SAM Developments to Support Transient Safety Analysis of Advanced non-LWRs

Nuclear Science and Engineering Division

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EXECUTIVE SUMMARY

The System Analysis Module (SAM) is under development at Argonne National Laboratory as a modern system-level modeling and simulation tool for advanced non-light water reactor safety analyses. It utilizes the object-oriented application framework MOOSE to leverage the modern software environment and advanced numerical methods. The capabilities of SAM are being extended to enable the transient modeling, analysis, and design of various advanced nuclear reactor systems. This report summarizes major fiscal year 2019 (FY19) progress in SAM code development, capability enhancements, demonstration, and validation to support transient safety analysis of advanced non-LWRs.

Rapid developments continued in FY19 to support various needs of the advanced reactor community, especially NRC and industry on the licensing safety analysis of advanced reactor designs. Significant changes provide enormous capability enhancements, bug fixes, and user friendliness improvements. Major code updates are summarized in Section 1, while three important enhancements are detailed in Section 3-5, including enhancements for coupling with other codes for multi-scale multi-physics simulations; developments of point-kinetics and reactivity feedback models; and development of heat-pipe-cooled micro-reactor simulation capabilities.

SAM code is enhanced for coupling with other codes for multi-scale multi-physics simulations of various advanced reactors. The code structure was updated so that it accepts both SAM input syntax and the standard MOOSE input syntax in a single input model (mixed input syntax style). This update enables the coupling of SAM with the other MOOSE-based codes. Several components and boundary conditions were added or updated to enhance the flexibility in modeling the conjugate heat transfer. For the accurate prediction of structure displacements, SAM was updated to include the MOOSE Tensor Mechanics (TM) module, which is a library that solves the mechanics problems. Another effort was pursued to enable the SAM and SAS4A/SASSYS-1 coupling capability at the solid-liquid interface for potential use of the Versatile Test Reactor (VTR) program.

Significant effort has been made to develop, implement, verify and demonstrate the point-kinetics module in SAM. Various reactivity feedback models were developed to work with the point-kinetics module, including fuel axial expansion, core radial expansion, fuel Doppler, and coolant density reactivity. Simplified thermal expansion models for the fuel pin and core restraint system (e.g. grid plate) were developed for the calculation of the reactivity feedback due to thermal expansion of various components. Extensive verification tests have been completed for the point-kinetics module and the separate reactivity feedback models. A coupling interface has been developed to enable the coupling of SAM with an external thermomechanical analysis module. Note that the simplified thermal expansion models in SAM are important for fast simulations in reactor safety analysis, while the coupled thermomechanics module provides accurate thermal expansion results for verification purposes. These new capabilities have been demonstrated by simulating the early stage of an unprotected loss-of-flow accident in a reference sodium-cooled fast reactor (SFR). This confirms that the major physics phenomena in the heat transport system of SFR are captured by SAM. The point-kinetics models, reactivity feedback models, and the coupling schemes are working as expected.

Because of the increasing interests in heat-pipe type micro-reactors, the capability of SAM has been extended to enable the modeling of conventional heat pipes and heat pipe type reactors. Two modeling options have been developed for the analysis of conventional heat pipes, depending on how heat is transported between the heat pipe wick and heat pipe vapor core. Both options assume that the vapor core of the heat pipe can be simulated as a superconductor of an extremely high thermal conductivity. The proposed modeling options are verified with a classical thermal resistance model. The temperature at different locations and the heat transport capacity of the heat pipe from the code predictions agree very well with the thermal resistance model.

Multi-physics phenomena of the heat-pipe-cooled micro-reactor are simulated using three submodules under NRC's Comprehensive Reactor Analysis Bundle (CRAB), its intended suite of non-LWR codes for confirmatory analysis. The MAMMOTH module is used to simulate the reactor kinetics behavior of the micro reactor; the SAM module is used to simulate the heat conduction in the reactor core and heat removal through the heat pipe heat exchangers and reactor cavity cooling system (RCCS); and the MOOSE Tensor Mechanics module is used to simulate the thermal expansion of the reactor core. The different sub-models are coupled together using MOOSE's MultiApp system and executed using the BlueCrab application. The multi-physics simulation capability has been demonstrated by a steady-state operation analysis, a failure of a single central heat pipe transient analysis, and a loss of heat sink transient analysis of a reference heat pipe reactor design. The fully coupled model is shown to work well.

Utilizing an application- and validation-driven development approach, SAM has been applied to selected demonstration or validation problems where the physics and scales of the problem may expand or increase with complexity. These demonstrations and validations lead up to the continuous assessment of the code capabilities and performance for a wide range of advanced reactor applications. Code validation activities in FY19 include using test data from Compact Integral Effects Test (CIET), Molten-Salt Reactor Experiment (MSRE), Natural convection Shutdown heat removal Test Facility (NSTF), and Minnesota Natural Circulation Loop. Overall, the results predicted by SAM are in good agreement with the experimental data. The successful validation of SAM against these selected data demonstrates that the computer code is well suited for thermal fluids analysis of FHR designs, coupled reactor kinetics, delay neutron precursor drift, and thermal transport modeling of the molten salt reactors, thermal fluids analysis of RCCS, and for simulation of experimental vehicle in test reactors.

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1 Introduction

An advanced system analysis tool, SAM (Hu 2017a, Hu et al. 2019a), is under development at Argonne National Laboratory for advanced non-LWR reactor safety analysis. It aims to provide fast-running, modest-fidelity, whole-plant transient analyses capabilities, which are essential for fast turnaround design scoping and engineering analyses of advanced reactor concepts. While SAM is being developed as a system-level modeling and simulation tool (Hu 2015, Hu 2017b), advanced modeling techniques including a reduced-order three-dimensional module (Hu 2019), pseudo 3-D conjugate heat transfer modeling in reactor core (Hu and Yu 2016), in addition to the advances in software environments and design, numerical methods.

SAM aims to be a generic system-level safety analysis tool for advanced non-LWRs, including Liquid-Metal-cooled fast Reactors (LMR), Molten Salt Reactors (MSR) or Fluoride-salt-cooled High-temperature reactor (FHR), and high-temperature gas-cooled reactor (HTGR). SAM takes advantage of advances in physical modeling, numerical methods, and software engineering to enhance its user experience and usability. It utilizes an object-oriented computational framework (MOOSE, Gaston et al. 2009), and its underlying meshing and finite-element library (libMesh, Kirk et al. 2006) and linear and non-linear solvers (PETSc, Balay et al. 2019), to leverage the modern advanced software environments and numerical methods.

