MSRE Transient Benchmark Development and Evaluation: NEUP Project Updates

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INTRODUCTION

Molten-Salt Reactor (MSR) is a class of advanced nuclear reactors with the unique feature that a molten salt mixture is used as both fuel and coolant of the reactor. MSR was among the original reactor designs back to the 1940's [1], and research on MSR has been conducted since then in pursuit of operation and safety advantages over water and other types of reactors. These advantages include: (1) its capability for online refueling, processing, and fission product removal, which eliminate the high costs for fuel fabrication and qualification, the need for reactor shutdown to refuel, and the need for large core excess reactivity; (2) a high coolant outlet temperature that supports high-efficiency downstream heat process; (3) a lower capital expenditure of the reactor vessel, thanks to the lower operating pressure; and (4) its inherent safety due to the liquid state and flowing nature of the fuel, allowing the fuel to be easily drained or pumped into a non-critical configuration when needed [2].

Because the liquid fuel also acts as the coolant in MSR, fission energy is predominantly released immediately into the coolant, and delayed neutron precursors and other fission products are all drifted by the fuel flow. Due to these unique physical features, MSR modeling is a particular challenge, and high-quality experimental data is desired for the validation of the computational models developed. Unfortunately, experimental data for MSR is very limited. The Molten Salt Reactor Experiment (MSRE), performed at Oak Ridge National Laboratory (ORNL) in the 1960s [3, 4], is currently the only collection of experimental data for this class of advanced reactor concepts. The University of California Berkeley (UCB) and ORNL have collaborated to build high-quality reactor statics models for the start-up zero power core of MSRE, including control rod worth measurement, reactivity coefficient measurement, and steady-state operating experiments [5]. This initial benchmark set for the MSRE was successfully developed and included in the 2019 edition of International Reactor Physics Experiment Evaluation Project (IRPhEP) handbook [6], whereas evaluations of MSRE transient experiments remain lacking. However, modeling accidental scenarios is crucial for MSR design and safety assessment, and transient

experiments performed in MSRE can provide precious data for the validation of the computational models.

Therefore, a new DOE NEUP project was recently established with the primary goal to develop a rigorous benchmark on the MSRE transient experiments and their associated uncertainties and to include them into IRPhEP handbook as a complementary to the current MSRE static benchmark. To have a thorough evaluation of the transient experiments performed at MSRE in the 1960s, the whole primary loop of MSRE will be modeled. The undocumented basic data will be regenerated from available experimental data by using advanced data-assimilation methods [7, 8] to facilitate the whole-loop modeling of the representative MSRE transients. Specifically, the following objectives will be achieved along with the MSRE transient benchmark development: (1) Specification of representative transient experiments and identification of missing data; (2) Regeneration of missing parameters through advanced dataassimilation methods; (3) Verification and validation of the experimental transient benchmark and uncertainty quantifications; (4) Documentation of the investigated experimental transients and submission for inclusion in the IRPhEP handbook.

The current efforts for this project mainly focus on the development of a simplified yet efficient multiphysics modeling and simulation platform to enable the transient analyses of MSRE experiments such as the pump startup test, pump coast down test, and thermal-convection heat-removal test. Both neutronics and thermal-hydraulics components are needed in the modeling platform. This summary gives an overview of the neutronics models in the platform and presents some preliminary results on the neutron and delayed neutron precursor (DNP) behavior in the entire primary loop of the MSRE. These results are obtained from the developed models using the COMSOL Multiphysics solvers [9].

METHOD

Governing Equations and Model Parameters

With standard notations, the time-dependent one dimensional (1D) two-group (2G) forward neutron diffusion equations for flowing fluid fuel at MSRE may be written as

$$\begin{cases} \frac{1}{v_1} \frac{\partial \phi_1}{\partial t} - \frac{\partial}{\partial x} \left[D_1 \frac{\partial \phi_1}{\partial x} \right] + \Sigma_{r,l} \phi_l = (1 - \beta) \left[v \Sigma_{f,l} \phi_l + v \Sigma_{f,2} \phi_2 \right] + \sum_{k=1}^K \lambda_k C_k, \\ \frac{1}{v_2} \frac{\partial \phi_2}{\partial t} - \frac{\partial}{\partial x} \left[D_2 \frac{\partial \phi_2}{\partial x} \right] + \Sigma_{a,2} \phi_2 = \Sigma_{s,l \to 2} \phi_l, \\ \frac{\partial C_k}{\partial t} + u \frac{\partial C_k}{\partial x} = \beta_k \left[v \Sigma_{f,l} \phi_l + v \Sigma_{f,2} \phi_2 \right] - \lambda_k C_k, \quad k = 1, \cdots, 6. \end{cases}$$
(1)

