Computational Modeling and Verification of MSR Transients via MSRE Reactivity Insertion Tests

M. Elhareef[1], T. Fei[2], and Z. Wu[1,*]

[1]Department of Mechanical and Nuclear Engineering,
Virginia Commonwealth University, Richmond VA 23284;

[2]Division of Nuclear Science and Engineering,
Argonne National Laboratory, Lemont, IL 60439.

[leave space for DOI, which will be inserted by ANS]

ABSTRACT

The liquid fueled Molten Salt Reactors (MSRs) are currently undergoing significant and extensive development with several computational codes being developed and validated. The Molten Salt Reactor Experiment (MSRE) is a reliable experimental data on verification and validation of the MSR simulation tools. In this work, a neutronics/thermal-hydraulics coupled computational model for MSRs is being developed for reactor transient analysis. The model employs one-dimensional (1D) formulations of mass, momentum, and energy conservation to model the heat and mass transfer in pipes and the transport of diluted species in MSR. The model also employs the reactor point kinetics model customized for flowing fuel to model the reactor power. A reactivity model is adopted to count the proper thermal feedback in the coupled system. The model is implemented in the pipe flow module using COMSOL Multiphysics. The developed computational model is applied to a set of MSRE reactivity insertion tests, which were conducted at 1MW, 5MW, and 8MW thermal power, respectively. The simulation results are graphically compared to the experimental results as well as other computational results from literature to provide validation and verification of the developed model. The results are generally shown in good agreement with the experimental and computational data with some unresolved discrepancies in the power response.

Keywords: Molten Salt Reactors; MSRE; COMSOL Multiphysics; circulating fuel point kinetics equation; coupled neutronics/thermal-hydraulics calculations.

1. INTRODUCTION

The interest in Molten Salt Reactors (MSRs) was renewed after considering it as one of the six Generation IV nuclear reactors chosen by the international forum (GIF) [1]. The liquid fueled Molten Salt Reactor (MSR) design employs a molten salt mixture as both fuel and coolant. This design gives this class of reactors unique features due to the flowing nature of the fuel. The flow of the fuel outside the core creates a strong coupling between the neutronics and thermal hydraulics characteristics of the reactor. The salt mixture carries the fuel and the fission products through the fuel circulation loop causing a fraction of the delayed neutron precursors to decay outside the active core. The flowing fuel also results in the redistribution of the delayed neutron source when the fuel salt flow rate changes. These features make

*zwu@vcu.edu

modeling this class of reactors challenging to the current LWRs modeling tools and demand the development of new tools that have the capability to model these features.

One crucial step in the development of new modeling tools is code validation. In this step, the code is tested against the available experimental data to verify the accuracy of the simulation results. The Molten Salt Reactor Experiment (MSRE) [2] represents the only extensive set of reliable experimental data source for MSRs. The MSRE was operated at ORNL between 1965 and 1969. The MSRE was a 10 MW thermal-spectrum reactor that is cooled by a FLiBe molten salt mixture and moderated by graphite. The MSRE had two operation phases. ^{235}U was used as fuel during the first phase while ^{233}U was used in the second phase. The objectives of this experiment were to demonstrate the MSR concept, verify the safety and serviceability of the liquid fuel; and test the materials under operation conditions. During its operation, several static, dynamic, and transient tests were conducted.

In this work, a neutronics/thermal-hydraulics coupled computational tool for MSRs is being developed. The Finite Element Method (FEM) based commercial tool COMSOL Multiphysics [3] is employed to solve the coupled Neutronics/Thermal-hydraulics model for the flowing fuel system. A set of reactivity insertion tests during the ^{233}U operation phase are used to validate the computational model. This paper is organized as follows: the mathematical model is provided in Section 2, an overview introduction of MSRE system and reactivity insertion test specifications are provided in Section 3, and the results and discussion are provided in Section 4 with some concluding remarks offered at the end of the paper.