Rapid development continued in fiscal year 2019 (FY19) to support various needs of the advanced reactor community, especially NRC and industry on the licensing safety analysis of advanced reactor designs. SAM is receiving increasing interests in the nuclear community for its use in advanced reactor design and safety analyses. Significant accomplishments in user engagements in FY19 include:

- In April of 2019, the US NRC has formally stated its intent to use the SAM code for advanced non-LWR design basis event analysis.
- Kairos Power formally adopted SAM to support its KP-FHR licensing application for safety analysis.
- SAM code licensees granted in FY19 include TerraPower, Southern Company Services, Applied Programming Technology, University of Michigan, Idaho State University, while the license agreement with BWX Technologies, Framatome, Moltex Energy, Virginia Commonwealth University, University of Wisconsin are undergoing.
- The SAM User's Guide (Hu et al. 2019a) is updated and released to all code users. It helps users understand the input description, core capabilities of the SAM code, as well as providing a number of tutorial problems.

In FY 19, the SAM code has gone through significant changes with enormous capability enhancements, bug fixing, and user friendliness improvements. A periodic release procedure has also been established in FY19. The major updates in V0.9.4 (in April 2019) and recent updates since then include:

- Advanced model development for thermal mixing and stratification in a large pool: three different (0D, 1D, and 3D) modeling approaches are pursued. Details can be found in Hu et al. (2018).
- Point kinetics and reactivity feedback modeling, including reactivity feedbacks due to core radial and axial thermal expansion feedbacks;

- Boundary condition update in boundary and junction components for improved code convergence;
- SAM input syntax updates that it supports mixed SAM-style and MOOSE-style input models;
- Mass transport model allow for tracking any number of species carried by the fluid flow;
- Form losses updates, which allowing for both forward and backward Re-dependent form losses;
- Updated core channel model, which can model both pin-bundles and prismatic block fuel and 1D channel flow assemblies;
- Mesh refinement allowed for the end element of fluid or structure components;
- Code enhancements allowing sensitivity coefficients in friction, heat transfer, and fluid property closure models;
- Enhanced *PBPipe* component which allows for multiple layers of heat structures, such as pipe wall and insulations;
- Heat Pipe component model, with 2D or 3D modeling of heat pipe wall and wick and 2D or 1D vapor core;
- Improved equation of state models with built-in Helium and Nitrogen models, and strong pressure-dependency properties;
- Enhancements to support flexible coupling with other external physics codes.

SAM also utilizes the application- and validation-driven code development approach. The code is being applied each year to selected demonstration or validation problems where the physics and scales of the problem may expand or increase with complexity in successive years. These validations lead up to the continuous assessment of the code capabilities and performance for a wide range of advanced reactor applications.

Code demonstration activities in FY19 include: the unprotected loss-of-flow transient simulation of a reference sodium-cooled fast reactor (SFR), to test both the recent developed point-kinetics and reactivity feedback models and multi-physics simulation of SFR transients; and the multi-physics simulations of a reference heat-pipe-cooled micro-reactor (HPR) design. Both demonstration simulations also resulted in reference plant models for SFR and HPRs, which can be further utilized and tested by code users to examine the SAM code capabilities and identify capability gaps for these types of reactors.

Code validation activities in FY19 include using test data from Compact Integral Effects Test (CIET), Molten-Salt Reactor Experiment (MSRE), Natural convection Shutdown heat removal Test Facility (NSTF), and Minnesota Natural Circulation Loop.

This report summarizes the FY19 progress in SAM code development, capability enhancements, demonstration, and validation to support transient safety analysis of advanced non-LWRs. This report is structured as follows: Section 2 provides an overview of the SAM code, summarizing the goals and objectives, software structure, the governing theory, as well as current capabilities of the code. Section 3 describes the recent enhancements in SAM for coupling with other codes for multi-scale multi-physics simulations of various advanced reactors. Section 4 provides a summary on the point-kinetics and reactivity feedback models in SAM, and the demonstration of the capabilities by simulating the early stage of the unprotected loss-of-flow accident in a reference SFR. These point-kinetics and reactivity feedback modeling capabilities

have also been demonstrated by simulating the early stage of the unprotected loss-of-flow (ULOF) accident in the Advanced Burner Test Reactor (ABTR). Section 5 provides a summary of the heat pipe models in SAM and the multi-physics coupling methodology for the heat-pipe-cooled microreactors. The coupled code capability has been demonstrated by both steady-state operation and transient simulation of a reference HPR design. The code validation efforts are summarized in Section 6.

2 SAM Overview

The System Analysis Module (SAM) is an advanced system analysis tool being developed at Argonne National Laboratory under the support of U.S. Department of Energy (DOE) Nuclear Energy Advanced Modeling and Simulation (NEAMS) program. It aims to be a modern system analysis code, which takes advantage of the advancements software design, numerical methods, and physical models over the past two decades. SAM focuses on modeling advanced reactor concepts such as SFRs (sodium fast reactors), LFRs (lead-cooled fast reactors), FHRs (fluoride-salt-cooled high temperature reactors), MSR (molten salt reactors), and HTGRs (high-temperature gas-cooled reactors). These advanced concepts are distinguished from light-water reactors (LWR) in their use of single-phase, low-pressure (except HTGRs), high-temperature, and non-unity Prandtl number coolants. This simple yet fundamental change has significant impacts on core and plant design, the types of materials used, component design and operation, fuel behavior, and the significance of the fundamental physics in play during transient plant simulations.

SAM is aimed to solve the tightly-coupled physical phenomena including heat generation, heat transfer, fluid dynamics, and thermal-mechanical response in reactor structures, systems and components in a fully-coupled fashion but with reduced-order modeling approaches to facilitate rapid turn-around for design and safety optimization studies. As a new code development, the initial effort focused on developing modeling and simulation capabilities of the heat transfer and single-phase fluid dynamics responses in reactor systems. This Section summarizes the goals and objectives, software structure, the governing theory, as well as current capabilities of the code. In the coming years, the SAM code will continuously mature as a modern system analysis tool for advanced (non-LWR) reactor design optimization, safety analyses, and licensing support.

2.1 Ultimate Goals and Objectives

The ultimate goal of SAM is to be used in advanced reactor safety analysis for design optimization and licensing support. The important physical phenomena and processes that may occur in reactor systems, structures, and components shall be of interest during reactor transients including Anticipated Operational Occurrence (AOO), Design Basis Accident (DBA), and additional postulated accidents but not including severe accidents. Typical reactor transients include loss of coolant accidents, loss of flow events, excessive heat transfer events, loss of heat transfer events, reactivity and core power distribution events, increase in reactor coolant inventory events, and anticipated transients without scram (ATWS).

As a modern system analysis code, SAM is also envisioned to expand beyond the traditional system analysis code to enable multi-dimensional flow analysis, containment analysis, and source term analysis, either through reduced-order modeling in SAM or via coupling with other simulation tools. Additionally, the regulatory processes in the United States is being evolved to a risk-informed approach that is based on first understanding the best-estimate behavior of the fuel, the reactor, the reactor coolant system, the engineered safeguards, the balance of plant, operator actions, and all of the possible interactions among these elements. To enable this paradigm, an advanced system analysis code such as SAM must be able to model the integrated response of all of these physical systems and considerations to obtain a best-estimate simulation that includes both validation and uncertainty quantification.

