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Verification and Validation Activities of Molten Salt Reactors Multiphysics Coupling Schemes at Idaho National Laboratory

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ABSTRACT

This paper presents the latest verification and validation activities in molten salt reactor modeling and simulation performed at Idaho National Laboratory. Multiphysics solutions are obtained by coupling the neutronics code Griffin, the thermal hydraulics code Pronghorn, and the system analysis code SAM, under the MOOSE framework. We present various multiphysics coupling schemes with these codes for molten salt reactor problems and provide verification and validation results. First, we present verification test results of the Griffin-Pronghorn coupled scheme for the CNRS benchmark. Then validation test results are presented for the Griffin-SAM coupled scheme for the pump startup and coast down transients of the Molten Salt Reactor Experiment. Finally, the Griffin-Pronghorn-SAM coupled scheme is demonstrated for the Molten Salt Reactor Experiment reactivity insertion transient using a domain-overlapping coupling algorithm between Pronghorn and SAM. The results of these various coupling schemes demonstrate the ability to capture the effect of fuel flow and the various feedback mechanisms important to MSRs.

Keywords: Multiphysics coupling, MSRs, DNPs, MSRE

1. INTRODUCTION

Molten salt reactors (MSRs) with liquid flowing fuel regained a wide interest worldwide for their safety features including low operating pressure, elimination of hydrogen evolution, and passive decay heat removal. The flow of the liquid fuel within the primary loop results in a strong coupling between neutronics and thermal-hydraulics since 1) the fuel generates and removes the heat from the active core and 2) the partial decay of delayed neutron precursors (DNPs) outside the core region alters the reactor kinetic response. This requires coupled multiphysics modeling and simulation to incorporate the strongly coupled physics and the accompanied DNPs transport.

Several efforts are ongoing at Idaho National Laboratory (INL) to develop modeling and simulation tools for advanced reactors to serve its mission of supporting the deployment of advanced reactors, including MSRs. The reactor multiphysics code Griffin [1] and thermal-hydraulics code Pronghorn [2], which are built upon the MOOSE (Multiphysics Object-Oriented Simulation Environment) framework [3], have been recently extended to handle the flowing fuel of MSRs with DNPs drift. Also, the System Analysis Module (SAM) [4] is being coupled to Griffin for MSRs analysis. Both Pronghorn and SAM are codes developed by the DOE Nuclear Energy Advanced Modeling and Simulation (NEAMS) program for analysis of advanced nuclear

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reactors. Pronghorn is mainly developed for analyzing multi-dimensional core flow conditions, while SAM is developed for system analysis including pumps and heat exchangers.

We demonstrate Multiphysics coupling schemes for different MSR applications. The Griffin-Pronghorn coupled scheme is utilized for problems that require multidimensional modeling of the reactor and the drift of the DNPs without considering the outer loop. While the Griffin-SAM coupled scheme is utilized for problems where the outer loop is modeled to capture the reactivity losses and the decay of the DNPs in that region. On the other hand, it is desirable to couple Pronghorn and SAM to obtain a self-consistent solution in the core and the outer loop which was performed with the domain-overlapping coupling approach and coupled to Griffin. Due to the multidimensional flow characteristics of MSRs it might be desirable to perform the modeling of the entire primary system with Pronghorn and couple to the system code via the heat-exchanger.

This work highlights recent verification and validation activities for different Multiphysics coupled schemes for MSR applications. First, the Griffin-Pronghorn scheme is verified against the MSR benchmark problem proposed by CNRS (Centre National de la Recherche Scientifique) [5], which covers several steps starting from steady state single physics solution to time dependent Multiphysics problem of fast spectrum liquid fuel MSR. The Griffin-SAM scheme is validated using the protected zero power pump transient test of the Molten Salt Reactor Experiment (MSRE) [6] to demonstrate the effect of the DNPs drift and decay outside the core. Finally, the Griffin-Pronghorn-SAM coupled scheme is tested and validated using a reactivity insertion transient of the MSRE which involves several feedback mechanisms.

