundamental understanding of low-velocity granular flows. Successful use of pebble fuel in salt coolants would bring major benefits for high-temperature reactor technology. Pebble fuels enable on-line refueling and operation with low excess reactivity, and thus simpler reactivity control and improved fuel utilization. If fixed fuel designs are used, the power density of salt-cooled reactors is limited to 10 MW/m<sup>3</sup> to obtain adequate duration between refueling, but pebble fuels allow power densities in the range of 20 to 30 MW/m<sup>3</sup>. This can be compared to the typical modular helium reactor power density of 5 MW/m<sup>3</sup>. Pebble fuels also permit radial zoning in annular cores and use of thorium or graphite pebble blankets to reduce neutron fluences to outer radial reflectors and increase total power production.

Combined with high power conversion efficiency, compact low-pressure primary and containment systems, and unique safety characteristics including very large thermal margins

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(>500°C) to fuel damage during transients and accidents, salt-cooled pebble fuel cores offer the potential to meet the major goals of the Advanced Reactor Concepts Development program to provide electricity at lower cost than light water reactors with improved safety and system performance.

Figure 3-6 provides a brief overview of the facility and its visualization capabilities. Further information can be obtained from Laufer and Buster [14].



Visual Image Sequence:



X-Ray Image Sequence:



Figure 3-6: Overview of the XPREX Facility at UCB [14]

# 3.2 Thermal Hydraulics Experimental Facilities and Data

The set of experimental facilities and data in the thermal hydraulics space for FHRs is diverse and growing. The primary experimental facilities are within the IRPs and are located at UCB, UNM, OSU, and UW. Other experimental data relevant to FHR benchmarking comes principally come from ORNL and SINAP, the two major research institutions researching and developing molten salt reactor technology associated with FHRs.

## 3.2.1 University of California, Berkeley

For safety and licensing purposes for pebble bed FHRs (PB-FHRs), it is important to accurately model the heat transfer coefficient between fuel pebbles and the flibe coolant in order to better estimate temperatures in a PB-FHR core. UCB has been performing scaled pebble-bed heat transfer experiments using simulant oils that match key non-dimensional parameters for flibe. Using temperatures throughout a scaled pebble-bed test section along with other experimental parameters, the interfacial heat transfer coefficient can be extracted as a function of position within the bed and time. The scaled pebble-bed test section is shown in Fig. 3-7. Correlations for interfacial heat transfer coefficients are available in the literature. Experimental interfacial heat transfer coefficients for this scenario have also been derived using experimental data outside the Mk1 PB-FHR's characteristic conditions. There is significant disagreement between the established correlations and the experimental ones, proving that it is important to perform tests and develop new correlations in the appropriate Re and Pr range.

UCB designed the first iteration of the compact integral effects test (CIET) facility (CIET 1.0) to reproduce the integral transient thermal hydraulic response of FHRs under forced and natural circulation operation. CIET 1.0 provides validation data to confirm the predicted performance of the DRACS in FHRs. The facility has two coupled flow circuits: the primary coolant flow circuit, which replicates the main and bypass flow



Figure 3-7. Pebble-Bed Test Section for Heat Transfer

**Coefficient Measurement** 

paths shown in Fig. 3-8, and the DRACS circuit. The two flow circuits exchange heat through the DHX. The facility uses Dowtherm A as a simulant fluid for flibe, at reduced geometric and power scales. Test loops for CIET 1.0 were fabricated from thin-walled (schedule 10) 304 stainless steel (SS) pipe and butt-welded fittings to minimize the mass and thermal inertia. The favorable power scaling with oil (10 kW into oil being equivalent to 625 kW into flibe), along with the simplicity of the construction for low-temperature operation compared to the complexity and safety requirements for tests with the prototypical salt and other prototypical reactor

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coolants, were a key element in enabling the CIET 1.0 facility to be constructed at much lower cost than previous IETs for other reactor classes.

Because the designs of FHR commercial prototype reactors will evolve, inherent distortions will exist between the CIET 1.0 facility and future FHR commercial prototype reactors. For transient response, such distortions may arise from non-matched relative coolant residence times between future FHRs and CIET 1.0 sub-systems, as well as the use of reduced flow area SS piping with non-scaled thermal inertia in CIET 1.0. However, while CIET 1.0 was scaled based on the earlier design of a 900-MWth channel-type pebble-bed advanced high-temperature reactor (PB-AHTR), and the pre-conceptual design of a 236-MWth Mk1 PB-FHR was completed after scaling and design of CIET 1.0 were already finalized, elevations of the main heat sources and sinks in CIET 1.0 and the Mk1 PB-FHR design reveal a reasonable agreement between the scaled model and prototype. Therefore, CIET 1.0 will provide useful validation data for integral transient behavior of a generic set of FHRs, and given the low cost of the CIET facility, final code validation for a future commercial prototype plant would likely include construction of a new CIET-type loop scaled to closely match the prototypical design.

For lack of detailed heat exchanger designs when scaling was performed and design decisions were made for CIET 1.0, the heat exchangers in the system are not scaled to any prototypical heat exchanger. Instead, their designs are based on functional requirements in terms of heat transfer performance, and only relative elevations of the heat sources and sinks are scaled to the 900-MWth modular PB-AHTR. However, the ability to control fan speeds on the two oil-to-air heat exchangers using variable frequency drives (VFDs), as well as to interchange the current oil-to-oil heat exchanger that couples the primary and DRACS flow loops with another scaled heat exchanger design, leaves great flexibility in heat removal options for the CIET 1.0 system. Similar to the heat exchangers, the primary pump on CIET 1.0 is not scaled to any prototypical pump. Instead, its design is based on functional requirements in terms of pump head and resulting flow rates in the system. All instrumentation, as well as the computer-controlled power supply and VFDs are integrated through the LabVIEW software and manually or automatically controlled from a central computer station. Figure 3-9 shows the computer-aided design



Figure 3-9. 3-D Rendering of CIET 1.0

rendering of the CIET 1.0 loop with the main components labeled.

Between 2011 and 2014, CIET 1.0 was designed, fabricated, filled with Dowtherm A oil and operated. Isothermal pressure drop tests were completed, with extensive pressure data collection to determine friction losses in the system. CIET-specific friction loss correlations were compared with handbook values, and empirically measured values were implemented in the system codes that are to be validated by CIET data. The project then entered a phase of heated tests, from parasitic heat loss tests to more complex feedback control tests and natural circulation experiments. In parallel, UCB has been developing thermal hydraulic models to predict FHR steady-state characteristics and transient response for a set of reference LBEs. The general strategy is to rely on existing general-purpose thermal hydraulic codes with a significant V&V basis for design and licensing by the U.S. Nuclear Regulatory Commission, such as RELAP5. However, UCB has also been developing a one-dimensional FHR advanced natural circulation analysis (FANCY) code for CIET 1.0 and FHR natural circulation modeling. FANCY results will be compared with RELAP5 and validated by data from CIET 1.0. Validation data will include steady-state forced and coupled natural circulation data in the primary loop and the DRACS loop, and thermal transients data (e.g., startup, shutdown, loss of forced circulation with scram and loss of heat sink with scram) [15].

#### 3.2.2 University of New Mexico

Due to the high volumetric heat capacity of fluoride salts, FHR heat exchangers commonly operate in the transition and laminar flow regimes where heat transfer coefficients can depend strongly on Reynolds number (Re) and potentially on Grashof number (Gr). Several reduced-scale experiments investigating heat exchanger phenomenology for FHRs are currently underway at UNM. A multi-flow regime heat transfer loop, shown in Fig. 3-10, has been constructed for use with Dowtherm A to collect data and validate current heat transfer correlations (or develop new, when necessary) for several promising heat exchanger concepts. In parallel, a simple water loop investigating hydrodynamics was constructed and has been testing directional heat exchanger concepts for the DHX, which have the potential to help minimize parasitic heat losses during normal operation of the plant and enhance heat extraction during accidents.