where u is the flow velocity and is assumed to be constant at this stage. The six-group DNP model is considered. The scope of this paper is limited to the *k*-eigenvalue mode calculation (i.e., steady-state), which is defined as

$$\begin{cases} -\frac{d}{dx} \left[D_1 \frac{d\phi_1}{dx} \right] + \sum_{r,l} \phi_l = \frac{1-\beta}{k_{eff}} \left[\nu \sum_{f,l} \phi_l + \nu \sum_{f,2} \phi_2 \right] + \sum_{k=1}^6 \lambda_k C_k, \\ -\frac{d}{dx} \left[D_2 \frac{d\phi_2}{dx} \right] + \sum_{a,2} \phi_2 = \sum_{s,l \to 2} \phi_l, \\ u \frac{dC_k}{dx} = \frac{\beta_k}{k_{eff}} \left[\nu \sum_{r,l} \phi_l + \nu \sum_{r,2} \phi_2 \right] - \lambda_k C_k, \quad k = 1, \cdots, 6. \end{cases}$$

$$(2)$$

The corresponding adjoint formulation of Eq.(2) can be derived and given by

$$\begin{cases} -\frac{d}{dx} \left[D_1 \frac{d\phi_1^*}{dx} \right] + \Sigma_{r,1} \phi_1^* = \frac{\nu \Sigma_{f,1}}{k_{eff}} \left[(1-\beta) \phi_1^* + \sum_{k=1}^6 \beta_k C_k^* \right] + \Sigma_{s,1 \to 2} \phi_2^*, \\ -\frac{d}{dx} \left[D_2 \frac{d\phi_2^*}{dx} \right] + \Sigma_{a,2} \phi_2^* = \frac{\nu \Sigma_{f,2}}{k_{eff}} \left[(1-\beta) \phi_1^* + \sum_{k=1}^6 \beta_k C_k^* \right], \\ -u \frac{dC_k^*}{dx} = \lambda_k \phi_1^* - \lambda_k C_k^*, \quad k = 1, \cdots, 6. \end{cases}$$

$$(3)$$

We are interested in the adjoint solutions as they will be used to produce adjoint weighted point kinetics parameters for MSRE transient analysis.

In this work, we follow one recent work by ORNL [10] and intend to predict the neutron and DNP distribution along the entire MSRE primary loop. We used the piecewise constant fluid velocity for each component in the loop provided in Ref. [10] as inputs to our model. It should be noted that we noticed some inconsistencies in the geometrical parameters and flow speeds provided in the reference. For instance, if the given flow speed (v) and component length (*l*) are used to calculate the residence time as

$$\tau = \frac{V}{Q} = \frac{A_{eff}l}{A_{eff}u} = \frac{l}{u}, \qquad (4)$$

where V is the component volume and Q is the volumetric flow rate. However, the calculated residence times greatly vary from the reported ones. Also, using a varying speed field in a 1D model clearly violates the flow continuity principle. To resolve these inconsistences, we first recalculate the flow speed in each segment to preserve the residence time. The geometrical parameters are provided in Table I. Note the pipe numbers in the table are consistent with the ones indicated in Ref. [10].

Table I. Geometrical Parameters of the MSRE Loop.

Component	τ (s)	<i>l</i> (m)	u (m/s)	
Lower Plenum	4.584	0.181	0.03948	
Core	8.809	1.498	0.17004	
Upper Plenum	4.266	0.174	0.040785	
Pipe 8-9	0.513	0.705	1.373872	
Pipe 9-10	0.273	0.376	1.375126	
Pump	0.412	0.566	1.37373	
Pipe 1-2	0.284	0.391	1.373538	
Heat Exchanger	2.292	5.897	2.572512	
Pipe 3-4	0.816	1.122	1.374086	
Outer Annulus	3.64	1.579	0.433704	

To overcome the limitation of the 1D model in accounting for the flow area changes along the primary loop, we rewrite Eq. (2) and (3) in terms of the DNP mass flow rate defined as:

$$\dot{m}_k = c_k Q = c_k u A \,. \tag{5}$$

Substituting Eq.(5) to Eq. (2), we have

$$\begin{cases} -\frac{d}{dx} \left[D_1 \frac{d\phi_1}{dx} \right] + \sum_{r,1} \phi_1 = \frac{1-\beta}{k_{eff}} \left[v \sum_{f,1} \phi_1 + v \sum_{f,2} \phi_2 \right] + \sum_{k=1}^6 \frac{\lambda_k}{Q} \dot{m}_k, \\ -\frac{d}{dx} \left[D_2 \frac{d\phi_2}{dx} \right] + \sum_{a,2} \phi_2 = \sum_{s_1 \to 2} \phi_1, \\ \frac{u}{Q} \frac{d\dot{m}_k}{dx} = \frac{\beta_k}{k_{eff}} \left[v \sum_{r,1} \phi_1 + v \sum_{r,2} \phi_2 \right] - \frac{\lambda_k}{Q} \dot{m}_k, \quad k = 1, \cdots, 6. \end{cases}$$
(6)

Similar equations can be obtained for the adjoint system.