2. GRIFFIN-PRONGHORN MULTIPHYSICS COUPLING

This section presents verification activities of the MSR flowing fuel capabilities performed at INL for the CNRS [5] MSR numerical benchmark with the Griffin-Pronghorn scheme. The following subsections provide a brief description of the benchmark, coupling scheme, and selected benchmark verification results.

2.1. Coupling Scheme

The analysis of the CNRS benchmark was performed with Griffin as the main application, which provides neutronics solutions of the power density and fission source to Pronghorn (sub-application) to obtain the fuel salt temperature, density, velocity, and pressure fields and the DNP distribution. The fuel salt temperature field and density are transferred to Griffin to update multigroup cross sections. The DNP distribution is also transferred and used to construct the total fission source, solve the neutron flux and the corresponding power density that is sent back to Pronghorn calculations. The parameters are exchanged between the two codes at each iteration to obtain a fully-converged solution, and the convergence of the global Picard iteration is checked based on the relative reduction of the flux residual of Griffin. The feedback mechanisms captured by this multiphysics coupling of Griffin-Pronghorn are related to the cross section changes by temperature and density and the DNP distribution changes by velocity. The Multiphysics coupling scheme of Griffin-Pronghorn under the MOOSE framework used in this work for MSR analysis is shown in Figure 1.

2.2. CNRS Benchmark Modeling

The benchmark problem was originally developed for the numerical verification of thermal-hydraulics codes for incompressible flow in a lid-driven cavity. It was recently extended for application to the fast-spectrum MSR benchmark developed by LPSC/CNRS-Grenoble [5] considering multiphysics coupling of neutronics and thermal-hydraulics codes to verify modeling approaches of coupled multiphysics codes for MSR steady-state and transient analyses. The geometry of the CNRS benchmark is shown in Figure 2 and it represents



Figure 1. Coupling scheme for Multiphysics core calculations of the CNRS benchmark using Griffin and Pronghorn.

a simple 2-D lid-driven cavity of a $2m \times 2m$ domain bare reactor with homogeneous fuel salt composition with U-235 as the fissile isotope [5].

The benchmark analysis is performed in three phases with progressively increasing complexity. Each phase is composed of one or more steps and can be summarized as:

- Phase (0) single physics steady-state: which verifies single physics steady-state calculations to confirm the soundness of each code before performing coupled calculations.
- Phase (1) steady-state multiphysics coupling: which focuses on verifying multiphysics-coupled steadystate calculations to assesses the impact of DNP drift on the reactivity and the delayed neutron source distribution with a constant velocity field and temperature profile.
- Phase (2) time-dependent multiphysics coupling which is dedicated to verifying multiphysics-coupled transient calculations and is a single-step phase. The heat transfer coefficient is changed in time by a sinusoidal perturbation with a constant amplitude and with varying frequencies with the subsequent change in power.



Figure 2. CNRS benchmark problem geometry [5].

2.3. Verification Test Results

The verification test results of Griffin-Pronghorn for benchmark steps are presented in Reference [7]. The Griffin-Pronghorn code system showed expected physics phenomena and produced consistent results with