The heat transfer loop is being used to perform a number of SETs on heat exchanger concepts. It was initially designed to test bayonet-style heat exchangers, which are inserted into the FHR coolant pool from the top and feature both the secondary (tube-side) feeder and outlet tubes attached to the top of the heat exchanger. Validation data will be collected for two conventional bayonet-style configurations: plain tubes and twisted tubes. Twisted tubes are a particularly promising technology to the development of the FHR due to their enhanced heat transfer as well as their self-supporting design, which eliminates the need for baffles and reduces hot spots and tube vibration.

The loop will be able to match shell-side Re and Pr for the primary-to-DRACS heat exchanger (DHX), as well as have the capability to test a range of Gr, and by extension, Rayleigh (Ra) and Richardson (Ri) numbers owing to the flexibility of the temperature conditions.

The same plain and twisted tube bayonet heat exchangers will also be tested in a novel directionally enhanced shell concept. Because the DRACS is passive and always operating, heat is perpetually being removed from the primary coolant through the DHX. These parasitic heat losses lower the effective reactor outlet temperature during normal operation, reducing the efficiency of the FHR. The hydrodynamics of a directional DHX has been empirically investigated using a simple water loop and has shown promising initial results. The design will be further optimized in conjunction with computational fluid dynamics and the resulting shell design will be implemented in the heat transfer loop and tested with the plain and twisted tube bundles



Figure 3-10. UNM Heat Transfer Loop

Finally, the loop will be configured to

test and provide data for a double-wall twisted-tube heat exchanger. Due to the relatively large quantity of tritium generated in FHRs relative to other reactor concepts and the high operating temperature, which encourages the transport of tritium through and out of the system, the use of double-wall heat exchangers utilizing an intermediate fluid such as lithium to capture the tritium is under consideration. By using a twisted outer tube, it is possible to take advantage of the higher shell-side heat transfer coefficients and more uniform shell-side flow while also enhancing heat transfer to the intermediate fluid flowing in the annulus. Two configurations will be tested at UNM: a double-wall exchanger with inner plain tube/outer plain tube and a double-wall exchanger with inner plain tube/outer twisted tube to determine the heat transfer enhancement possible with the twisted-tube version [15].

### 3.2.3 University of Wisconsin – Madison

The University of Wisconsin – Madison was primarily involved in investigating materials phenomena in the FHR class in the previous IRP. However, as part of this IRP-2, a portion of their research and study will be developing thermal hydraulic loops for the investigation of thermal hydraulic phenomena present in FHRs as well as continuing their investigations of the molten salt chemistry and corrosion. Fluid loops are able to be used for SETs as well as IETs.

### 3.2.4 Georgia Tech-Led IRP

A high-temperature DRACS test facility (HTDF) that is being constructed at The Ohio State University (OSU) is shown in Fig. 3-11 (in red), along with the low-temperature DRACS test facility (LTDF) that is currently in operation (Fig. 3-11 in gray). Both the HTDF and LTDF are scaled down from a 200-kW prototypic DRACS design for a pebble bed reactor design by following a rigorous scaling analysis [16]. The HTDF employs FLiNaK and KF-ZrF<sub>4</sub> as the primary and secondary coolants, respectively. With the HTDF, the DRACS performance in

terms of its capability of removing decay heat under prototypic reactor conditions can be

evaluated. 1-1/2" and 1-1/4" Schedule 40 pipes are used for the primary and secondary loops, respectively. The HTDF core is simulated with 7 electric cartridge heaters with a total nominal power of 10 kW. The DHX employs a shell-and-tube heat exchanger design containing 80 5/8" BWG-18 tubes at a length of 0.325 m. Due to the large temperature difference between the secondary salt and ambient air, plain tubes are used for the NDHX. A total of 36 1/2" BWG-16 tubes are adopted in a staggered array in two rows. A vortex diode design that will exhibit desired pressure drop characteristics for both the forward and reverse flow directions has been obtained via a parametric CFD study [17], [18]. The diode design employs converging/diverging nozzles and a disk-shape chamber with a diameter of 6.6 cm and thickness of 1.56 cm [18]. In addition, a cantilever sump pump for high-temperature applications has also been employed in the HTDF. The nominal design conditions for steady-state operation of the HTDF are summarized in Table 3-1.



The HTDF will be fully instrumented with gauge pressure transmitters to monitor the cover gas pressure in all the salt tanks, capacitance level sensors to monitor the tank salt levels, and thermocouples (N-type) to measure/monitor the salt temperatures along the loop, as well as in the tanks. High-temperature clamp-on ultrasonic flow meters from Flexim will be employed to measure the flow rates. The same flow meters have been provided to ORNL for a similar application with temperature up to 700°C. For the differential pressure measurement, in-house designs utilizing commercial differential pressure transmitters have been developed, which will require accurate control of the salt-Ar interface in the pressure sensing lines.

	Primary Salt (FLiNaK)	Secondary Salt (KF- ZrF4)	Air
$T_{hot}$ (°C)	722.1	665.3	110.0
$T_{cold}$ (°C)	677.9	589.7	40.0
$\Delta T$ (°C)	44.2	75.6	60.0
m (kg/s)	0.120	0.127	0.142

The LTDF uses water as both the primary and secondary coolants. The LTDF is intended to examine the couplings among the natural circulation/convection loops, provide OSU experience before building the HTDF. 1-1/4" and 3/4" Schedule 40 pipes are used for the primary and secondary loops, respectively. The LTDF core is simulated with 3 electric cartridge heaters with

a total nominal power of 2 kW. The DHX employs a shell-and-tube heat exchanger design containing 80 3/8" BWG-18 tubes at a length of 0.356 m. For the NDHX, to enhance the air-side heat transfer, totally 52 5/8" BWG-20 finned tubes with a length of 0.99 m have been employed in a staggered array in two rows. In the LTDF, a fluidic diode simulator consisting of two parallel branches is used to simulate the forward and reverse flow directions. In each branch, the globe valve provides the desired flow resistance while the ball valve opens or closes the corresponding branch based on the flow direction. In addition, a vertical inline recirculation pump has been employed in the loop that simulates the intermediate heat transfer loop, enabling the study of the pump trip process experimentally. The nominal design conditions for steady-state operation of the LTDF are summarized in Table 3-2.

	Primary Water (1.0 MPa)	Secondary Water (0.1 MPa)	Air
$T_{hot}$ (°C)	76.5	65.2	40
$T_{cold}$ (°C)	63.7	34.8	20
$\Delta T$ (°C)	12.8	30.4	20
m (kg/s)	0.038	0.016	0.102

Table 3-2. Nominal Design Conditions of the LTDF

The LTDF is fully instrumented. T-type thermocouples are used to measure the temperatures at the inlets and outlets of all the heat transfer components (core, DHX, and NDHX), and differential pressure transmitters from Honeywell are employed to measure the pressure drops over the fluidic diode simulator and the throttling valve in the secondary loop. A gauge pressure transmitter is also utilized to monitor the pressure of the primary loop as it is pressurized. Clampon ultrasonic flow meters from Flexim are installed for the flow rate measurement. The flow meters have been demonstrated to function well in the LTDF. The LTDF is currently in operation and data are being acquired which will be used to benchmark a computer code that has been developed for the DRACS design and thermal performance evaluation [17].

### 3.2.5 Oak Ridge National Laboratory

The Liquid Salt Test Loop facility at ORNL has been constructed to support the development of the fluoride-salt-cooled high-temperature reactor concept. It is capable of operating at up to 700°C and incorporates a centrifugal pump to circulate FliNaK salt through a removable test section. A unique inductive heating technique is used to apply heat to the test section, allowing heat transfer testing to be performed. An air-cooled heat exchanger removes the added heat. Supporting loop infrastructure includes a pressure control system, a trace heating system, and a complement of instrumentation to measure salt flow, temperatures, and pressures around the loop. Facility parameters are given in Table 3-3.