2. MATHEMATICAL MODELS

A quasi one-dimensional (1D) model is used for the fluid flow in pipes and for the DNP concentration. With standard notations, the conservation equations for the mass, momentum, and energy of the salt flow can be described as [4]

$$A\frac{\partial \rho}{\partial t}+\frac{\partial}{\partial z}\left(A\rho u\right)=0, \tag{1a}$$

$$\rho\frac{\partial u}{\partial t}+\rho u\cdot\frac{\partial u}{\partial z}=-\frac{\partial p}{\partial z}-f_D\frac{\rho}{2d_h}u|u|+F, \tag{1b}$$

$$\rho_f c_p^f A\left(\frac{\partial T_f}{\partial t}+u\frac{\partial T_f}{\partial z}\right)=\dot{q}_{source}^f+A\frac{\partial}{\partial z}\left(k_f\frac{\partial T_f}{\partial z}\right). \tag{1c}$$

The heat source term $\dot{q}_{source}^f$ accounts for the heat generation in the core and the heat transfer between the fuel and the moderator matrix in the core and with the secondary coolant in the HEX respectively. The energy balance of the graphite in given by the 1D heat equation:

$$\rho_m c_p^m\frac{\partial T_m}{\partial t}=\dot{q}_{gen}^m+\frac{\partial}{\partial z}\left(k_m\frac{\partial T_m}{\partial z}\right). \tag{2}$$

The DNP concentration in the fuel circulation loop is described by the 1D drift-diffusion model:

$$A\frac{\partial c_k}{\partial t}+Au\frac{\partial c_k}{\partial z}=\frac{\partial}{\partial z}\left(AD_k\frac{\partial c_k}{\partial z}\right)+A\beta_i\sum_g \nu\Sigma_{fg}\varphi_g-A\lambda_k c_k,\quad k=1,\cdots,6. \tag{3}$$

Here c_k is the concentration of the k^{th} family precursor in units of *precursors/m^3*, and D_k is the diffusion coefficient of the k^{th} family and is considered constant and equal $10^{-9}m^2/s$.

The power shape is obtained by means of 1D, leakage-corrected diffusion model [5] at the steady state flowing core condition. The power shape is considered constant during any transient. The power magnitude is obtained using the point kinetics equation for circulating fuel:

$$\frac{dn}{dt} = \frac{\rho(t) - \beta_M}{\Lambda} n(t) + \frac{1}{\Lambda} \sum_{k=1}^{6} \beta_{M,k} \frac{\tilde{C}_k(t)}{\tilde{C}_{k0}} \tag{4}$$

where $\beta_{M,k}$ is the effective DNP fraction of the k^{th} family at steady state flowing conditions and is given by:

$$\beta_{M,k} = \frac{\lambda_k \int_0^L c_k(z,0)\, dV}{(1-\beta) \int_0^L \sum_g \Sigma_{f,g} \varphi_g(z,0)\, dV + \int_0^L \sum_k \lambda_k c_k(z,0)\, dV}, \tag{5}$$

$\rho(t)$ is total reactivity and is given by:

$$\rho(t) = \rho_{ext}(t) + \alpha_f \left(\tilde{T}_f - \tilde{T}_{f0}\right) + \alpha_m \left(\tilde{T}_m - \tilde{T}_{m0}\right), \tag{6}$$

where $\rho_{ext}(t)$ is the external reactivity such as reactivity contribution from control elements, α_f and α_m are reactivity feedback coefficients for the fuel and moderator, respectively. Other lumped feedback parameters are defined as:

$$\tilde{T}_f = \frac{1}{L} \int_0^L T_f(z,t)\, dz, \tag{7a}$$

$$\tilde{T}_m = \frac{1}{L} \int_0^L T_m(z,t)\, dz, \tag{7b}$$

$$\tilde{C}_k = \int_0^L c_k(z,t)\, dV. \tag{7c}$$

The mathematical model is implemented in COMSOL pipe flow module [6] coupled with the coefficient form PDE.