the reference codes under all conditions for all test cases and benchmark steps. Here we just show a part of the result for steady state and transient problems. Table I provides comparisons of the reactivity change of step 0.2, 1.1, 1.2, and 1.3. Step 0.2 compares the steady-state neutronics solutions for stationary fuel. Step 1.1 assesses the impact of DNP drift on the reactivity and the delayed neutron source distribution with the fixed velocity field from Step 0.1 and a constant temperature of 900 K. Step 1.2 adds in the temperature feedback to Step 1.1 and assesses its impact on the reactivity and fission rate density distribution. Step 1.3 assesses the ability to perform a fully-coupled simulation including the velocity fields for a system without forced convection, namely the lid velocity being zero, where the flow is only driven by the buoyancy effect caused by the temperature gradient. For all the steps, the Griffin-Pronghorn solution matches very well with the reference solution within few *pcm*. Also Figure 3 shows the flow speed and DNP density distributions depending on the lid velocity for a case of 1.0 GW power, which is a qualitative verification of the fully-coupled DNP drift simulation. The degree of DNP dispersion depends on their half-lives: the first-group DNPs, which have the longest half-life, are largely dispersed following the fluid as they can last long enough to be carried away by the fluid. The latter-group of DNPs are more centered at the cavity following the fission rate distribution due to their shorter half-lives [7].

In summary, all the steady-state multiphysics phenomena expected in a flowing fuel MSR are well-captured by the Griffin-Pronghorn code system. The external momentum source, buoyancy effects, DNPs drift, and temperature feedback are all considered properly in a fully-coupled manner. This completes the verification of the steady-state flowing fuel simulation capability of the Griffin-Pronghorn code system.

| | Step 0.2 | Step 1.1 | Step 1.2 | Step 1.3 |
|-------------|--------------|---------------------|---------------------|---------------------|
| Code | $ ho_{0.2}$ | $\rho - \rho_{0.2}$ | $\rho - \rho_{1.1}$ | $\rho - \rho_{0.2}$ |
| CNRS-SP1 | 411.3 | -62.5 | -1152.0 | -1220.5 |
| CNRS-SP3 | 353.7 | -62.6 | -1152.7 | -1220.7 |
| PoliMi | 421.2 | -62.0 | -1161.0 | -1227.0 |
| PSI | 411.7 | -63.0 | -1154.8 | -1219.6 |
| TUD-S2 | 482.6 | -62.0 | -1145.2 | -1208.5 |
| TUD-S6 | 578.1 | -60.7 | -1122.0 | -1184.4 |
| Avg. (Std.) | 443.1 (77.8) | -62.1 (0.8) | -1148.0 (13.7) | -1213.5 (15.4) |
| Griffin | 465.7 | -61.4 | -1149.3 | -1212.0 |
| Diff. | 22.6 | 0.7 | -1.3 | 1.5 |

Table I. Steady state reactivity change at different benchmark steps in *pcm* [7].

Phase 2 is dedicated for time-dependent coupling of the fully coupled system to verify the transient analyses capabilities considering a wave or sinusoidal perturbation in the system. Figure 4 presents the comparison of power gain and phase shift at different frequencies. The power gain computed by Griffin shows good agreement with the references, where the maximum discrepancy is less than 1.2%. For the phase shift, the discrepancy increases to (7-10%) in the lowest frequencies. However, the Griffin-Pronghorn values fall within the reference range in all frequencies. Therefore, the Griffin-Pronghorn code system is sound for fully-coupled transient simulations as well [7].

3. GRIFFIN-SAM MULTIPHYSICS COUPLING

This section presents validation activities of the MSR flowing fuel capabilities performed at INL for the MSRE experiment [6] performed with the Griffin-SAM code system. The following subsections provides a brief description of the coupling scheme and validation test results of the pump startup and coast-down transients.



Figure 3. CNRS benchmark problem geometry [7].



Figure 4. CNRS benchmark problem geometry [7].

3.1. Coupling Scheme

To address the impact of the fuel salt flow and its decay in the outer loop, a Multiphysics model is developed for the core and outer loop that consists of three components: (1) Griffin neutronics model, (2) SAM multi-D core model, and (3) SAM 1-D outer loop model. Here the SAM multi-D solver is used as a placeholder for Pronghorn upon completion of the domain-overlapping work that is presented in Section 4.