ONRL Liquid Salt Test Loop Parameter	Description
Salt	FLiNaK
Operating Temperature	700°C
Flow Rate	$\leq$ 4.5 kg/s
	$\approx$ 3.5 m/s (1 in. pipe ID)
Operating Pressure	Near Atmospheric
Material of Construction	Inconel 600
Operating Run Time Life	2+ years
Primary Piping ID	2.667 cm (1.05 in)
Loop Volume	72 liters
Trace Heating	$\approx 20 \text{ kW}$
Thermocouples	47 (8 in bed)
Pressure Gauges	1 in salt
	2 in gas spaces
Flow Rate Measurement	Ultrasonic Flow Meter
Salt Level	1 radar – sump tank
	2 H-T/C – sump and surge tanks (1 each)

#### Table 3-3. ONRL Liquid Salt Test Loop System Parameters

The goals of this facility (shown in Fig. 7) include providing infrastructure (operational knowledge and equipment) to test high temperature salt systems, developing a nonintrusive inductive heating technique that can be used for thermal/fluid experimentation, measuring heat transfer characteristics in a molten salt-cooled pebble bed, and demonstrating the use of silicon carbide as a structural material for use in molten salt systems [17].



Figure 7. ORNL liquid salt test loop.

ORNL was also the location of the molten salt reactor experiment project, and can provide legacy data that can be used for verification of experimental data and validation of computer models.

## 3.2.6 Shanghai Institute of Applied Physics (SINAP)

The TMSR-SF1 is an experimental test reactor designed to enable the development of the Chinese Academy of Sciences' Thorium Molten Salt Reactor (TMSR) solid fuel molten salt reactor (also referred to as a fluoride salt cooled high temperature reactor, or FHR). The purpose of this test reactor is to verify the feasibility and safety of the solid fuel molten salt reactor concept, and to enable the subsequent design and licensing of a demonstration commercial reactor design by providing a comprehensive experimental platform. The TMSR-SF1 adopts a conservative design approach, where reactor safety is the primary consideration in the design, taking into account the basic research capabilities.

SINAP has designed and built several test loops to support their development process. The three principal loops SINAP has constructed are the HTS Test Loop, FLiNaK Test Loop, and FLiBe Test Loop. The purpose of these loops includes basic instruction on the experimental method, design, and construction of molten salt loops; thermal hydraulics of molten salt; the development of equipment to operate and measure the salt loop properties; and the exploration of chemistry concerns for molten salts that include fluoride and beryllium.

The TMSR-SF0 is an electrically heated simulator for solid fuel molten salt reactors. As a comprehensive experimental platform, its primary function is to provide data and experience to support TMSR-SF1 licensing and provide practical experience for SF1 design, start up, operation and maintenance, including verification of TMSR -SF1 thermal-hydraulic design and safety programs and other key engineering and technical solutions; testing and test SF1 key equipment; to simulate and experiment SF1 start up, operation and accident conditions; and maintenance. TMSR-SF0 will also provide experimental evidence for verification and validation for solid fuel molten salt reactor thermal hydraulics and safety analysis codes.

Based on the above considerations, the TMSR-SF0 is designed as a full-scale, 1:1 geometrically scaled simulator for the TMSR-SF1. The key materials, technologies and equipment used in the SF0 have the same design with SF1, and the plant layout is also basically the same. The main differences between the SF0 and SF1 are that SF0 graphite fuel pebbles are not loaded with nuclear fuel, the coolant is heated by electrical heating elements with a total power greater than 1MW. The electrical heating is currently expect to use heating rods installed in channels in the graphite reflector. In addition, FLiNaK is used as the primary salt instead of FLiBe to simplify the safety issues involved in using beryllium. Taking into account the needs of thermal-hydraulic experiments and the low radiation levels, the SF0 core and loop have more instrumentation. In addition, the loop has a flow control valve and shut-off valves to facilitate experiments. From the long-term development considerations, SF0 will include pebble fuel recirculation test equipment.

### 3.2.7 Additional Facilities and Data

Due to increasing international interest in FHRs and in MSRs in general, as well as general interest in molten salt applications, resources for this IRP are constantly increasing in number and variety. Additional resources identified during the workshop include several different salt loops at the University of Geneva, Russian and Indian (BARC) salt loops, fuel salt experiments at the Institute of Trans-Uranium Elements (ITU) in Karlsruhe, several facilities at INL including an experimental facility to validate velocity fields for CFD and possible future salt loop(s), and in the more distant future, solar energy storage experiments at MIT on how light/radiation is absorbed in salts.

## 3.3 Materials Experimental Facilities and Data

### 3.3.1 MIT reactor capabilities to support material irradiation for FHR development

Besides using the MIT reactor to support neutronic experiments and analysis as described in Chapter 3.1.1 it is a powerful facility for material irradiation experiments as slightly touched upon in Chapter 3.1.1. The MITR has several slots that may be used for irradiation experiments.

Facility	Size	Neutron Flux (n/cm2-s)					
In-core	3 available, Max in-core volume ~ 1.8" ID x 24" long	Thermal: 3.6x1013 Fast: up to 1.2x1014 (E>0.1 MeV)					
Beam ports	Various radial: 4" to 12" ID	Thermal: 1x1010 - 1x1013 (source)					
Vertical irradiation position	2 vertical (3GV) 3" ID x 24" long	Thermal: 4x1012 - 1x1013					
Through ports	One 4" port (4TH), One 6" port (6TH).	Avg. thermal: 2.5x1012 to 5.5x1012					
Pneumatic Tubes	One 1" ID tube* (1PH1)	Thermal: up to 8x1012					
	One 2" ID tube* (2PH1)	Thermal: up to 5x1013					
Fission Converter Beam Facility (FCB)	Beam aperture ~ 6" ID	Epithermal: ~ 5x109					
Thermal Beam Facility (TNB)	Beam aperture ~ 6" ID	Thermal: up to 1x1010					

Table 3-4: Overview of Slots Available for Irradiation Experiments at the MITR

Different capsules of which two (FS-1 and FS-2) are displayed here have been successfully operated in the past at various high temperature conditions and may be suitable to support material irradiation to support FHR development.

## FS-1

- 1000 hours at 700°C
- 6 chambers, 5 specimen types (SS316, Hastelloy-N, SiC, SiC/SiC<sub>f</sub>, TRISO)
- Used a single capsule in the ICSA
- 120g of flibe



Figure 3-12: FS-1 Capsule Head

## FS-2

- 300 hours at 700°C
- 6 chambers, 6 specimen types (SS316, compact graphite, IG110-U, SiC/SiC<sub>f</sub>, C/C, TRISO), 2 fluoride potentials
- Used a dedicated facility
- 327g of flibe



Figure 3-13: FS-2 Entire Capsule (without head)

A large number of online and post-irradiation tools are available that support irradiation experiments carried out at the MITR.

Online irradiation tools include: Temperature, gas radioactivity, flow rate, pressure, residual gas analyzer (mass spectrometer), tritium measurement and capture, double-compensated ion chambers, redundant water/glycol bubblers for scintillation, gamma spectroscopy (portable HPGe), self-powered neutron and gamma detectors.

Post irradiation tools include: Neutron activation analysis, hot cell facilities, sample extraction, physical examination, mass photography, inert glove box with ventilated furnace, optical profilometry, optical microscopy, SEM/EDS, thermal diffusivity.