3. MSRE DESCRIPTION

3.1. MSRE system and parameters

During the MSRE operation, the fuel salt enters the cylindrical reactor vessel through an annular volute around the top of the cylinder and flows downwards between the vessel and the graphite matrix. A dished head at the bottom forces the flow in the upward direction through stadium-shaped passages in the graphite matrix to the top head. The fuel then flows the suction line of the primary pump and then discharge to the shell side of a U-tube heat exchanger. A secondary fluoride melt (LIF-BeF2, 66-34 mole %) is used to cool the fuel salt [7]. The coolant salt is circulated in the tube side in the HEX and then travels to the suction line of the coolant pump before it dissipates heat to air through the radiator. The salt volume in the secondary loop is 45.83 ft^3. A schematic representation of the MSRE salt circulation loops is shown in Figure 1.

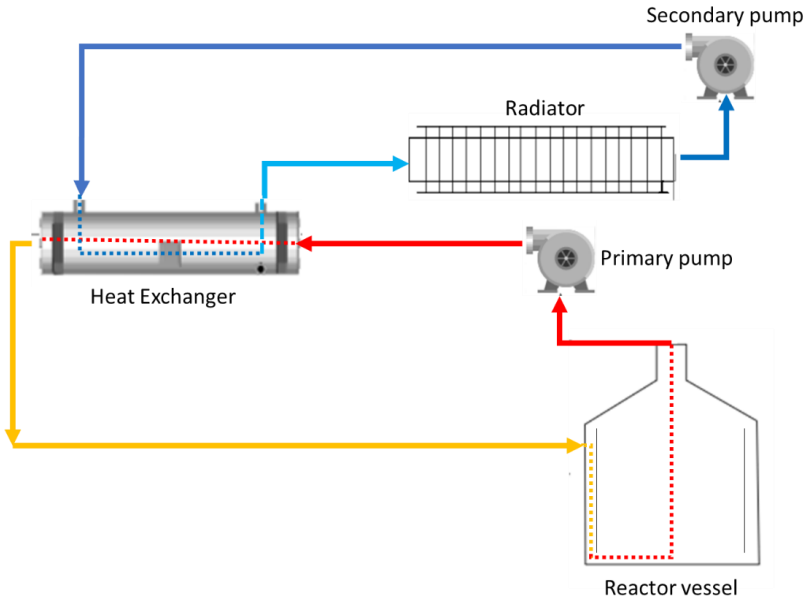

Figure 1 Schematic representation of the MSRE salt circulation loops.

To cast the MSRE geometry into 1D representation, the physical length of each component is used. An effective flow area is calculated to preserve the salt volume inside each component. The MSRE primary loop geometrical parameters are summarized in Table I. The thermophysical parameters of the fuel salt and the coolant salt are listed in Table II.

Table I. Geometrical parameters of the MSRE fuel circulation loop [7].

Component	Length [m]	Effective flow area [m²]	Volume [m³]	Residence time [s]
Lower plenum	0.34	0.827	0.2832	3.7
Core	1.67	0.425	0.7080	9.3
Upper plenum	0.35	0.850	0.2973	3.9
Line 100 (vessel to pump) horizontal	1.83	0.013	0.0232	0.3
Line 100 (vessel to pump) vertical	0.81	0.045	0.0363	0.5
Pump	1.94	0.060	0.1161	1.5
Line 101 (pump to HX)	1.79	0.013	0.0227	0.3
Heat exchanger	2.44	0.071	0.1727	2.3
Line 102 (HX to vessel)	4.92	0.013	0.0623	0.8
Distributor + downcomer	2.36	0.116	0.2747	3.6
Total			1.9963	26.3

Table II. Thermophysical properties of the MSRE fuel salt and coolant salt [8].

Property	Unit	Fuel salt	Coolant salt
Density ρ	kg/m^3	$2553.3-0.562T$	$2146.3-0.488T$
Heat Capacity c_p	$J/kg\cdot K$	2009.66	2390.0
Thermal conductivity k	$W/m\cdot K$	1.0	1.1
Dynamic viscosity μ	$Pa\cdot s$	$8.4\times10^{-5}e^{\frac{4340}{T}}$	$1.16\times10^{-4}e^{\frac{3455}{T}}$

The thermophysical parameters of the MSRE graphite are given in Table III.