The parameters needed by each model component to obtain a Multiphysics coupled solution are transferred between model components at each calculation point or time step. Figure 5 shows the coupling scheme and the transferred parameters between the main-app and the sub-apps. Griffin (mani-app) provides the power density and fission source distributions to SAM Multi-D (sub-app). The power density distribution is used to obtain fuel and moderator temperatures, density, pressure, and velocity fields. While the fission source distribution is used to calculate the DNP distribution. SAM multi-D and 1-D models exchange parameters

at the downcomer outlet and the top core outlet pipe to obtain core inlet temperature, density, pressure, temperature, and DNP values [8]. The fuel salt and moderator temperatures and densities are transferred to Griffin from SAM to update the cross sections and the fuel salt isotopic densities for proper feedback calculations. Also, the DNPs is transferred to determine the delayed neutron source and construct the total fission neutron source in the core region considering their decay in the outer loop.



Figure 5. Coupling scheme for Multiphysics analysis using Griffin and SAM [8].

3.2. MSRE Experiment Modeling

A multiphysics reference plant model of the MSRE was developed using the MOOSE framework. The MSRE neutronics model was developed considering a 2-D axisymmetric domain in R-Z coordinate using the multigroup diffusion approximation to the linearized Boltzmann transport equation. The thermal-hydraulics model of the MSRE, developed using the SAM code. In this model, the core region is represented by a 2-D porous media approximation and the outer loop is modeled with 1-D/0-D fluid channels to solve the mass momentum and energy equations along with the DNP equations to account for the drift of the DNPs within the core and its decay in the outer loop. These models are coupled using the MultiApp system to obtain Multiphysics solution and to address the right feedback mechanisms considering the effect of the DNP redistribution and decay, fuel expansion, and temperature feedback. Figure 6 shows the core and outer loop models of the MSRE experiment [8].

3.3. Validation Results

Pump transient tests of the MSRE were performed at zero power to evaluate the impact of the flow rate changes on the reactivity during pump start-up and coast down transients. In these tests, the reactor was fueled with U - 235, and the reactor was operated at a low power level to ensure that the DNP losses were the only feedback mechanism. Initially, the equilibrium conditions of the system were established with minimal flow at the critical state.

During the experiment, the fuel flow rate in the primary loop was increased or decreased by adjusting the primary pump head. The control rod positions were adjusted to maintain a constant low power and eliminate any thermal feedback effects. The control rod movement was compensating for the reactivity loss or gain due to the redistribution of the DNPs in the core and their decay outside the core. Multiphysics transient calculations were performed for the MSRE to simulate the pump start-up and coast down tests. Figure 7 shows the a comparison of the reactivity losses calculated by the Multiphysics coupled model and the experimental values that was generated from converting the control rod position data into a reactivity data.



Figure 6. Developed multiphysics model for MSRE analysis using Grifiin and SAM [8].

During the protected pump start-up test, the flow of fuel that starts outside the core leads to reactivity loss due to the decay of the DNPs outside the core and the losses increase with the increasing flow velocity which requires more control rod withdrawal to maintain criticality. The oscillatory behavior is observed due to undecayed fuel flowing back and decays in the core region. The positive reactivity effect of the recirculated precursors entering the core is clearly seen 13 seconds after pump start-up. While in the protected pump coast-down transient, the reactivity increases with decreasing fuel flow rate due to the decay of the DNPs in the core region. Therefore, the compensated reactivity continues to decrease and reaches zero when all the precursors decay in the core which requires insertion of the control rod to maintain criticality. For both cases, the calculated values agree with measured values except for the pump start-up case where the oscillatory behaviour is slightly overestimated. This might be attributed to excluding the control rods from the current model and the simplifications that were made to perform this transient [8].

4. PRONGHORN-SAM OVERLAPPING DOMAIN COUPLING

This section presents validation test results for reactivity insertion transient of the MSRE experiment performed with the Griffin-Pronghorn-SAM coupled code system using a domain overlapping scheme for thermal-hydraulic analysis. The following subsections provide a brief description of the coupling scheme and validation test results of the simulated transient [9].