Figure 3-14: Brief Overview of the Neutron Activation Analysis Tools and the Inert Glove Box

Irradiation may be of particular advantage for combined effects testing that may simulate conditions very similar to what can be expected in certain reactor regions. More specifically the following areas may achieve the most representative conditions:

- In-situ tritium production
- Radiolysis products in flibe
- Other activation products (e.g. <sup>16</sup>N, <sup>19</sup>O)
- Neutron damage (swelling, creep, conductivity, ductility)

Keeping these areas in mind the most promising and therefore potential future materials FHR experiments conducted at the MITR may be in the following three areas:

- Corrosion/compatibility (materials in static or flowing flibe under irradiation, combination of irradiation and thermal gradients (corrosion product transport)
- Tritium production (real-time tritium partitioning, flux, temperature, and chemistry effects on cover gas composition)
- Core behavior (structural and compact graphite stability, TRISO performance)

### 3.3.2 Materials corrosion in molten FLiBe and salt redox potential

### **3.3.2.1** Experimental facilities and designs for corrosion tests

The first stage of structural materials corrosion in molten FLiBe focuses on the static corrosion tests performed in purified ORNL FLiBe at 700°C. Due to the toxicity of beryllium in FLiBe and the hygroscopicity of fluoride salts in general, molten salt corrosion tests are inherently challenging in regards to experimental design, data gathering, and safety[20], [21]. A series of preparatory apparatus and experimental facilities have been successfully built for safely handling salt to conduct corrosion tests, at the University of Wisconsin-Madison:

1. An atmosphere-controlled glove box has been outfitted with oxygen and moisture monitors, a high temperature heater control system, a gas purifier, and an exhausting system (Figure 3-15).

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- 2. The FLiBe purification and transferring system mainly consists of a pure nickel canister, pure nickel transfer tubes, a T-type filter (40 microns pore size), and a trace heating on all transfer tubes.
- 3. The molten salt dripping system mainly consists of a pure nickel canister with a "V" shaped hole on the bottom, a "V" shaped graphite plug, a pure nickel rotation bar connected to the graphite plug, trace heaters, and a digital balance. Accuracy is about 0.1g of liquid salt (Figure 3-15).
- 4. The graphite baking system is composed of a high temperature ceramic furnace, a temperature control system, and a gas (10% H<sub>2</sub> balanced N<sub>2</sub>) flowing system. The baking process was performed at temperatures above 850°C.
- 5. The static corrosion system mainly includes a computer-controlled ceramic furnace, multiple thermocouples monitoring salt temperatures, an alumina container, and a temperature gradient rod heater for melting salt from top to bottom.
- 6. The corrosion samples collection system consists of a stainless steel reservoir with four pins, a stainless steel mesh (0.76mm x 0.76mm) held by pins, and a temperature controlled furnace.



Figure 3-15: Atmosphere-controlled glove box, and molten salt dripping system

The next stage of the materials corrosion tests in molten FLiBe will be performed in a convection loop equipped with a diamond window for online monitoring of molten salt conditions. Compared to the static corrosion tests, this flow loop needs much more FLiBe. To perform corrosion tests in the loop, UW will melt and purify a batch of about 38kg of FLiBe. This large scale salt purification system requires a series of facilities that have been successfully built by UW molten salt group.

### 3.3.2.2 Graphite effect on structural alloys corrosion in molten FLiBe

Graphite will be widely used in the FHR core as the matrix material of fuel pebbles, and will be in direct contact with molten salt in reactor. The static corrosion tests in graphite crucibles revealed carbon particulates in the molten salt even though the graphite crucible was cleaned and baked prior to filling. These carbon particulates were transported from crucible walls via the molten salt on to the surface of alloys being tested. This deposited carbon subsequently reacted with metallic components in the alloys such as Cr and Mo to form carbides (Figure 2). Some

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carbon also diffused into the bulk alloy to form to form carbide phases, such as  $Cr_3C_2$ ,  $Cr_7C_3$ ,  $Cr_{23}C_6$ ,  $Mo_2C$ , and  $Al_4C_3$ , in the near-surface regions of the alloy. In the 3000 hour corrosion tests of 316 stainless steel in molten FLiBe in the graphite crucible at 700°C, the carbide-containing layer extended deeper than 50 microns. This carbide layer seemed to stabilize Cr in the alloys. However, the carbides might influence other properties of alloys in the molten salt. For example, the hardness and thermal conductivity of the alloys' surface layer changes due to the formation of carbides on and in the alloys. During the MSRE program, carburization was found in the Hastelloy N that was in intimate contact with graphite parts, but it was not considered to be a concern because a sacrificial shim was placed between the graphite and metal[22]. Is it reasonable to neglect this issue for the FHR? Or is it necessary to investigate the carburization phenomenon?



Figure 3-16: Surface and cross-sectional SEM images of Hastelloy N tested in molten FLiBe in graphite crucible at 700°C for 1000 hours.

### 3.3.2.3 Microstructural evolution during corrosion in molten FLiBe

Since the corrosion of alloys in molten salts takes place at high temperatures (700°C for the FHR), the microstructure of the alloys can evolve. This microstructural evolution during corrosion increases the complexity of the corrosion rate evaluation. It is therefore important to separate the thermal effects from molten salt effects on the final corrosion results to fully understand the corrosion behavior of alloys in molten fluoride salt. Although the microstructural instability of alloys at high temperature has been investigated [23, 24, 25], it is a challenge to quantify each factor on the final corrosion because both effects occur simultaneously.

### 3.3.2.4 Model development for predicting corrosion attack

It is desirable to develop a model for predicting corrosion attack of alloys in molten fluoride salt. As previously mentioned, corrosion tests in high temperature molten fluorides is challenging work. Running long-term corrosion tests not only requires durable and reliable facilities, but are also costly. Under the assumption of thermal diffusion controlled corrosion[26], [27], UW developed a simplified model to calculate the maximum Cr depletion distance which was selected as a criterion to evaluate the corrosion attack depth. The calculated overall Cr depletion profiles reasonably fit experimental results. However, to precisely model the corrosion of alloys in high temperature molten fluoride salts, many factors must be considered. For example, in most alloys, the grain boundary diffusion ( $D_{gb}$ ) predominantly contributes to the overall diffusion coefficient ( $D_{eff}$ ) [28], [29]. It is not well-known how the grain boundary precipitate changes the Cr diffusion through the grain boundary during high temperature corrosion in molten salt.

#### 3.3.2.5 Redox potential measurements of molten FLiBe

A compact electrochemical probe (

Figure 3-17) has been developed to measure the redox potential in flibe via an in-situ dynamic beryllium electrode as described by Afonichkin et al[30]. The dynamic reference electrode removes the need for the ion permeable container used in typical electrochemical cells, creating a simpler, more robust probe, which has the potential to operate in varying depths. This probe is capable of operating on a loop, or static system at salt temperatures exceeding 500 °C. Only robust materials proven to be inert are in contact with the salt. The probe has been well-characterized in Li<sub>2</sub>BeF<sub>4</sub> salt over wide variety operating conditions, yielding redox measurements with an accuracy of  $\pm 4$  mV.



Figure 3-17: UW beryllium reduction probe cutaway drawing

Part	Description				
1	Vitreous Carbon Anode				
2	Molybdenum Electrodes				
3	PTFE Ferrule				
4	<sup>1</sup> / <sub>4</sub> " Swagelok Fittings				
5	Boron Nitride Spacer				
6	Viton O-Ring				

Table 3-5. Part List of UW Probe Design

A measurement begins by applying a voltage to a submerged cathode, creating a current between the molybdenum cathode and submerged glassy carbon anode, forcing beryllium fluoride to reduce as beryllium at the cathode. After sufficient plating, the circuit is opened, allowing beryllium to donate electrons to the salt, reforming beryllium fluoride. As the beryllium recombines, it creates a distinct voltage on the cathode which can be referenced and compared to the potential on a third, submerged molybdenum indicator electrode, yielding the redox potential. After the beryllium reference reaction diminishes, the potential between the cathode and indicator electrode relaxes back to near zero volts. A small "hump" during relaxation is normally observed which is thought to be due to plated metallic impurities (Figure 3-18).



Figure 3-18: Measured plateau region voltages shown to be repeatable through several runs

### 3.3.3 Ultrasonic Enhancement of Inert Gas Sparging

Ultrasonic enhancement of inert gas sparging to better understand how mass transfer out of the working fluid maybe supported is performed at UNM. The principles of rectified diffusion is used in two set-ups (flow cell 1 and 2) with a third one planned. The figures below illustrate the idea showing flow cell 1:





#### Figure 3-19: Brief Overview of Flow Cell 1

Bubbly flow is pumped up towards the face of the ultrasonic horn. The design of the configuration makes sure that bubbles will interact with the near field. The frequency used is usually in the magnitude of 20 kHz. Due to primary radiation forces the ultrasonic energy at flow cell one is in pulsing mode.