Table III. Thermophysical properties of the MSRE moderator [9].

Parameter	Unit	Value
Density ρ	kg/m^3	1860
Heat Capacity c_p	$J/kg\cdot K$	1758.456
Thermal conductivity k	$W/m\cdot K$	58.8

The reactor dynamic parameters of the MSRE during for the ^{233}U fuel are given in Table IV.

Table IV. Reactor dynamic parameters used of the MSRE for the ^{233}U fuel [10].

Group	Decay constant $\lambda_i\left[s^{-1}\right]$	Delayed Neutron fraction $\beta_i\left[\times10^{-4}\right]$
1	0.012	2.28
2	0.034	3.85
3	0.139	6.64
4	0.325	7.36
5	1.130	1.36
6	2.500	0.88
Prompt neutron generation time $\Lambda\left[s\right]$		4×10^{-4}
Fuel salt temperature coefficient of reactivity $\alpha_f\left[\mathrm{pcm}/K\right]$		-11.034
Moderator temperature coefficient of reactivity $\alpha_m\left[\mathrm{pcm}/K\right]$		-5.814

3.2. MSRE reactivity insertion tests

The purpose of the MSRE reactivity insertion tests was to determine the response of the reactor to external reactivity insertion. The experimental tests were conducted by withdrawing the control rod to insert a predefined reactivity while fixing all other parameters and measuring the reactor power response. The tests were conducted at three power levels and the corresponding reactivity insertion are listed in Table V. It's important to note that the magnitude of the inserted reactivity for the 1MW and the 8MW tests are reversed with each other in the original document (i.e., Ref. [11]). The presented data in Table V is the corrected version. It was shown that the experimental measurements for the reactivity insertion test have a large noise level [11]. This noise was attributed to the existence of a large void percentage circulating in the primary loop.

Table V. External reactivity insertion in the MSRE reactivity insertion tests [11].

Power [MW]	External reactivity ρ_{ext} [pcm]
1	24.8
5	19
8	13.9

To simulate the reactivity insertion test, both the primary and secondary loops are modeled. The reactor core is modeled as a single heated channel. The primary side heat exchanger is modeled as a single cooled channel while the secondary side is modeled as a U-tube pipe with heated walls. Both the primary and secondary pumps are modeled by a fixed flow-rate points. The ultimate heat sink (i.e., the radiator) is molded by assuming fixed air ambient temperature at the radiator. Each of the primary loop, secondary loop, and graphite matrix is defined as a separate component.

The primary loop is defined in the pipe flow module which is used to model the fluid flow, heat transfer, and the transport of the DNPs. Heat generation in the fuel salt is modeled by assuming a fixed power-shape function that is obtained by solving the steady-state, 2G neutron diffusion equation [5]. The magnitude of the power is modeled using the PKE. A similar approach is used to model the production rate of the DNPs in the reactor vessel. The heat generated directly in the fuel salt is assumed to be 93.7% of the total core power. The remaining power is generated in the graphite matrix. Heat is transferred between the graphite matrix and the flow channel through heat convection assuming a constant heat transfer coefficient which is calibrated to match the designed temperature drop between the graphite and the fuel salt at nominal conditions which is $28^{\circ}F$ [12]. Heat transfer between the primary and secondary salt is modeled using a wall heat transfer boundary condition.

The secondary loop also modeled in the pipe flow module. The heat transfer between the secondary salt and the air in the radiator is modeled by assuming a fixed heat transfer coefficient and fixed air temperature ($100^{\circ}F$). The fixed heat transfer coefficient is considered a function of the initial power of the reactor. This is equivalent of adjusting the radiator door opening to keep the salt temperature within the operational limits. The temperature of graphite matrix is modeled using the 1D heat conduction equation. The heat generation in graphite is 6.3% of the core power. The graphite matrix is subject to the convection boundary condition.