4.1. Coupling Scheme

The coupling of thermal-hydraulic model was performed with a domain overlapping scheme between the thermal-hydraulic core solver (Pronghorn) and the system code (SAM) using MOOSE's MultiApp system [9]. The coupling scheme utilizes a fixed point iteration with alternating solves between SAM and Pronghorn in which parameters are exchanged between the codes before executing either of the codes. In the Multiphysics



Figure 7. Comparison calculated reactivity losses by Griffin-SAM and measured values data during pump start-up and coast down tests [8].

coupled model, Griffin is the main-app and it provides neutronics solution of the core region to Pronghorn which is a sub-app that can call SAM as sub-sub-app. Figure 8 shows the coupling scheme and the transferred parameters between the main-app and the sub-apps.



Figure 8. Multiphysics coupling scheme of Griffin-Pronghorn-SAM.

4.2. MSRE Experiment Modeling

The MSRE core and primary loop are strongly interacting which makes the core conditions (i.e., temperature and DNPs) determine the fission rate distribution and the fission rate distribution determines the change in temperature and DNPs in the core. The core conditions feed the inlet conditions for the primary circuit where a negligible amount of fission happens but the DNPs decay is significant. The outlet conditions for

the primary circuit are the inlet conditions for the temperature and precursors at the core inlet. Thus core and primary circuit are coupled via thermal and neutronics feedback.

The Pronghorn model of the core is R-Z axisymmetric that includes the downcomer, lower plenum, core, upper plenum, and top outlet pipe. Conjugate heat transfer is modeled between the core, upper plenum, and downcomer with the core barrel. The SAM model includes the reactor primary loop, heat exchanger, and a single pipe that combines the core, lower plenum, and upper plenum. The flow exits the heat exchanger and enters the downcomer towards the lower plenum [9].

4.3. Validation Results

The developed coupling scheme was validated using a reactivity insertion transient of the MSRE. In this transient, the reactor was operated at 5 MWth power when a step positive reactivity equivalent to 19 pcm was inserted by withdrawing the control rod. In the Griffin model, the reactivity insertion is achieved by adjusting the fission reaction rate to match the inserted reactivity as the model doesn't account for control rods. The power evolution during the transient is depicted in Figure 9 considering different models: (1) point kinetics and SAM standalone model, (2) domain-segregated coupling between SAM and Pronghorn, and (3) the domain overlapping approach discussed in this section.

After the reactivity insertion, the reactor power increases which leads to an increase of the fuel salt and graphite temperature. The temperature increase results in a negative feedback due to Doppler effect and thermal expansion of the fuel salt, thus reducing the reactor power again. After this, an oscillatory power behaviour is observed due to the flow back of unheated fuel salt into the core and the decay and redistribution of the DNPs in the core region with a time constant similar to the circulation time of approximately 25 seconds. For the models integrating Pronghorn, a closer agreement with the measured data is observed at the peak power region. This is mainly due to the multidimensional temperature resolution in the core, which improves the accuracy in capturing the temperature feedback [9].



Figure 9. Comparison of measured and calculated power evolution after 19 pcm reactivity insertion of the MSRE at 5.0 MW [9].

5. SUMMARY

This paper presents Multiphysics coupling schemes of the MOOSE based reactor multiphysics application Griffin and thermal hydraulics applications Pronghorn and SAM. This is followed by verification test results using the fast spectrum MSR benchmark problem known as CNRS and validation test results using the MSRE experimental data for zero power pump transient tests and reactivity insertion transients. These various coupling schemes demonstrated the modeling capabilities of liquid fuel MSRs, ability to capture the drift of the DNPs, and the resulting strongly coupled feedback mechanisms. Further verification and validation tests will be performed in the future and more detailed modeling of the complicated geometries will be incorporated to simulate more realistic designs to help and support the mission of new MSRs designs.

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