Flow cell 2 has a similar set up but is slightly smaller than flow cell 1. The principle is the same and again 20 kHz is used as the acoustic wavelength.





Figure 3-20: Brief Overview of Flow Cell 2

Preliminary results optical results using a high speed camera show potential improvement in the sparging mass transfer. See pictures below.



Figure 3-21: First Results of the High Speed Camera

However, a need for more accurate design has been identified to account for the bubble to bubble radiation or secondary Bjerkens forces.

### 3.3.4 System Models of Materials Chemistry, Activation, Tritium and Transport (MATT)

MIT (J. Stempien) as part of its first IRP has developed a model of TRITium Diffusion EvolutioN and Transport (TRIDENT) with benchmarking using existing experimental data. TRIDENT integrates the effects of the tritium production, chemical redox potential, tritium mass transfer, tritium diffusion through pipe walls, and selective Cr attack by tritium fluoride. Systems for capturing tritium from the coolant were proposed and simulated with TRIDENT. The capabilities of this system model relative to other models is summarized below.

	TRIDENT	TMAP4/7	ORNL- 4575	ТРАС	ORNL- TM-4804	SFR/FUS- TPC	THYTAN
Time- dependence	Х	Х		Х		Х	Х
T Transport	Х	Х		Х	Х	Х	Х
T production model in flibe	Х						
Other T production (ternary fission etc.)		User must define		Х		Х	Х
Reactor system-level model	Х	User may build		Х	Х	Х	Х
Reactor Coolants	flibe/flinak	flibe/He/ Pb/Pb-Li	flibe	Не	Flibe	Na/Pb- Li	Не
Redox Dependence	Х		Х		X		
Isotope Exchange		Х		Х	X	X	X
Corrosion Reactions	Х		X				
Corrosion Product Mass Transport	Х		Х				
Model of T sorption on graphite	Х				Х		
Online pebble refueling effects	Х						
T permeator system model	Х						
T removal to purge gas	Х	User may define			Х	Х	
Counter- current gas stripping	Х						
Secondary loop model	Х			Х	Х		Х

Comparison of TRIDENT features critical for FHR analysis with features of other codes.

### 3.3.5 Planned corrosion research at Georgia Tech

Project related facilities include multiple furnaces for molten salt experiments (up to 1000°C). Tests can be carried out under inert gas atmosphere. A glove box with controlled atmosphere will be used glove box to prepare salts and prepare samples for tests.

Other related facilities in our group include electrochemical equipment like potentiostats, and Electrochemical Impedance equipment. Thermal balance for high temperature oxidation studies under gaseous environments. Access to surface characterization methods including SEM, EDS, XPS etc.

Three types of tests are planned in our group at Georgia Tech:

- Corrosion under static conditions in pure FLiNaK
- Exposure tests will be conducted at 700°C and 850°C in graphite crucibles with Ar cover gas.
- Commercial Ni-based alloys (including Hastelloy-N, Hastelloy-X, Hastelloy-B, Haynes-230, Inconel-617, Inconel 625, Incoloy-800H, Inconel 625, and Ni-201) and austenitic stainless steel grades 304L, 316L, 347, and 321. Pure metals Ni, Fe, Cr, Mo, and Mn.
- Results will be compared to those of FLiNaK exposure tests done at the UW and other groups as well as tests done in MS loop at ORNL.

Impurity and redox condition effects on corrosion behavior of selected alloys:

- Levels of impurities such as excess fluoride, oxides, HF, or excess reactive metal (Zr) will be systematically controlled and their effects investigated using electrochemical measurements during exposure tests.
- Commercial Ni-based alloys (including Hastelloy-N, Hastelloy-X, Hastelloy-B, Haynes-230, Inconel-617, Inconel 625, Incoloy-800H, Inconel 625, and Ni-201) and austenitic stainless steel grades 304L, 316L, 347, and 321. Pure metals Ni, Fe, Cr, Mo, and Mn.
- Initially a pseudo reference electrode (Mo) will be used. Work will also develop and use Ni based reference electrodes for molten salts.

Effect of Flow on Corrosion in Molten Salts

- Flow rate effects will be investigated using the rotating electrode method. The rotating sample will spin at different speeds to simulate different flow rates. These tests will be done at different temperatures and different time periods.
- Five alloys with the best corrosion behavior based on the results of other experiments will be tested.

• Results will be compared with ORNL loop test results as well as with the static tests done at Georgia Tech.

### 3.3.6 Relevant material research capabilities at Ohio State University

### Glove box Systems Equipped with Electrochemical Cell and Gamry Potentiostat:

To ensure accurate results, it must be ensured the experiments are conducted within an inert environment. This is accomplished by conducting the experiment within a glove box. In using a glove box, the environment will be in an inert Argon gas with sensors to ensure minimal  $H_2O$  and  $O_2$  contamination. Therefore, all the tests related to molten salt will be conducted in glove box system. Recently, the PI's molten salt Lab at OSU has designed and fabricated two glove box systems, and the two systems will be in operation in Mar.2015.

The first glove box system is from Innovative Technologies, and is a custom glove box. This glove box box has an internal working dimension of 96'' x 65'' x 31'' (width x height x depth). The glove box will be placed on a small stand to allow the ideal height for testing. The glove box has eight gloves to work from that are configured in, 2 rows of four. When on the stand, the bottom row of gloves are at standing height (48 inches above the ground) to allow for work on the floor of the glove box, and the upper gloves (at 72 inches from the ground) are to work on the adjustable shelves for material storage. It was determined that the lower gloves could be used when operating the furnace by standing on the ground. The upper gloves can be used to perform material preparation by standing on a small platform that could be set on the ground. This extended height is ideal because it allows longer electrodes to come from the furnace, enough space to work above the furnace, and enough room left over to store materials.

The second glove box is also from the same company, but a standard box, Innovative Technologies PureLab 1950. This glove box has an internal working dimension of 76 x 35 x 31 (inches for Width x Height x Diameter). The glove box has four gloves to work from with adjustable shelves for material storage. This glove box will also include a well on the glove box. This well is added to allow a furnace to sit within for testing. By adding a well, the top of the furnace, where most of the manipulation is done for the experiment is at glove level. This is to allow more room above the furnace to allow more room for the removing the samples. The well can also be closed when making preparations to materials to allow for the full range of the inside floor spacing.

Both of glove box systems come with a gas purification system to recirculate argon gas and a heat exchanger to moderate temperature within the box. It contains filters with enough absorption capacity for 30 liters of  $O_2$  and 1300 grams of  $H_2O$ and sensors to measure the content between 0 - 1000 ppm for both impurities to ensure the correct conditions are met when testing. These sensors are viewed and controlled via a touch screen interface. It also has antechambers to allow materials to be transferred into the glove box while the environment is maintained.



Figure 3-22: Modulated Speed Rotator

Both glove box systems are equipped with custom designed electrochemical cells for conduct molten salt-related experiments. In the cells, the temperature can research as high as 750°C.

### Modulated Speed Rotator

The lab also equipped with 3 modulated speed rotators which can be applied control the working electrode rotating speed, then to identify the flow effects on the materials corrosion. The rotation rate of the electrode may be read from the LCD display on the front panel, and the rate may be adjusted using the knob located just below this display. The rotation rate is adjustable over a range from 50 to 10,000 RPM and is accurate to within 1% of the reading on the display. A voltage output signal that is proportional to the rotation rate is available on the front panel. This signal may be used to monitor the rotation rate using an external voltmeter or data acquisition system.