The system of equation is solved using a fully coupled scheme. The Generalized alpha method is used for time stepping. The initial conditions for each test are obtained by a stationary step followed by a time dependent step with zero reactivity insertion to insure that the simulation starts from exact steady state.

The circulating DNP fractions (Eq. (5)) at steady state flowing conditions are listed in Table VI.

Table VI. The effective DNPs fraction for the ^{233}U load at nominal flow rate.

Group	1	2	3	4	5	6	total
$\lambda\ [s^{-1}]$	0.0126	0.037	0.139	0.325	1.35	2.5	-
$\beta/10^{-5}$	22.8	78.8	66.4	73.6	13.6	8.8	264.0
$\beta_M/10^{-5}$	15.5	53.8	49.6	64.8	13.4	8.8	205.9

4. RESULTS AND DISCUSSIONS

The core response to the reactivity insertion at 5MW is shown in Figure 2 as an example for the reactor response. As shown in the figures, the MSRE configuration has slower response at lower power levels. The results show that the prompt power increase is accompanied by a rapid increase in the fuel temperature. Following the prompt peak, the negative reactivity feedback balances the external reactivity which causes a plateau in the power response. After about 25 seconds, the hot fuel generated in the prompt power increase returns to the core causing rapid power decrease. This is followed by oscillations with a period of 25 seconds until the core returns to its initial power. These oscillations are associated with the circulation of the hot salt plug that was produced during the prompt temperature rise. The moderator temperature increases gradually until steady state condition is achieved.

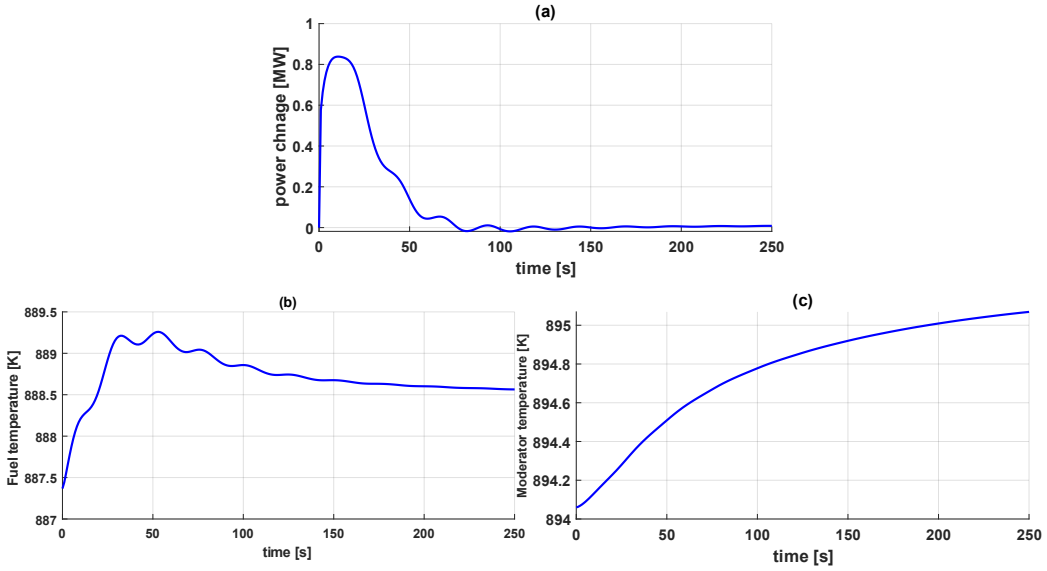

Figure 2. Calculated response for 19.0 pcm reactivity insertion at 5MW, (a) is the power change, (b) is the core fuel average temperature, and (c) is the moderator average temperature.

Serval models were developed for the MSRE transients and their results for the reactivity insertion tests are available in literature. In the following part, a comparison between these models and their results for the MSRE reactivity insertion tests is discussed.