The delayed neutron fractions, decay constants, and homogenized cross sections used in the model were generated by SERPENT [11] following the MSRE developed in Ref. [12]. The two-group homogenous cross sections were generated by assuming one homogenized region for the core. The cutoff energy for the thermal group is 0.625 eV. The cross section and DNP data are summarized in TABLE II and TABLE III, respectively.

TABLE II. Homogenized Cross Sections of the MSRE Core.

Parameter	Value		
<i>D</i> ₁ [<i>cm</i>]	1.18219		
$D_2[cm]$	0.840635		
$\Sigma_{r,1} [cm^{-1}]$	0.004591		
$\Sigma_{a,2} [cm^{-1}]$	0.008244		
$\Sigma_{s,1\rightarrow 2} [cm^{-1}]$	0.003326		
$\nu \Sigma_{f,1} [cm^{-1}]$	0.000698		
$\nu \Sigma_{f,2} [cm^{-1}]$	0.010374		

Group	1	2	3	4	5	6
eta / 10 ⁻⁵	20.7	106.9	104.1	296.2	86.2	30.8
$\lambda [s^{-1}]$	0.012	0.031	0.109	0.317	1.35	8.64

TABLE III. DNP Parameters Used in the Analysis.

COMOL Multiphysics Implementations

The generic partial differential equation (PDE) solvers embedded in the COMSOL Multiphysics platform [9] was called to solve the governing equations for MSRE models. The general eigenvalue coefficient form PDE model in COMSOL takes the following form

$$\lambda^2 e_a \hat{\phi} - \lambda d_a \hat{\phi} + \nabla \cdot \left(-c \nabla \hat{\phi} - \alpha \hat{\phi} + \gamma \right) + \beta \cdot \nabla \hat{\phi} + a \hat{\phi} = f , \qquad (7)$$

where the coefficients must be defined to match the MSRE diffusion model, and $\hat{\phi}$ needs to be set as a vector of eight unknowns

$$\hat{\boldsymbol{\phi}} = \left[\boldsymbol{\phi}_1, \boldsymbol{\phi}_2, \dot{\boldsymbol{m}}_1, \cdots, \dot{\boldsymbol{m}}_6\right]^T \tag{8}$$

to cover all the unknowns in the model. For this purpose, ϕ_1 and ϕ_2 represents the neutron flux for group 1 and 2, respectively. And $\dot{m}_k (k = 1, \dots, 6)$ represents the DNP mass flow rate. The same approach is used to solve the adjoint problem.

The system of equations was assumed to be subjected to the zero-incoming neutron flux and the corresponding zerooutgoing adjoint flux at the entrance of the lower plenum and the exit of the upper plenum. Following the COMSOL generic forms, the boundary conditions are given as

$$-\vec{n}\cdot\left(-c\nabla\hat{\phi}\right) = -q\hat{\phi}\,,\tag{9}$$

where the constant parameter q is given as

$$q = \left[\frac{1}{2}, \frac{1}{2}, 0, \cdots, 0\right]^{T}.$$
 (10)

The periodic boundary condition was assumed for the DNP equations by implying the continuity of DNP mass flow rate

$$\dot{m}_k(0) = \dot{m}_k(L),$$
 (11)

where L is the total length of the primary loop..

The *k*-eigenvalue of the system is obtained based on the ARPACK (ARnoldi PACKage) search algorithm. The algorithm uses Implicitly Restarted Arnoldi Method (IRAM) to search for a few eigenvalues and the corresponding eigenfunctions in a predefined search region. We searched for the closest eigenvalue to 1.0 with relative tolerance for convergence equals to 1.0E-6.

RESULTS

We used a pre-defined, piecewise constant velocity filed as input parameters in the 1D model. The velocity field distribution along the different components of the primary loop is given in Table I. The volumetric flow rate is set to be $Q = 1200 \ gpm = 0.0756 \ m^3/s$.