### ThermoCalc Software

The PI's lab has ThermoCalc software license. ThermoCalc is a software based on CALPHAD (CALculation of PHAse Diagrams) approach to calculate the multicomponent thermodynamics and phase diagrams. It has two main components: the internally-consistent thermodynamic databases, and application itself, which determine the range and properties of a multi-component system that can be calculated. Current, the software has many databases including databases for molten salt, stainless steel, Ni-base alloys, Zr-base alloys and aqueous solutions which will benefit our proposed research. In addition, the capabilities of ThermoCalc may be extended by adding your own databases or retrieving the multicomponent thermodynamic data and phase equilibrium results through the software development kits, such as the TQ-Interface, TC-API, and TC-Toolbox for MATLAB, and combing them with your own application programs.

### Materials Characterization Tools

The Institute of Materials Research (IMR) of the university has a range of scanning and electron microscopes for performing fracture surface analysis, chemical analysis (SEM/EDX), X-ray diffraction, electron backscattered diffraction (EBSD), and conventional transmission electron microscopy (TEM), and facilities for fabricating bulk and thin film characterization samples.

### 3.3.7 Relevant material research opportunities at ORNL

As needed, the Corrosion Science and Technology Group has access to personnel and facilities housed within the ORNL's Materials Science and Technology Division (MSTD), which is a large, diversified materials research division with over 300 employees. The division consists of 19 research groups encompassing 6 major technical themes: theory and modeling at multiple scales; designed synthesis of structural alloys and ceramics, specialized crystals, and condensed matter physics systems; structural characterization via electron, ion, photon, and neutron sciences; comprehensive physical and mechanical property characterization; interactions with extreme environments; and applied materials physics. The division also houses 3 program offices and 2 major user facilities: the High Temperature Material Laboratory (HTML) and the Shared Research Equipment (SHaRE) User Facility and Program. These facilities offer world-class capability for the manufacture, processing, characterization and evaluation of the physical,

mechanical, thermal, and environmental properties of materials and are available to the proposed research program.

An extensive array of arc-casting and related metals processing facilities are available to manufacture model alloys for this study including casting, hot rolling, cold rolling, heat treatment/quenching, and machining capabilities such as electoral discharge machining. For characterization of mechanical properties, numerous high-temperature electromechanical, servo-hydraulic, and lever-arm dead load machines are available to conduct creep and creep fatigue testing. Several machines were upgraded to allow testing in corrosive environments such as steam and molten salt. For evaluating surface reaction and rate limiting reactions, MSTD houses electrochemical test systems, high-temperature autoclaves, inert glove boxes, and an array of welding tools including electron beam that ensure controlled environment and allow for creating specialized test articles. MSTD also houses x-ray diffractomers and an array of optical and electron microscopes for the evaluation of surface morphology, surface micro-chemistry, and crystallinity of surface products. In addition, there is access to neutron diffraction, if needed.

Characterization equipment that may be employed include 6 state-of-the-art scanning and transmission electron microscopes (STEM/TEM) with aberration-correction, EELS, EFTEM, EDS, electron holography, HRTEM, and HAADF capabilities. Three field emission gun scanning electron microscopes with BSE, OIM/EBSD, and EDS capabilities, electron probe microanalysis (EPMA), and XPS and Auger electron spectroscopy including in-situ fracture capability to study failure surfaces are available. Atom probe tomography (APT) for 3D atomic scale resolution of precipitate chemistry is also available.

### 3.4 FHR Benchmark Data Management: NE-KAMS

Advanced modeling and simulation (M&S) for nuclear energy development involves significant processing and use of digital data. To assess the reliability of M&S results, computational and experimental data are needed for V&V. To estimate error limits of computational and experimental outcomes, a considerable amount of data must be processed for UQ. To ensure successful nuclear M&S development:

- significant data and related information from diverse sources of computations and experiments must be efficiently managed and correctly used with great accuracy and consistency;
- communications between modelers and experimentalists must be conducted on a mutually understood base;
- information and knowledge generated must be adequately preserved for future reference; and
- unnecessary research and development (R&D) redundancies must be readily identified and eliminated for cost- and time-efficiency.

It is apparent that the immensity and diversity of data involved in advanced nuclear M&S poses a great challenge to satisfying these needs and requirements.

To rise to the challenge, it was proposed that a multi-faceted knowledge management system is needed to support V&V and UQ of M&S for nuclear energy development. Such a system must provide a comprehensive and web-accessible knowledge base with V&V and UQ expertise and resources for establishing confidence in the use of M&S for nuclear reactor design, analysis, and licensing. It should offer support to development and implementation of standards, requirements and best practice for V&V and UQ that enable scientists and engineers to assess the quality of their M&S while facilitating access to computational and experimental data for physics exploration. It should also serve as a platform for technical exchange and collaboration, enabling credible computational models and simulations for nuclear energy applications. Furthermore, it must be able to assist positioning programs of the Department of Energy (DOE) to share the costs associated with development and application of M&S, capture and preserve the V&V, UQ and M&S knowledge and data, and provide value-added tools and utilities while leveraging its knowledge-sharing ability to educate young scientists and engineers in government, industry, and academia.

The concept of such a multi-faceted knowledge management system has attracted great interest and gained strong support from stakeholders across industry, academia, and government for the development of NE-KAMS. Nevertheless, the cost and time required for the development became a serious issue, as it became obvious that an advanced, sophisticated, and robust system that could meet these high requirements would demand significant resources and years of development time. Due to the pressing needs of several DOE M&S projects and increasingly strained budgets, initiation of such a development seemed funds- and time- prohibitive, unless an existing "launching pad" could be found.

An extensive search was conducted by the Nuclear Energy Advanced Modeling and Simulation (NEAMS) Program to identify potential candidates. After thorough scrutiny and evaluations, it was concluded that the relational database infrastructure at ORNL established through the Gen IV Materials Handbook Project could best meet the requirements. The Handbook has been used by DOE for data collaboration among nine signatories representing more than ten countries involved in Generation IV Nuclear Reactor development since 2009, and its infrastructure has provided a solid foundation for the spinoffs of the Nuclear System Materials Handbook Database, the Nuclear Concrete Materials Database, the ASME Materials Database, and several other smaller databases. The infrastructure that has evolved, along with the expertise and experience accumulated through these projects, can enabled rapid development and implementation of major features and functionalities that are highly desired for NE-KAMS, which include 1) high traceability of complicated relations between data; 2) robust but flexible access control applicable to every level of data hierarchy in a database to meet information control requirements of different projects; 3) versatile reorganization of large quantities of digital data in various desired formats; 4) efficient data transfer between data storage and computational models; and of pragmatic importance, 5) the capability to become operational in less than six months.

Development of NE-KAMS officially started in mid-June 2012 with a collaboration among Idaho National Laboratory (INL), Bettis Atomic Power Laboratory (BAPL), Argonne National Laboratory (ANL), Sandia National Laboratories (SNL), and ORNL. As the development continues, more collaborators are expected to join in the project [31].

The FHR IRP-2 proposes to use the NE-KAMS database as the project's data management system. The benefits of controlling the data management through NE-KAMS is the ability to access all experimental data from anywhere, to compare data from different experiments directly, and to store all experimental data securely.

# 4 Candidate Benchmarking Exercises

The purpose of the candidate benchmarking exercises in the three subject areas serve several purposes, including to begin defining the scope of phenomena that are possible to explore through benchmarking, which phenomena are most desirable to explore, and how the exercises should begin and then progress throughout the span of the project.

## 4.1 Neutronics Candidate Benchmarking Exercises

IAEA (IAEA-TECDOC-1694) and OECD/NEA IRPhE HTGR benchmarks provide helpful guidelines for setting up benchmarks and experimental campaigns, but overall they are not fully relevant for near term FHR neutronic benchmarking efforts. Three stages of code-to-code comparison may be used for neutronics benchmarking in IRP-2. The code-to-code comparison may consist of three phases, with the detailed down selection of problems being performed by the neutronics working group later:

### 1. Code capabilities check

The purpose of this phase is to test code capabilities and quantify discrepancies on simple test problems. Because the nearest-term neutronic test data for FHRs is expected to be provided by the SINAP TMSR-SF1 test reactor, which will use pebble fuel, pebble geometries will also be the primary initial focus for IRP-2 neutronics benchmarking. Two models will be used: (1) unit cell with reflective boundary conditions comprising one pebble and corresponding coolant volume, with low-enriched uranium and no fission products; (2) horizontal cross section (infinite long) of the TMSR-SF1 that includes an active core region and reflector (this is similar to what was done by IAEA for gas cooled reactors, but replace cubic model with infinite cylindrical model).