ORNL [10] developed a model that used a multi-region lumped representation of the MSRE components including the secondary loop. The core region was represented by nine regions. In this model, a two-seconds time lag component was added to the exit of the reactor vessel to compensate for the insufficient mixing in the model. Zanetti et. al. [13], used a multiscale representation of the MSRE where the core is divided into three radial channels. The core channels are molded as 3D components while the remaining components

are modeled as 0D. Zanetti et. al. [14] developed a 1D model for the MSRE using SCALE code. The code was extended by including the 1D DNP and decay heat advection-diffusion equation. Both the primary and secondary loops are considered. A SAM model of the MSRE reactivity insertion tests was also used. The model was limited to the primary loop components and the fixed HEX inlet temperature was imposed on the secondary salt. The input files of the SAM model can be found in the NRIC virtual test bed repository [15]. All the mentioned models used the point kinetics equation to model the reactor power.

The results of the current work compared to the experimental results and the four models described above are shown graphically in Figure 3 Figure 4 and Figure 5 for the reactivity insertion tests at 8 MW, 5 MW, and 1 MW respectively. For the 1 MW test, only the results from the SCALE model are available.

For the three cases, all the models converge essentially to the same power level except for SAM model which converges to a slightly higher power level. This is mainly due to the adoption of the fixed HEX inlet temperature boundary condition. On the other hand, more variations are observed in the initial response.

For the 8MW test, the current model overestimates the prompt power rise compared to the experimental data. However, the prompt peak is in good agreement with the other models. The fuel prompt temperature change is in good agreement among all models except for ORNL model which shows larger fuel temperature rise. The discrepancy in the prompt power between the current model and both Zanette and SCALE models may be a result of the adoption of different reactivity feedback coefficients in these models. There is good agreement between the current model and SAM model. A similar behavior is also observed for the 5 MW test. For this test, more discrepancy in the graphite temperature is observed for Zanette and SCALE models. For the 1MW test, good agreement in the power response is observed among the available models. The fuel temperature oscillations are more visible in the current model compared to the SAM model and it's not observed in SCALE model.

The large noise level exists in the measured response and the lack of uncertainty quantification of the measurements renders the estimation of errors in the simulated results difficult. An uncertainty quantification step is required to provide the best estimate of the measured data and the uncertainty interval which are needed to evaluate the error metrics of the computational model. The uncertainty quantification of the experimental measurements is the subject of an ongoing study.

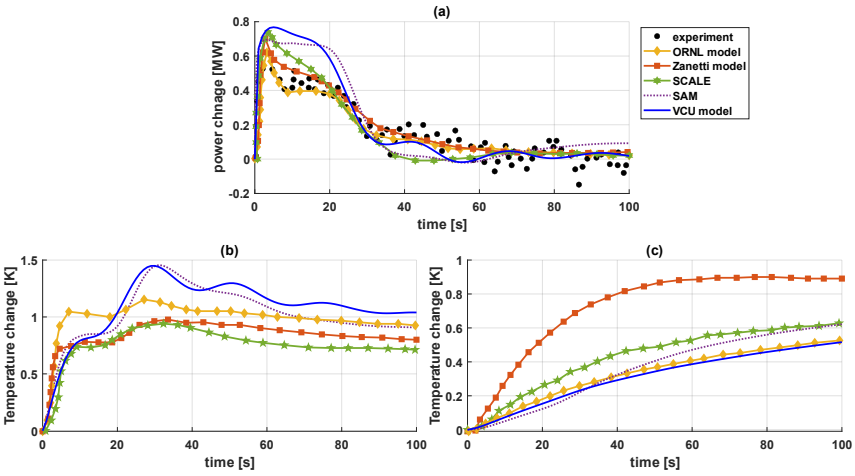

Figure 3. The response to a 13.9 pcm reactivity insertion at 8 MW initial power, (a) is the power response, (b) is the change in the salt average temperature in the core, and (c) is the change in the moderator average temperature.