The SAM code is aimed to provide improved-fidelity simulations of transients or accidents in an advanced non-LWR, including three-dimension resolutions as needed or desired. This will encompass the fuel rod, the fuel assembly, the reactor, the primary and intermediate heat transport system, the balance-of-plant, the containment. Multi-dimension, multi-scale, and multi-physics effects will be captured via coupling with other simulation tools, and computational accuracy and efficiency will be state-of-the-art. Uncertainty quantification will be integrated into SAM numerical simulations. Legacy issues such as numerical diffusion and stability in traditional system codes will be addressed and the code will attract broad use across the nuclear energy community based on its performance and many advantages relative to the legacy codes. The integrated architecture will provide a robust toolset for decision making with full consideration of the various disciplines and technologies affecting an issue.

2.2 Software Structure

SAM is being developed as a system-level modeling and simulation tool with higher fidelity (compared to existing system analysis tools), and with well-defined and validated simulation capabilities for advanced reactor systems. It provides fast-running, modest-fidelity, whole-plant transient analyses capabilities. To fulfill its objectives, SAM utilizes the object-oriented application framework MOOSE (Gaston et al. 2009) and its underlying meshing and finite-element library libMesh (Kirk et al. 2006) and linear and non-linear solvers PETSc (Balay et al. 2019), to leverage the available advanced software environments and numerical methods. The high-order spatial discretization schemes, fully implicit and high-order time integration schemes, and the advanced solution method (Jacobian-free Newton–Krylov (JFNK) method, Knoll and Keyes 2004) are the key aspects in developing an accurate and computationally efficient model in SAM.

The software structure of SAM is illustrated in Figure 2-1. In addition to the fundamental physics modeling of the single-phase fluid flow and heat transfer, SAM incorporates advances in the closure models (such as convective heat transfer correlations) for reactor system analysis developed over the past several decades. A set of Components, which integrate the associated physics modeling in the component, have been developed for friendly user interactions. A flexible coupling interface has been developed in SAM so that multi-scale, multi-physics modeling capabilities can be achieved by integrating with other higher-fidelity or conventional simulation tools. The code coupling with STAR-CCM+, SAS4A/SASSYS-1, Nek5000, BISON, and Mammoth/RattleSnake have been demonstrated, while the coupling with PRONGHORN and PORTEUS codes are ongoing or planned.

Figure 2-1. SAM Code Structure

2.3 Governing Theory

2.3.1 Fluid dynamics

Fluid dynamics is the main physical model of the SAM code. SAM employs a standard one-dimensional transient model for single-phase incompressible but thermally expandable flow. The governing equations consist of the continuity equation, momentum equation, and energy equations. A three-dimensional module is also under development to model the multi-dimensional flow and thermal stratification in the upper plenum or the cold pool of an SFR.

2.3.2 Heat transfer

Heat structures model heat conduction inside solids and permit the modeling of heat transfer at interfaces between solid and fluid components. Heat structures are represented by one-dimensional or two-dimensional heat conduction in Cartesian or cylindrical coordinates. Temperature-dependent thermal conductivities and volumetric heat capacities can be provided in tabular or functional form. Heat structures can be used to simulate the temperature distributions in solid components such as fuel pins or plates, heat exchanger tubes, and pipe and vessel walls, as well as to calculate the heat flux conditions for fluid components. Flexible conjugate heat transfer and thermal radiation modeling capabilities are also implemented in SAM.

2.3.3 Closure Models

The fluid equation of state (EOS) model is required to complete the governing flow equations, which are based on the primitive variable formulation; therefore, the dependency of fluid properties and their partial derivatives on the state variables (pressure and temperature) are implemented in the EOS model. Some fluid properties, such as sodium, air, salts like FLiBe and FLiNaK, have been implemented in SAM. It can also utilize the fluid properties available in the MOOSE Fluid Properties Module. Empirical correlations for friction factor and convective heat transfer coefficient are also required in SAM because of its one-dimension approximation of the

flow field. The friction and heat transfer coefficients are dependent on flow geometries as well as operating conditions during the transient.

2.3.4 Mass transport model development

The mass transport modeling capability is needed to model sources and transport of particles for a number of applications, such as tritium transport, delayed neutron precursor drift, radioactive isotope transport for molten salt fueled/cooled systems. A general passive scalar transport model has been implemented in SAM, and it can be used to track any number of species carried by the fluid flow.

2.3.5 Reactor Kinetics model development

SAM employs a built-in point-kinetics model, including reactivity feedback and decay heat modeling. Various reactivity feedback models have been developed and integrated with the point-kinetics module, including fuel axial expansion, core radial expansion, fuel Doppler, and coolant density reactivity. Since this development is a relatively new effort, enhancements of the reactivity feedback modeling are also needed to include additional reactivity feedback mechanisms.

2.3.6 Numerical Methods

SAM is a finite-element-method based code. The “weak forms” of the governing equations are implemented in SAM. It uses the Jacobian-Free Newton Krylov (JFNK) solution method to solve the equation system. The JFNK method uses a multi-level approach, with outer Newton’s iterations (nonlinear solver) and inner Krylov subspace methods (linear solver), in solving large nonlinear systems. The concept of ‘Jacobian-free’ is proposed, because deriving and assembling large Jacobian matrices could be difficult and expensive. The JFNK method has become an increasingly popular option for solving large nonlinear equation systems and multi-physics problems, as observed in a number of different disciplines (Knoll and Keyes 2004). One feature of JFNK is that all the unknowns are solved simultaneously in a fully coupled fashion. This solution scheme avoids the errors from operator splitting and is especially suitable for conjugate heat transfer problems in which heat conduction in a solid is tightly coupled with fluid flow.

2.4 Overview of Current Capabilities

To develop a system analysis code, numerical methods, mesh management, equations of state, fluid properties, solid material properties, neutronics properties, pressure loss and heat transfer closure laws, and good user input/output interfaces are all indispensable. SAM leverages the MOOSE framework and its dependent libraries to provide JFNK solver schemes, mesh management, and I/O interfaces while focusing on new physics and component model development for advanced reactor systems. The developed physics and component models provide several major modeling features:

1. One-D pipe networks represent general fluid systems such as the reactor coolant loops.
2. Flexible integration of fluid and solid components, able to model complex and generic engineering system. A general liquid flow and solid structure interface model was developed for easier implementation of physics models in the components.
3. A pseudo three-dimensional capability by physically coupling the 1-D or 2-D components in a 3-D layout. For example, the 3-D full-core heat-transfer in an SFR reactor core can be

modeled. The heat generated in the fuel rod of one fuel assembly can be transferred to the coolant in the core channel, the duct wall, the inter-assembly gap, and then the adjacent fuel assemblies.