Calculations to be performed (all conditions are fixed in the benchmark definition) for both models will provide reactivity (infinite multiplication factor), average flux, average neutron spectrum, radial leakage (for the cylindrical model only), and power distribution in the following conditions:

- a. Fully homogenized fuel/coolant<sup>+</sup>
- b. Heterogeneous coolant/pebble, homogeneous inner pebble (mixing pebble shell, matrix and TRISO)<sup>+</sup>
- c. Fully resolved double heterogeneity<sup>+</sup>
- d. Ordinate bed<sup>+</sup>
- e. Random bed<sup>+</sup>

### 2. Criticality and reactivity worth tests

These benchmark problems will assess mostly criticality and reactivity worth for first core using a TMSR-SF1 fuel core 3D model (this ideally would be a completion of the 2D model used in phase 1) with uniform conditions (zero power, uniform temperature):

- a. Number of pebbles required to achieve criticality for a fixed enrichment<sup>+</sup>
- b. Enrichment necessary to reach criticality for a fixed bed<sup>+</sup>
- c. Coolant temperature reactivity worth<sup>+</sup>
- d. Fuel temperature reactivity worth<sup>+</sup>
- e. Graphite (matrix and shell) reactivity worth<sup>+</sup>
- f. Control system reactivity worth<sup>+</sup>
- g. Single (or cluster) pebble reactivity worth (space dependent) \*

Besides reactivity, these tests should also provide power distribution and flux spatial (and energy) distribution in selected locations in the core and in the reflector to emulate actual or potential sensor locations. All these evaluations should be repeated at full power and cold shutdown conditions.

### 3. Dynamic tests

This phase will include time dependent evaluations, such as:

- a. Burnup with fixed bed<sup>+</sup>
- b. Burnup with once-through bed\*
- c. Burnup with continuous refueling\*
- d. Transients (RIA, LOFA, others?)\*

Computationally, these evaluations (excluding a) could be quite complex; therefore better gauge of the existing modeling capabilities during phase 1 and 2, and before making a final decision needs to be considered.

### 4.2 Thermal Hydraulics Candidate Benchmarking Exercises

The key thermal hydraulic phenomena that have been identified in previous FHR work that are important to address in benchmarking exercises include natural circulation, including passive decay heat removal; heat transfer in high Pr coolants, including enhanced heat transfer surfaces such as pebble beds and twisted tubes; heat/flow distributions in critical components such as bypass flow in the reactor; heat exchanger performance; conduction in the fuel and the reactor structures; and radiation heat transfer in molten salts. These phenomena are meant to bound the thermal hydraulics space that this IRP can perform benchmarking exercises within. The exercises that are actually performed over the course of the project will be down-selected from this space based on the importance of the phenomena, the quality of the data available, current knowledge gaps, and licensing concerns. The down-selection to a realistic set of benchmarking exercises will be a critical process, and will be one of the initial steps taken by the thermal hydraulics working group.

The ability to identify key phenomena for a given technology is necessary for defining the scope of benchmarking activities. The proposed method is through the use of phenomena identification and ranking tables (PIRTs), which are an element of the EMDAP which comes from NRC Regulation Guide 1.203. During the development of the practical set of benchmarking exercises, it may be necessary to supplement the PIRT process with a more limiting evaluation

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method that takes into account existing validation data sets, operating experimental facilities, and the resources of IRP-2.

The first exercise posed during the workshop discussions is meant to be an example of an initial problem that can be chosen during the beginning of IRP-2 because of its study of fundamental FHR thermal hydraulic phenomena and the knowledge gap it represents.

Candidate exercise one (CE1) explores steady-state natural circulation flow in a loop. The purpose is to validate the relevant performance models against experimental data for validation. This is a critical first step before more advanced models/scenarios can be explored. This exercise is able to be performed on many experimental facilities, including CIET 1.0, the UNM Heat Transfer Loop, thermal hydraulic loops developed at UW, the OSU DRACS test loops, the Liquid Salt Test Loop at ORNL, and the thermal hydraulic loops at SINAP. The ability to perform CE1 on several test facilities and validate several models should lead to very accurate and flexible natural circulation models. It is important to note that this is a relatively straightforward test to perform in isolation (without coordinated benchmarking with other universities or partners), and there may already be work underway or work completed that can be included in this effort.

Candidate exercise two (CE2) is meant to represent a mature benchmarking exercise that should be performed towards the end of the project after more fundamental areas are fully explored and essential knowledge gaps have been filled. CE2 is a transient response, time-at-temperature study for loss-of-forced-circulation (LOFC) transients, both with and without scram (ATWS). The purpose is to determine the time the system remains above a certain temperature threshold during a LOFC transient in the FHR, both with or without a full scram occurring. The significance will be the ability to address the LBE initiating event, "decrease in reactor coolant system flow rate," and that the data can be used to address the limiting safety cases of structural integrity during transients. The experimental facility used in this exercise is the CIET facility (UCB) and the figures of merit include the peak bulk coolant outlet temperature, the time at temperature for metallic and ceramic structures, the temperature difference across the DRACS, and the time to establishment of natural circulation.

SETs are an important part of benchmarking as they directly support the IETs by exploring individual phenomena in isolation. This allows IETs to test how different thermal hydraulic phenomena interact in a system. Examples of SETs would be tests to provide pressure drop correlations and heat transfer coefficients for integral test facilities. An example of a SET would be the exploration the bi-directional shell –side heat transfer in the DHX with buoyancy effects using both plain and twisted tube geometries within the DHX. The purpose of this exercise is to address the lack of data for buoyant flows in twisted tubes. The bi-directional flow component data is necessary because of the flow reversal present in the DHX. Data can be provided for a range of Re and Pr which will give heat transfer correlations for several different candidate salts over a range of operating conditions. CE1 will use the DHX Heat Transfer Loop at UNM, and the figures of merit are heat transfer enhancement due to twisted-tubes and the effect on heat transfer due to local buoyancy forces for up- and down-flow (degrading/enhancing).

The ability to instrument SETs extensively to generate high-quality data for loss coefficients, and component characterization and other system characteristics and state parameters, will be important as system characteristics such as loss coefficients represent the majority of uncertainty.

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Comparison of uncertainty from different sources be valuable, particularly in developing future PIRTs for FHRs.

In general, there will be serious scrutiny on the scaling practices applied to justify using simulant fluids in the place of molten salt. Therefore verifying the similitude between the selected simulant fluids and the working salts will be critical in establishing the application of scaled experiments for validation of FHR evaluation models, particularly for licensing purposes. A good method of proving similitude will be to use diverse data from multiple experimental facilities using both oil and salt, or data compared to multiple evaluation models. An important aspect in data diversity is that the characterization of uncertainty will be different. If a diverse data set can be used to validate a diverse set of evaluation models to a high degree of acceptability by licensing bodies, this will be a significant step towards understanding and applying molten salts in reactor systems.

## 4.3 Materials Corrosion, Activation, Tritium, and Transport (MATT) Candidate Benchmarking Exercises

Materials corrosion, materials and coolant activation, tritium behavior and transport of tritium and corrosion products in an FHR are tightly coupled as shown in Fig. 4-1 for the TRIDENT code to model these effects that was described earlier.