The forward flux, forward DNP concentration, adjoint flux, and adjoint DNP concentration are shown in Fig. 1 to Fig. 4, respectively. Note the dashed lines separate different components in the primary loop. The value of $k_{eff} = 0.96809$ for both forward and adjoint systems.



Fig. 1. Flux distribution for the MSRE primary loop.



Fig. 2. DNP concentration in the MSRE primary loop.



Fig. 3. Adjoint flux distribution for MSRE primary loop.



Fig. 4. Adjoint DNP concentration in MSRE primary loop.

The neutron flux and DNP solutions are normalized to the same power rate with constant flow velocity assumed. The DNP is calculated in the form of DNP mass flow rate (see Eq.(6)), and the corresponding DNP concentration is obtained by dividing the DNP mass flow rate by the volumetric flow rate. As can be seen from Fig. 2 and Fig. 4, mainly due to the DNP drifting effect, both the forward and adjoint solution of DNP concentrations are shown with asymmetric characteristics in the axial direction in the core, and different group of DNP has shown with different level of skewness in the distribution profile.

The limitation on the 1D representation was overcame by solving for the mass flow rate instead of directly solving for the concentration. In the later approach, the concentration is non-physical due to the lost information regarding the changing cross sections between segments.

SUMMARY & FUTURE WORK

As part of the neutronics model development for the MSRE transient benchmark evaluation project, the steadystate 1D 2G neutron diffusion model coupled with six DNP groups was established with a representative MSRE 1D geometry, and solved by the COMSOL Multiphysics platform. Both the forward and adjoint system of equations were solved. The homogeneous cross sections and DNP data were generated using Serpent code. The core, lower plenum, and upper plenum were considered as one homogenized region. The zero incoming flux (zero outgoing adjoint) is considered as boundary condition for this homogenized region. Periodic boundary conditions were considered for the DNP mass flow rate. A piecewise constant fluid flow, in which the speed changes discontinuously between regions, was considered in the model.

As an ongoing NEUP project, many works are scheduled ahead to be accomplished in the near future. On the computational model aspect, the current 1D 2G model is expected to be expanded to 2D/3D multigroup models for more precise predictions. The zero-incoming flux boundary condition will be relaxed to account for more accurate leakage effect of the core. The system level thermal hydraulics model is also expected to be developed to provide a multiphysics coupling calculation capability for the benchmark development. The selected MSRE transient experiments will be examined carefully to eventually develop a rigorous transient benchmark for the IRPhEP handbook.

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REFERENCES

- E. P. WIGNER, A. M. WEINBERG, G. YOUNG, "Preliminary Calculations on a Breeder with Circulating Uranium," In: A. M. Weinberg (eds) Nuclear Energy. The Collected Works of Eugene Paul Wigner, Vol A / 5. Springer, Berlin, Heidelberg (1992).
- 2. T. J. DOLAN, *Molten Salt Reactors and Thorium Energy*, Woodhead Publishing (2017).
- R. C. ROBERTSON, "MSRE Design and Operations Report Part 1: Description of Reactor Design," ORNL-TM-728, ORNL (1965).
- B.E. PRINCE et al., "Zero-power Physics Experiments on the Molten-Salt Reactor Experiment," ORNL-4233, ORNL (1968).
- M. FRATONI et al., "Molten Salt Reactor Experiment Benchmark Evaluation (NEUP Project 16-10240)", Tech. Report, University of California Berkeley (2020).
- 6. J. BESS et al., "The 2019 Edition of the IRPhEP Handbook," *Trans. Am. Nucl. Soc.*, **121**, 1565 (2019).
- C. LU and Z. WU, "A Preliminary Study on the Use of the Linear Regression Method for Multigroup Cross-Section Interpretation," *Nucl. Sci. Eng.*, **195**(4) (2021).
- C. LU et al., "Enhancing the 1-D SFR Thermal Stratification Model via Advanced Inverse Uncertainty Quantification Methods," *Nucl. Tech.*, 207(5) (2020).
- 9. COMSOL Multiphysics Reference Manual, COMSOL Multiphysics® (2014).
- K. LEE et al., "Transient Convective Delayed Neutron Precursors of ²³⁵U for the Molten Salt Reactor Experiment", *PHYSOR 2022 proceedings*, (2022).
- J. LEPPÄNEN et al., "The Serpent Monte Carlo code: Status, development and applications in 2013," Ann. Nucl. Energy, 82 (2015).
- 12. D. SHEN et al., "Reactor Physics Benchmark of the First Criticality in the Molten Salt Reactor Experiment," *Nucl. Sci. Eng.*, **195**(8) (2021).