4. Pool-type reactor specific features such as liquid volume level tracking, cover gas dynamics, heat transfer between 0-D pools, fluid heat conduction, etc. These are important features for accurate safety analyses of SFRs or other advanced reactor concepts.
5. A computationally efficient multi-dimensional flow model is under development, mainly for thermal mixing and stratification phenomena in large enclosures for safety analysis. It was noted that an advanced and efficient thermal mixing and stratification modeling capability embedded in a system analysis code is very desirable to improve the accuracy of advanced reactor safety analyses and to reduce modeling uncertainties.
6. A general mass transport capability has been implemented in SAM based on the passive scalar transport. The code can track any number of species carried by the fluid flow for various applications.
7. An infrastructure for coupling with external codes has been developed and demonstrated. The code coupling with STAR-CCM+ (Hu et al. 2014), SAS4A/SASSYS-1 (Fanning and Hu 2016, Brunett et al. 2019), Mammoth/RattleSnake (Hu et al. 2019b), Nek5000, and BISON (Martineau et al. 2018) have been demonstrated, while the coupling with PRONGHORN, RattleSnake, and PORTEUS codes are undergoing.

The examples of SAM simulation results of advanced reactors are shown in Figure 2-2 to Figure 2-4 for SFR(Hu et al. 2014), FHR (Ahmed et al. 2017), MSR (Zhang and Hu 2018), and HTGR (Vegendla et al. 2019).

(a) SAM model with 61 core channels

(b) Coupled SAM and CFD code simulation

Figure 2-2. SAM simulation results of an SFR

Figure 2-3. SAM simulation results of an FHR

(a) Power
(b) Coolant temperature
Figure 2-4. SAM simulation results of a simple MSR primary loop during a postulated loss-of-flow transient

(a) Fluid and solid temperature

(b) Coolant velocity

(c) Maximum heat structure temperatures during transient

Figure 2-5. SAM simulation results of a reference HTGR primary loop during a postulated pressurized conduction cooldown (PCC) transient

3 SAM Enhancements for Multi-Scale Multi-Physics Coupling

This Section summarizes the recent enhancements in SAM for coupling with other codes for multi-scale multi-physics simulations of various advanced reactors.

3.1 SAM Input Syntax Update

Previously, the input syntax of SAM was customized from the standard MOOSE's input syntax because of the special feature of a system level analysis code. The input syntax of SAM's input model was thus different from that of the other MOOSE-based codes. This was not a problem until the current needs for the coupling between SAM and the other MOOSE-based codes. In FY19, the SAM code structure was updated so that it accepts both SAM input syntax and the standard MOOSE input syntax in a single input model (mixed input syntax style). This update enabled several major enhancements in the capability of coupling SAM with the other MOOSE-based codes.

SAM supported two types of input syntax previously, i.e. the MOOSE native syntax and the SAM syntax with the embedded Component system taking care of the mesh generation, variable and physics objects (Kernel, Materials, BCs, etc.) creation, etc., using “-m”, or “-i” command line options. This distinction brought in issues when SAM was coupled with the other MOOSE based codes through the MultiApp system of MOOSE, i.e. “-m” option was not able to be passed to the sub Apps. After recent code updates, the “-i” option now supports both the SAM input syntax and the original MOOSE syntax. This update enables us to perform SAM-SAM coupling through the MultiApp system with one app using the MOOSE input syntax and the other using the SAM input syntax. This is a critical update which enables more complex and highly coupled multi-physics modeling and simulations.

3.2 Flexible Coupling with External Solid and Liquid Components

A major effort in performing a coupled simulation between different components is related to the conjugate heat transfer at the boundary surface. In order to enhance SAM's flexibility in modeling the conjugate heat transfer, several components/boundary conditions were recently added/enhanced, including:

1. *HeatStructureWithExternalFlow*. This new component was added into SAM for coupling with an external flow from an external fluid flow solver. The external fluid flow solver can be SAM itself or a different code. This new component models a SAM heat structure, which takes the boundary conditions at one side from an external flow solver. The main external variables this component takes are the external flow temperature and heat transfer coefficient.
2. *HeatTransferWithExternalHeatStructure*. This new component was added into SAM for coupling with an external heat conduction solver. The external heat conduction solver can be SAM itself or a different code. This new component models a typical 1D fluid flow component, which takes the external wall temperature and heat transfer coefficient from the external heat conduction code.
3. *PBCoupledHeatStructure*. This component was enhanced to be more flexible in terms of conjugate heat transfer. The major enhancement was the additional option to take

the external variable of either heat flux or fluid temperature and heat transfer coefficient as the boundary conditions. These external variables can be in the form of an *AuxVariable* and would be applied in a new *CoupledConvectionBC*. These external variables are usually taken from a coupled heat conduction solver or a fluid flow solver.

4. *CoupledConvectionBC*. This new type of boundary condition was added into SAM to take an *AuxVariable* of either heat flux or temperature and heat transfer coefficient for modeling the convective boundary condition. These variables are usually taken from a coupled heat conduction solver or fluid flow solver.
5. *CoupledRadiationHeatTransferBC*. In order to model the heat transfer from the reactor vessel to the Reactor Cavity Cooling System (RCCS) system, a radiation heat transfer boundary condition was added into SAM, called *CoupledRadiationHeatTransferBC*. It takes the temperature of the vessel outer surface and the temperature of inner surface of RCCS system for the coupling between the reactor core and the RCCS system sub-Apps. It can also be used to model the general radiation heat transfer between two solid surfaces while the two solid domains are modeled in separate SAM models.

These enhancements enabled many of the recent coupled code simulations.

3.3 Linking and Coupling with MOOSE's Tensor Mechanics Module

The analysis of the transient behavior of a nuclear reactor requires the coupled simulation of reactor kinetics and thermal-hydraulics of the reactor core, especially for those unprotected transients where the reactor scram system may not function properly. Reactivity feedbacks due to the thermal deformation, such as the fuel axial expansion and core radial expansion, is important for transient analyses of advanced reactor concepts. However, the accurate prediction of the fuel axial expansion and core radial expansion requires the coupling of SAM with an external thermomechanical analysis module, see Figure 3-1.

In order to achieve this capability, SAM was updated to include the MOOSE Tensor Mechanics (TM) module, which is a library for simplifying the implementation of the simulation tools that solve the mechanics problems. In the update, the Tensor Mechanics module library was linked in the SAM executable and became directly available to SAM. In order to perform a coupled SAM and Thermomechanics analysis, two new features were added into SAM, including:

1. *MultiAppCoordSwitchNearestNodeTransfer*: one application of the Tensor Mechanics module is the prediction of the axial displacement in the fuel. The coupling between SAM and TM is through the MOOSE's MultiApp system. The fuel temperature from SAM's heat structure will be transferred to the TM app for calculation of the axial displacement. This is a mesh-based data transfer, which requires the mesh in SAM's heat structure and the mesh in TM app being the same. For performance reasons, axisymmetric simulation option was used in both SAM and TM. In SAM, the heat structure is modeled as the real geometry, i.e. axisymmetric RZ coordinated defined in YZ mesh; however, the axisymmetric mesh in TM is always in XY mesh. This conflict caused the mismatch in the mesh-based data transfer. In order to resolve this issue, a customized *MultiAppCoordSwitchNearestNodeTransfer* was added into SAM, which will perform a nearest node data transfer based on any configuration of 2D mesh in

SAM and TM. This is achieved by a canonical transformation of the coordinate in the master and sub app when searching for the nearest node.