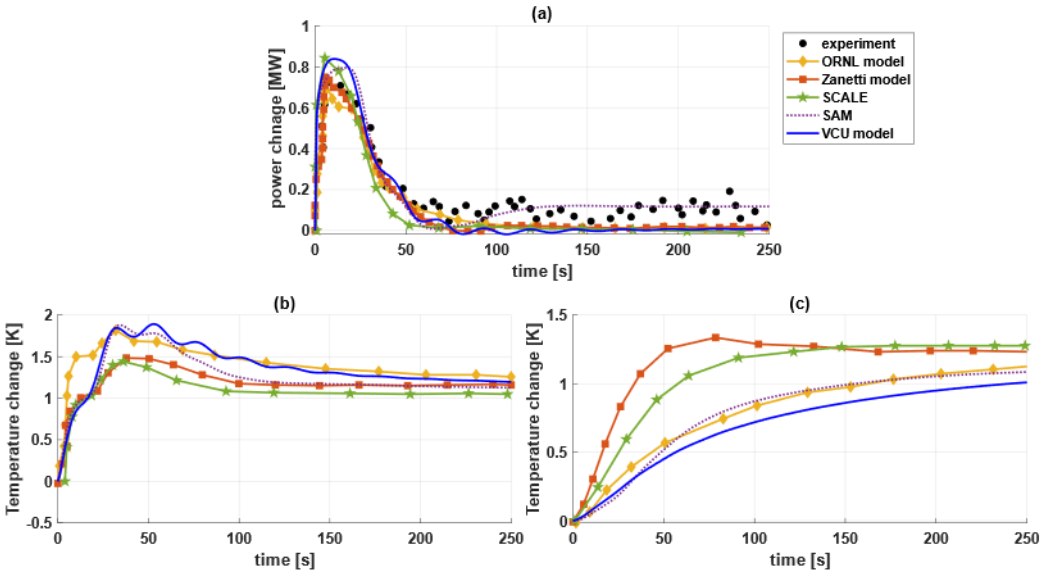

Figure 4. The response to a 19.0 pcm reactivity insertion at 5 MW initial power, (a) is the power response, (b) is the change in the salt average temperature in the core, and (c) is the change in the moderator average temperature.

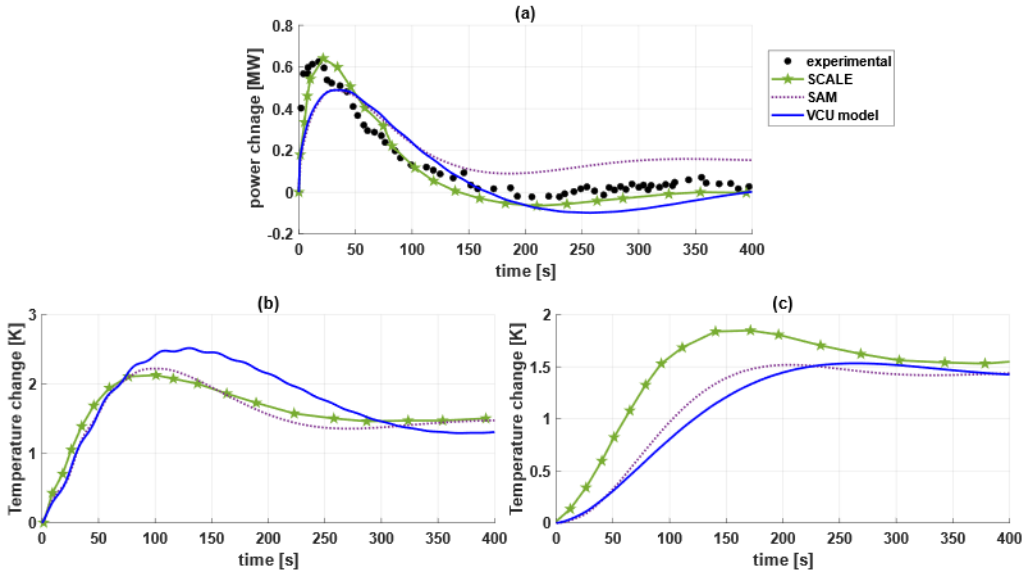

Figure 5. The response to a 24.8 pcm reactivity insertion at 1 MW initial power, (a) is the power response, (b) is the change in the salt average temperature in the core, and (c) is the change in the moderator average temperature.