Figure 4-1: TRIDENT Model of Materials, Tritium, and Corrosion Behavior in the FHR

Neutron radiation of fluoride salts containing lithium and or beryllium generate tritium fluoride ( ${}^{3}$ HF). The salt redox potential then determines how much is remains as TF and how much is converted into T<sub>2</sub>. The TF can cause metallic corrosion in the FHR heat exchangers and particularly the selective corrosion of chromium from the metal. The T<sub>2</sub> can diffuse through metals and determines tritium release rates. Carbon in the fuel absorbs both TF and T<sub>2</sub> but its absorption capacity is limited. As a consequence tritium generation, metal (chromium) corrosion and deposition rates around the loop as a function of temperature, transport of tritium inventory, and tritium releases to the environment are tightly coupled and cannot be separately modeled. TRIDENT addresses all of these phenomena. At the current time the lack of good experimental data, particularly integrated tests, is a major limitation. Benchmarking is to address this challenge by finding new sources of data, refine models where required, and enable long-term predictions of system behavior.

Of particular interest for material benchmarking is material- and more specifically tritium mass transport in FHRs. Three a scales:

1) **Fuel**: Chemical interactions based upon temperature, neutron damage, graphite properties, FLiBe saturation, reactive species ratios (ex: [T<sub>2</sub>]/[TF]), and mass transfer characteristics.

- 2) **Core**: Concentration drops from salt flow rate, TH considerations, and product generation rates.
- 3) **System**: Core outlet concentrations, additional sinks/barriers, temperature, corrosion, permeability of HXs may be regarded in more detail. TRIDENT is the current state of the art model that we are aware of but benchmarking will help identify other possible models and where information is lacking

Further information on the three benchmarking areas is provided in table below:



- Convective specie fluxes
- Bulk concentrations



#### **FHR Core** Height Inputs: Temperature and flow distributions Temperature out Bulk generation Flow \_ rates Generation Outputs: $\Delta c_{core}$ Core outlet concentrations Core concentration drop cin



### **FHR Loop**

### Inputs:

- Concentration additions/drops through loop
- Permeation rates
- Corrosion rates

### Outputs:

- Tritium release fraction
- Product distributions



Figure 4-4: Material Candidate Benchmarking Exercise "Loop"

# 5 Proposed Path Forward

Overall, the most critical outcome of the first IRP-2 workshop is to define the path forward to continue FHR research and development efforts under the new DOE IRPs. This includes how to divide and coordinate research between IRP partner universities and how to structure future workshops.

### 5.1 Technical Area Working Groups

Three clear technical areas emerged during workshop preparation and discussions: neutronics; thermal hydraulics; and materials corrosion, activation, tritium and transport (MATT). These three technical areas create a clear division of FHR phenomena that encompass the most important phenomena required for FHR licensing and commercial development. Based on recommendations from the workshop participants on the division of FHR phenomena into these three technical areas, the IRPs propose to form three working groups to organize future research efforts within the broader FHR benchmarking campaign.

Each working group will consist of students and professors from FHR IRP partner universities with related interests in the technical area of the working group as well as universities and organizations that fall outside the formal IRP organization. Additionally, each working group will have its own advisory committee consisting of professors, national laboratory scientists, and other technical area experts to help guide research efforts. Beyond providing guidance, the oversight of an expert advisory committee will help facilitate collaboration and mentorship between established experts within the Nuclear Engineering field and students in Nuclear Engineering, ensuring a high degree of knowledge transfer and continuation of FHR development capability. Developing an advisory committee will be one of the first tasks for each working group. However, identifying working group chairs to run and hold accountable sub-groups is a necessary first-step before technical efforts can be coordinated. Charters for the working groups can then be developed, designating responsibilities and powers the groups have.

The flexibility of having the FHR evaluation model benchmarking efforts divided among three technical area working groups also allows for more contact and collaboration through video-conferencing, side meetings at conferences related to the working groups' technical area, and other more frequent interactions. This will be critical for maintaining communication and progress within working groups in between the larger FHR benchmarking workshops, which are proposed to meet approximately annually. The IRP partner universities, including the GT-led IRP, are tentatively divided into working groups as follows<sup>2</sup>:

- Neutronics: UCB, GT, MIT
- Thermal Hydraulics: UCB, OSU, UNM, UW
- Materials Corrosion, Activation, Tritium, and Transport: UW, MIT, GT, OSU

Each working group will identify two lead faculty members who will co-chair the group. The responsibilities of the lead faculty will include: developing a working group charter, communication and coordination within the working group as well as with the other working groups, organization of working group resources, prioritization of benchmarking efforts, coordination and integration of the working group advisory committee, and other managerial duties. Working group co-chairs may be faculty from either IRP.

During the beginning of the combined IRP efforts, the working groups will primarily work separately as their technical areas are relatively disparate. However, sharing individual experiences with benchmarking efforts with the other working groups will be critical in further development of benchmarking best practices and creating positive communication practices. Also, as the understanding of FHR phenomena advances during the course of the IRPs, the more complex phenomena will require coupled development between working groups, e.g. thermal hydraulics – neutronics coupling to understand complex FHR transient behaviors that will be important for licensing efforts. Sub-working groups may be necessary to facilitate this cross-working group collaboration, and will be explored further during subsequent workshops as benchmarking efforts advance.

In practice, benchmarking activities within each working group will include participation from organizations outside of the IRP partner universities both domestically and internationally. Outside collaboration will serve several purposes, primarily: (1) providing additional credibility to benchmarking campaign results as more diverse experimental data, model predictions, and applications of FHR phenomena are contributed by additional benchmarking participants; (2) providing high-quality experience to students through their collaboration with professionals and experts in the Nuclear Engineering field on a reactor design and development project of significant depth and breadth; and (3) acquiring international attention and interest in the advancement of FHR technology development.

### 5.2 Future Workshop Organization

Future MIT-led IRP benchmarking workshops are proposed to have two complimentary components: (1) a full IRP discussion component where all participants involved in FHR IRP research efforts and contributing experts can meet to discuss topics pertinent to the IRPs at large, and (2) separate breakout sessions consisting of working group members and their respective

<sup>&</sup>lt;sup>2</sup> Texas A&M University has an established and impressive expertise in instrumentation and control, and as such does not readily fall into the proposed working group structure. TAMU's role in this benchmarking campaign has yet to be established, and they may contribute to FHR technology development and understanding in other, equally important ways.

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advisory committees to discuss topics pertinent to only the respective working group in more detail. This workshop structure is a much more efficient use of participants' time while still encouraging collaboration and enthusiasm for FHR research within and outside the IRPs.

The proposed agenda for future MIT-IRP benchmarking workshops is a half-day of welcome activities to allow all participants to arrive, a day dedicated to breakout sessions to discuss more specific topics within the working groups, followed by a second day dedicated to general IRP discussion.

The following tentative schedule for MIT-IRP benchmarking workshops is suggested:

- Second FHR Benchmarking Workshop
  - Date: April 13-15, 2016 (preceding the ICAPP meeting April 17-20 in San Francisco)
  - Location: UC Berkeley/San Francisco
- Third FHR Benchmarking Workshop
  - Date: February, 2017
  - Location: TBD
- Fourth FHR Benchmarking Workshop
  - Date: October, 2017
  - Location: TBD

The proposed dates for holding the subsequent three workshops are approximately based on the proposed MIT-IRP milestone schedule, but ideally can be coordinated with other large events to facilitate maximum participation. The date and location for the second FHR benchmarking workshop is chosen to directly precede the ICAPP 2016 conference in San Francisco. SINAP/ORNL combined meetings on the ORNL campus are also ideal for coordinating the IRPs' workshops as many of the key contributors will be present and ORNL has excellent facilities to host an FHR workshop. Each workshop may also consider hosting an ANS 20.1 FHR Safety Standard Meeting the day before the workshop.

The GT-IRP is also planning to hold workshops focused on performing V&V and PIRT-like activities for each of the three technical areas. The first neutronics workshop will be held at Georgia Tech on December 7-10, 2015. These workshops will be complimentary to the benchmarking focused workshops organized by the MIT-IRP, and there will be participation from both IRPs in both sets of workshops.

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