2. *HeatStructureLayeredAverage*: both the fuel Doppler and the fuel axial expansion reactivity feedback models requires a stack of radially averaged fuel temperature. This average can be performed using the *LayeredAverage* UserObject of MOOSE, which was however based on the Cartesian mesh. A customized *HeatStructureLayeredAverage* UserObject was added into SAM for handling the cylindrical heat structures.

Figure 3-1. Schematic of coupling of SAM and Thermomechanics (TM) module

3.4 SAM-SAS Coupling Interface

Under the support of an Argonne LDRD project, an effort was pursued to enable the SAM-SAS4A/SASSYS-1 coupling capability at the solid-liquid interface for potential use of the Versatile Test Reactor (VTR) program. A coupling boundary (Figure 3-2, left) has been identified at the VTR test vehicle and primary coolant interface, where SAS4A/SASSYS-1 (SAS) treats primary coolant thermodynamics, while SAM treats all thermodynamic and reactivity behavior within the test vehicle, including the vehicle walls (Brunett et al. 2019). Essential to this integrated tool is its newly developed capability to properly model the conjugate heat transfer process which ensures equality of temperatures and heat fluxes at the vehicle wall interface while ensuring energy conservation.

The coupling interface between SAM and SAS4A/SASSYS-1 was achieved through a new non-geometrical component. This interface accepts the primary coolant temperature and heat transfer coefficient at the fluid-solid interface from SAS and returns the wall temperature and wall heat flux to SAS4A/SASSYS-1. Additionally, the interface accepts the total power deposited in the test vehicle. This power can then be distributed to any component within SAM that will accept a heat source. At the beginning of an iteration, the external data is supplied by SAS4A/SASSYS-1 and read into SAM memory. This data is then mapped to the interface boundary mesh within SAM using the built in MOOSE linear interpolation routine. Upon completion of the heat transfer calculation, SAM calculates the wall temperature and heat flux at the fluid-solid interface boundary on the SAS4A/SASSYS-1 mesh and send them back to the external source (Figure 3-2, right) (Brunett et al. 2019).

Figure 3-2. Definition of the coupling boundary interface, boundary condition options, and the data transfer scheme between SAS4A/SASSYS-1 and SAM

The previously mentioned enhancement in the *PBCoupledHeatStructure* is essential for this coupled simulation. In order to achieve this new coupling scheme, several new capabilities/features were added into SAM, including:

1. *SASInterface*. This is a new non-geometrical component added into SAM for the data transfer between SAM and SAS4A/SASSYS-1. It handles the reading/writing of the data between SAS4A/SASSYS-1 and SAM as required by the coupling scheme (Figure 3-2, right). It accepts the primary coolant temperature and heat transfer coefficient from SAS and apply them to the coupled heat structure in SAM. It also returns to SAS the wall temperature and wall heat flux from the coupled heat structure in SAM. Both file-based data transfer and FIFO-based (First In First Out) data transfer were achieved in this interface.
2. *SASInterfaceControl*. This is a customized control class which is derived from MOOSE's Control system for the transient coupled simulation. It is used to control the global parameter, e.g. the reactor power from SAS4A/SASSYS-1, in the *SASInterface*.
3. *CoupledSASExecutioner*. This is a customized transient executioner added into SAM for achieving the coupling scheme as is shown in (Figure 3-2, right).

This new coupling interface was successfully demonstrated by the simulation of Unprotected Loss of Heat Sink (ULOHS) accident of the Versatile Test Reactor, Figure 3-3 (Brunett et al. 2019). The coupling interface was shown to work very well in the transient simulation.

Figure 3-3. ULOHS VTR coolant temperature (left) and test vehicle temperature (right) from the coupled simulation

4 Point Kinetics and Reactivity Feedback Modeling

The analysis of the transient behavior of a nuclear reactor requires the coupled simulation of reactor kinetics and thermal-hydraulics of the reactor core, especially for those unprotected transients where the reactor scram system may not function properly. The point-kinetics model has been widely used for reactor safety analysis due to its simplicity to capture the transient behavior. Various reactivity feedback models have been developed and integrated with the point-kinetics module, including fuel axial expansion, core radial expansion, fuel Doppler, and coolant density reactivity. The reactivity feedback models in SAM are similar to the respective models used in SAS4A/SASSYS-1. This Section first presents the brief theory of the point-kinetics module and reactivity feedback models. A number of verification tests have been performed where the code simulations are compared to the analytical model results, with details discussed in Hu et al. (2019c).

The reactivity feedback due to the thermal deformation, such as the fuel axial expansion and core radial expansion, is important for SFR transient analysis. Simplified thermal expansion models for the fuel pin and core restraint system (e.g. grid plate) are developed and verified in SAM. Additionally, a coupling interface is developed to couple SAM with external thermomechanical analysis modules for more accurate predictions of the thermal expansion of different components during the transients. The current coupling interface has been tested with the Tensor Mechanics module from MOOSE.

These point-kinetics and reactivity feedback modeling capabilities have also been demonstrated by simulating the early stage of the unprotected loss-of-flow (ULOF) accident in the Advanced Burner Test Reactor (ABTR). Both the stand-alone SAM and coupled SAM and Tensor Mechanics simulations are performed. It is confirmed that the major physics phenomena in the heat transport system of the ABTR reactor are captured by SAM, and the point-kinetics model, reactivity feedback models, and the coupling schemes are working as expected.

4.1 Point-kinetics and Reactivity Feedback Models

In the point-kinetics model, it is assumed that the reactor power can be separated into space and time function. The assumption is adequate when the space distribution remains nearly constant during the transient. The point-kinetics model shown in Equation (4-1) and (4-2) has been widely used for the transient safety analysis of stationary fuel reactors.

$$\frac{dn}{dt} = \frac{\rho_{ext} - \tilde{\beta}_{eff}}{\Lambda} n + \sum_i \lambda_i C_i \quad (4-1)$$

$$\frac{dC_i}{dt} = \frac{\beta_i}{\Lambda} n(t) - \lambda_i C_i \quad (4-2)$$

where $n(t)$ is the total neutron population, normalized by the neutron population at full fission power; C_i is the magnitude of delayed-neutron precursor population i , normalized by the neutron population at full fission power; $\tilde{\beta}_{eff}$ is the total effective delayed-neutron fraction while β_i is the fraction for delayed neutron precursor i ; ρ_{ext} is representing the net reactivity feedback; Λ is the prompt neutron generation time (t). The normalized fission power and delayed-neutron precursor population are solved simultaneously.