5. CONCLUSIONS

A computational model for MSRs was developed and implemented using COMSOL Multiphysics. The model employs a 1D pipe flow model for the fluid flow and the transport of diluted species, and the point kinetics equation for the core power. The model was used in benchmarking the reactivity insertion tests

conducted during the MSRE operation. This set of tests were conducted by inserting a step reactivity of a predefined magnitude and observing the power response. To simulate this set of tests, a model of the MSRE primary loop and secondary loop was developed with a fixed ambient temperature at the ultimate heat sink (i.e., the radiator) was imposed. The results of the simulation are in good agreement with the experimental data. The model results were also verified against other results in literature. There is general agreement among the computational results with unresolved discrepancies in the power and temperature evolutions. The current results may be enhanced by employing a multichannel representation of the reactor core and/or higher spatial-resolution model for the neutronics behavior.

ACKNOWLEDGMENTS

This work is performed with the support of U.S. Department of Energy's Nuclear Energy University Program (NEUP) with the Award No. DE-NE0009162.

REFERENCES

[1]. Gen IV International Forum - GIF, 2010 Annual Report. OECD Nuclear Energy Agency, (2010).

[2]. P. N. Haubenreich, and J. R. Engel, "Experience with the Molten-Salt Reactor Experiment, Nuclear Applications and Technology," **8**(2), 118-136 (1970).

[3]. COMSOL Multiphysics® v. 6.1. www.comsol.com. COMSOL AB, Stockholm, Sweden.

[4]. N. E. Todreas and M. S. Kazimi. *Nuclear Systems. Volume 1 Thermal Hydraulic Fundamentals*. 2nd ed., Taylor & Francis, London (2011).

[5]. M. Elhareef, Z. Wu, and M. Fratoni, "A Consistent One-Dimensional Multigroup Diffusion Model for Molten Salt Reactor Neutronics Calculations," *Journal of Nuclear Engineering*, 4(4):654-667, (2023).

[6]. Pipe Flow Module User's Guide, COMSOL Multiphysics® v. 6.1. COMSOL AB, Stockholm, Sweden, (2022).

[7]. R. C. ROBERTSON, "MSRE Design and Operations Report Part 1: Description of Reactor Design," ORNL-TM-728, ORNL (1965).

[8]. S Cantor, "Physical Properties of Molten-Salt Reactor Fuel, Coolant, and Flush Salts," Technical Report ORNL-TM-2316, Oak Ridge National Laboratory, Oak Ridge, TN, (1968).

[9]. R. B. Briggs, "Molten-Salt Reactor Program Semi-annual Progress Report," ORNL, Oak Ridge, Tennessee, ORNL-3708, (1964).

[10]. R. C. Steffy and P. J. Wood, "Theoretical Dynamic Analysis of the MSRE with U-233 Fuel," Oak Ridge National Laboratory, ORNL-TM-2571, July (1969).

[11]. R.C. Steffy Jr., "Experimental Dynamic Analysis of the MSRE with U-233 Fuel," ORNL-TM-2997, Oak Ridge National Laboratory, April (1970).

[12]. R. B. Briggs, "Molten-Salt Reactor Program Semi-annual Progress Report," ORNL, Oak Ridge, Tennessee, ORNL-3369, 1962.

[13]. M. Zanetti, A. Cammi, L. Luzzi, "Extension of The FAST Code System for The Modelling and Simulation of MSR Dynamics," in Proceedings of ICAPP 2015, Nice, France, May 03-06, (2015).

[14]. M. Zanetti et al., "An innovative approach to dynamics modeling and simulations of the Molten Salt Reactor Experiment". Proc. Int. Conference PHYSOR 2014, Kyoto, Japan (2014).

[15]. The National Reactor Innovation Center's (NRIC) Virtual Test Bed Repository, https://github.com/idaholab/virtual_test_bed/tree/devel/msr/msre/reactivity_insertion, Date cited: Jan (2024).