4.1.1 Fuel Axial Expansion Reactivity Feedback

In advanced nuclear reactors (e.g. sodium-cooled fast reactor), the fuel, especially metallic fuel, expands or shrinks within the cladding in response to the fuel temperature changes during the transient. The geometry changes of the fuel impose a positive or negative reactivity feedback, which affects the prompt fission power calculation in the point-kinetics model.

The fuel axial expansion model is developed to consider the reactivity feedback in response to the fuel temperature changes during the transient. The fuel reactivity is integrated over the core channels (Equation (4-3)), and the difference between the transient and initial values (Equation (4-4)) is provided to the point-kinetics model for the calculation of fission power (Fanning 2012).

$$R_A(t) = \int_{z=0}^{z=L} \rho_f(z, t) \times r_f(z) \times A \, dz \quad (4-3)$$

$$\Delta R_A(t) = R_A(t) - R_A^{ss} \quad (4-4)$$

where R_A is the axial expansion feedback in the unit of $\Delta k/k$; $\rho_f(z, t)$ is the fuel density at transient time t in the unit of kg/m^3 ; $r_f(z)$ is the fuel reactivity coefficient in unit of $\Delta k/k / kg$; L and A are the fuel length and cross-section area, respectively. The integration will consider the transient axial displacements in the fuel pin, which will be provided by either coupled thermomechanical analyses or SAM standalone calculations. The coupling scheme was briefly discussed in Section 3.3. In case the coupled displacements are not provided, a simple thermal expansion model in SAM is used to calculate the displacements.

4.1.2 Core Radial Expansion Feedback Reactivity

Due to temperature changes in the cooling system, the reactor core experiences radial thermal expansion, which impose a positive or negative reactivity feedback. For most advanced nuclear reactor design, there are also core restraint systems (e.g. Grid Plate, Above Core Load Pad, Top Load Pad), and the geometry of the reactor core during the transient is also affected by those constraint systems (Figure 4-1).

Figure 4-1. Restraint Systems in Typical SFR and Core Radial Expansion

A core radial expansion model has been developed to consider the reactivity feedback in response to the thermal expansions of the reactor core during a transient. The current model implemented in SAM is able to consider the expansion effects based on multiple restraints (Figure 4-1). The reactivity feedback due to the expansion effects at different elevations are weighted by user-defined factors (Fanning 2012).

$$\Delta R_{RC}(t) = \sum_n^N \left(\frac{\Delta R}{R} \right)_n \times w_n \times \rho_{RC,n} \quad (4-5)$$

where ΔR_{RC} is the core radial expansion feedback in the unit of $\Delta k/k$; $\Delta R/R$ is the relative change in the radius of reactor core; ρ_{RC}^n is core radial expansion coefficient at position n in the unit of $\Delta k/k$ per $\Delta R/R$; w_n is the user-defined weighting factor; N is the total number of restraints. The displacement of individual constraint system is provided by either an external thermomechanical calculation or SAM standalone calculation. In case the displacement of individual constraint system is not provided by external calculations, the internal thermal expansion model will be initialized to calculate the displacement of individual constraint system.

4.1.3 Fuel Doppler Reactivity Feedback Model

The fuel Doppler reactivity model is implemented in SAM to consider the reactivity feedback in response to fuel temperature changes during a transient. The Doppler reactivity feedback is integrated over the core channels (Equation (4-6)) and provided to the point-kinetics model for the calculation of fission power.

$$R_D(t) = \sum_n^N \alpha_D^n \times \ln[T_f^n(t) / T_f^n(0)] \quad (4-6)$$

where R_D is the fuel Doppler reactivity feedback in the unit of $\Delta k/k$; α_D^n is the fuel Doppler reactivity coefficient of node n in unit of $\Delta k/k$; $T_f^n(t)$ and $T_f^n(0)$ are the fuel temperature of node n at the time of t and the beginning, respectively; N is the total number of the nodes. The Doppler reactivity coefficient is generated from the neutronics calculations by perturbing the corresponding axial nodes in all the assemblies in a single core. All the assembly nodes on the same axial level are lumped together. The Doppler reactivity coefficients are provided as user inputs in SAM simulations. With user-provided fuel Doppler reactivity coefficients, the fuel temperature changes during the transient impose a positive or negative reactivity feedback on the fission power.

4.1.4 Coolant Density Reactivity Feedback

The coolant density reactivity model is developed to consider the reactivity feedback in response to the coolant temperature changes during the transient. The coolant density reactivity feedback is integrated over the flow channels (Equation (4-7)), and the difference between the initial and transient values (Equation (4-8)) is provided to the point-kinetics model for the calculation of fission power.

$$R_{CD}(t) = \sum_n^N \alpha_c^n \times \rho_c^n(t) \times V_c^n \quad (4-7)$$

$$\Delta R_{CD}(t) = R_{CD}(0) - R_{CD}(t) \quad (4-8)$$

where $R_{CD}(t)$ is the integrated coolant reactivity at time t in the unit of $\Delta k/k$; α_c^n is the coolant density reactivity coefficient of node n in unit of $\Delta k/k$ per kg; $\rho_c^n(t)$ is the coolant density of node n at the time of t ; V_c^n is the coolant volume of node n ; N is the total node number in the flow channel. Together with user-provided coolant density reactivity coefficients, the reactivity feedbacks in response to the coolant temperature changes during the transient impose a positive or negative impact on the fission power.

4.1.5 Coupling with Structure Mechanics Models

The coupling between SAM and the external thermomechanics modules would be necessary, as it provides the option to accurately calculate the thermal expansion of different components (e.g. grid plate and fuel pin). This capability is developed to provide more accurate predictions of the fuel axial expansion and core radial expansion in Equation (4-3) and Equation (4-5), respectively. The coupling of SAM and the thermomechanics module is achieved through MOOSE's MultiApp mechanism (See Section 3.3). The Tensor Mechanics module from MOOSE is currently coupled with SAM for the calculation of thermal expansion in fuel pin and core restraint system.

4.2 Demonstration of Reactivity Feedback Mechanisms

The heat transport system of the ABTR preconceptual design is used to demonstrate the point-kinetics and reactivity feedback modeling capabilities in SAM. The major components in the ABTR heat transport system are the reactor core, inlet/outlet plenum, cold/hot pool, pump, direct reactor auxiliary cooling system (DRACS), and intermediate heat transfer system (IHTS). In the

SAM model, the reactor core is modeled with 5 core channels (CH1 to CH5), the DRACS is modeled with one heat exchanger (DHX), and the IHTS is modeled with two heat exchangers (IHx and NaHX).

In the ULOF accident, the reactor remains at full power initially and is reduced later due to the inherent negative reactivity feedback. As the coolant flow rate decreases, reactor temperatures increase within the first minute. During this time, the peak fuel and cladding temperatures rise. This increase in temperatures provides the driving force for establishing the natural circulation flow, which will then reduce the peak fuel and cladding temperatures. The reactor seeks equilibrium with the available heat sink by reducing power. This will reduce the reactor temperature and establish a quasi-equilibrium condition. However, the reactor system will continue to heat slowly until the decay heat falls below the heat rejection capacity of the DRACS system. When decay heat production falls below the DRACS capacity, the system temperature starts to decline.

Figure 4-2 shows the histories for the total reactor power, the heat removal rate from the IHTS (IHx) and DRACS (DHX) heat exchangers, and the coolant flow in the hot channel (CH1). Figure 4-3 shows the transient peak fuel, peak cladding, CH1 coolant outlet, cold pool, and hot pool temperatures. Figure 4-4 shows the transient radial core expansion, axial fuel expansion, coolant density, and Doppler reactivity feedbacks. The coolant and cladding temperatures increase significantly during the first 30 seconds, which contribute to the negative radial and axial reactivities. The negative radial and axial reactivities are the main factors to bring down the reactor power and fuel temperatures. For this demonstration case, the coolant density and Doppler effect bring in positive reactivity, but in a smaller magnitude. The flow coast-down by the inertia of the primary pumps ends at approximately 450 seconds when the natural circulation has not yet been fully established. Shortly after this point, the peak fuel, peak cladding, and coolant temperatures begin to rise to form a second temperature peak. The increased temperatures become the driving force to increase the natural circulation flow rate.

The radial and axial expansion reactivities from the SAM standalone simulation and the coupled SAM and Tensor Mechanics module simulation are compared in Figure 4-5. In the SAM standalone simulation, the radial core expansion and axial fuel expansion are calculated internally by SAM; while in the coupled simulation, the core radial expansion and fuel axial expansion are provided by the Tensor Mechanics module. The reactivities from the SAM standalone simulation match well with that from the coupled simulation except for the bias in the fuel axial expansion reactivity. The bias in the reactivity significantly affects the reactor power, which in turn affects the fuel temperature and axial reactivity. The bias comes from the approximations made in the internal models for calculating the axial displacement, including the general plane-strain assumption and the use of cross-sectional averaged temperature, which is currently approximated with the temperature at a few nodes. Improvement on the fuel axial expansion reactivity feedback model will be implemented later.

Figure 4-2. ABTR ULOF transient reactor power, heat removal rate, and flow rate

Figure 4-3. ABTR ULOF transient temperatures.

Figure 4-4. ABTR ULOF transient reactivity feedbacks

Figure 4-5. ABTR ULOF transient reactivity feedbacks from SAM standalone simulation and coupled simulation

5 Heat Pipe Reactor Modeling

5.1 Heat pipe modeling

The need for power at remote locations away from a reliable electrical grid is an important niche for nuclear energy. Heat pipe-cooled fast-spectrum nuclear reactors are well suited for these applications (McClure et al. 2015). The key part of the heat pipe reactors is the heat pipes used to cool the reactor core. The heat pipe makes use of the phase change of the working fluid and transport a large amount of heat from the evaporator to the condensation end with very small temperature drops (Faghri, 1995). The essential part in the analysis of a heat pipe type reactor is the modeling of heat transport in the heat pipe.

Because of the increasing interests in heat-pipe type micro-reactors, the capability of SAM has been extended to enable the modeling of the conventional heat pipe and the heat pipe type reactor (Hu et al. 2019d). Two modeling options are developed for the analysis of the conventional heat pipe, depending on how the heat transfer between the wick and vapor core is modeled, i.e. 2D-RZ heat conduction and 3D-1D coupling. In the 2D-RZ heat conduction approach, the heat pipe wall, heat pipe wick, and heat pipe vapor core are modeled as axisymmetric 2D-RZ blocks, with all heat being transported through heat conduction. In the 3D-1D coupling option, the heat pipe wall and wick will be modeled as the 3D heat structure while the vapor core will be modeled as a 1D heat structure representing the heat conduction in a superconducting material. The essential idea behind these two options is that the vapor core of the heat pipe can be simulated as a superconductor of extremely high thermal conductivity.

In the 2D-RZ heat conduction approach, the wall region is modeled as the normal container material, the wick is modeled as a solid material using an effective thermal conductivity, and the vapor core is modeled as a superconducting material with an ad-hoc very large thermal conductivity. Flexible boundary conditions are provided at the evaporator and condenser wall surface for coupling with the other components of the reactor system. The modeling methodology in SAM was verified with the thermal resistance model (Hu et al. 2019d). Figure 5-2 shows the comparison of average temperature at different locations from SAM prediction and the resistance model, and the comparison of the heat transport capacity (i.e. Q in the figure) from SAM prediction and the resistance model.

Figure 5-1. A conventional heat pipe in axisymmetric coordinate and the classical thermal resistance model

Figure 5-2. Heat pipe steady-state verification results

5.2 Multi-physics modeling and simulation of heat pipe micro reactor

The heat pipe cooled micro reactor poses a number of modeling challenges that are substantially different from those of traditional LWRs, including:

- Use of a fast neutron spectrum;
- Possible usage of metallic fuel;
- Enhanced neutron leakage due to streaming through the heat pipe vapor core;
- Large negative reactivity feedback effects due to thermal expansion of both the fuel and the core support plate;
- Passive conduction cooldown with vessel cooling system for decay heat removal.

Meeting these challenges requires not only an advanced thermal fluid or reactor kinetics analysis capability but a fully coupled multi-physics approach involving reactor kinetics, thermomechanics, 3D heat transfer, and heat pipe modeling. The nonlinearities brought by the different physics needs to be resolved through a coupling approach. It would be ideal to solve the different physics simultaneously; however, it is quite challenging or unfeasible. A common approach to resolve the nonlinearities is to apply the so-called tight coupling approach. The tight coupling consists of solving each physics problem separately and ensures the global convergence through Picard iterations. The main challenge in the tight coupling lies in the transfer between different physics problems. The MOOSE's MultiApp system (Gaston et al. 2015) provides an efficient framework for this purpose.

The full suite of non-LWR codes for confirmatory analysis at NRC is known as the Comprehensive Reactor Analysis Bundle (CRAB). It makes use of existing NRC codes, and integrates them with several codes developed through the DOE-NE's Nuclear Energy Advanced Modeling and Simulation (NEAMS) program. This modeling and simulation effort of a heat pipe

micro reactor utilize several MOOSE-based submodules under CRAB, including SAM, MAMMOTH/Rattlesnake, and MOOSE's Tensor Mechanics module.

5.2.1 Multi-physics coupling models

The numerical model consists of the following sub-models coupled to each other through the MOOSE MultiApp system. A schematic representation of interrelation is given on Figure 5-3.

- RK: one whole-core, 3-D MAMMOTH input with homogenized blocks to solve the linearized Boltzmann transport equation. The multigroup cross-sections are computed with a heterogeneous Serpent model. A Super Homogenization (SPH) correction is applied to run transport-corrected diffusion. The main purpose of this input is to compute the power density distribution and transfer it to the other physics.
- HC: one whole-core, 3-D SAM input for the heat conduction calculation in the reactor core. It models the heat conduction in the core and convection at its boundaries. It takes the power density from the RK model and calculate the solid temperature in different regions (e.g. fuel, reflector, reactor vessel, plate, etc.).
- HPs: 192 instantiations of a SAM input for modeling the individual heat pipe. Each individual heat pipe is coupled to a cooling pipe to model the secondary heat exchangers. The individual heat pipe takes the thermal heat from the fuel cell by conduction across the heat pipe evaporator wall. The condenser wall of the heat pipe is coupled with a cooling pipe through conjugate heat transfer.
- RCCS: a SAM input for modeling the reactor cavity cooling system. It takes the radiation heat from the reactor vessel and transport it to a coupled cooling pipe. Under the circumstance that the heat removal through the heat pipes is not available, the RCCS plays the key role in taking the heat out of the reactor core.
- TM-Fuel: 192 instantiations of a Tensor Mechanics input for modeling the axial expansion of the fuel elements. It takes the fuel temperature from the HC and return the axial expansion for reactivity feedback calculation in RK. There is one sub-model for each individual fuel cell.
- TM-Plate: a Tensor Mechanics input for modeling the radial expansion of the reactor core. It takes the solid temperature in the support plate from the HC and returns the radial expansion for reactivity feedback calculation in RK.
- Joint: a dummy input model to initiate the simulation flow of the HC and TM. This model is added to the coupling chain because of the difference in the meshes used by the RK and HC model. It also avoids the direct communications between TM sub-Apps and the HC sub-App so that the TM sub-Apps will not participate the Picard iterations needed for HC, HPs, and RCCS sub-Apps.

Figure 5-3. Schematic of the multi-physics coupling method for heat pipe micro reactors

The multi-physics model was shown to work very well in the steady state simulation of a reference heat-pipe micro-reactor core. Figure 5-4 shows the cross-sectional view of the solid temperature profiles in the reactor core. Figure 5-5 (left) shows the average fuel temperature in different fuel cells. The distribution of the average fuel temperature keeps very well the symmetry of the reactor core. Figure 5-5 (right) shows quantitatively the heat removal rate of the individual heat pipes. It is seen that the profile is closely following that of the power density of individual fuel cell. The heat pipe heat removal rate near the center of the core is about 1.5 times of that near the periphery of the core.

Figure 5-4. Steady state solid temperature profile. Horizontal cut view (left) and vertical cut view (right).

Figure 5-5. Distribution of average fuel temperature at different fuel cells (left) and heat removal rate at different heat pipes (right) at steady state

5.2.2 Simulation of single heat pipe failure

Transient behavior of the system with a failure of a single heat pipe near the center of the reactor core was simulated. The numbering of the heat pipes and fuel cells near the center of the reactor core is shown in Figure 5-6. In this simulation, the heat pipe with ID = 1 (HP1) is assumed failed at the start of the transient. The failure is modeled by a sudden drop in the flow rate of the attached micro heat exchanger, which will bring in a sudden drop to the heat removal rate by this heat pipe. Because of the failure of HP1, the temperature of the fuel in this fuel cell (FC1) will increase. In addition, the temperature of fuel in the neighboring fuel cells and the heat removal rate in the neighboring heat pipes will increase accordingly.

Figure 5-6. IDs of heat pipes and fuel cells near the center of the reactor core

The single heat pipe failure transient results are shown in Figure 5-7, Figure 5-8, and Figure 5-9. Figure 5-7 shows the average fuel temperature in FC1, FC2, FC8, and FC9. The heat removal rate of HP1 drops to a much lower level, which causes the increase of the average fuel temperature in FC1. The extra heat in the FC1 starts being transported to its neighboring fuel cells, which causes the increase of the average fuel temperatures in FC2, FC8, and FC9. Figure 5-8 shows the total power of the reactor. Because of the increase in the fuel temperature, a negative reactivity due to the fuel axial expansion and Doppler effect, the reactor power starts to drop following the single heat pipe failure. However, since the negative reactivity caused by the single heat pipe failure is minor, the reactor power is observed to stabilize to a new lower level at the end of the transient, 500 s in the current simulation. Figure 5-9 shows the distribution of the average fuel cell temperature at the start and end of the transient. The temperature increase in the neighboring fuel cells of the failed HP is very limited (~ 20 C), indicating that there would not be any cascading effects leading to the failure of the neighboring fuel cells.

Figure 5-7. Transient average fuel temperature in FC1, FC2, FC8, and FC9

Figure 5-8. Transient reactor power following the single heat pipe failure event

Figure 5-9. Average fuel temperature at the start (left) and end (right) of single heat pipe failure transient

5.2.3 Simulation of unprotected loss of heat sink event

This test simulates the transient behavior of the system with a loss of heat sink (LOHS) event. The loss of heat sink is modeled by a sudden drop in the secondary flow rate (to 0.1% of nominal condition). The simulation is started with a null transient of 200s and followed by the sudden drop in the secondary flow rate. The transient results are shown in Figure 5-10 and Figure 5-11. Figure 5-10 shows the total reactor power, power to the heat pipes, and the power to the RCCS; Figure 5-11 shows the transient average temperature at different blocks. After the start of the transient, the heat transferred to the heat pipes drops quickly to a lower level. The fuel temperature starts to increase accordingly, which brings in strong negative reactivity to the reactor core, and the reactor power starts to drop. During the early stage of the transient, the heat removal rate from the RCCS changes little, as the reactor vessel temperatures increases very slowly. The radiation heat transfer from the vessel outer surface will surpass the reactor power as the vessel wall temperature continues increasing and the reactor power continues decreasing at the later stage of the transient.

Figure 5-10. Transient reactor power and heat removal rate

Figure 5-11. Transient average solid temperature of different blocks

6 Code Validation Efforts

SAM utilizes the application- and validation-driven code development approach. The code is being applied each year to selected demonstration or validation problems where the physics and scales of the problem may expand or increase with complexity in successive years. These validations lead up to the continuous assessment of the code capabilities and performance for a wide range of advanced reactor applications. Code validation activities in FY19 include using test data from Compact Integral Effects Test (CIET), Molten-Salt Reactor Experiment (MSRE), Natural convection Shutdown heat removal Test Facility (NSTF), and Minnesota Natural Circulation Loop.

6.1 Code Validation using CIET Test Data

The CIET experimental loop is a test facility that is designed, built and operated at University of California, Berkeley, with the aim to reproduce the thermal-hydraulics response of fluoride salt-cooled high-temperature reactors under forced- and natural-circulation conditions. Among many available experiments, three sets of CIET experiments with distinctive characteristics were selected for SAM validation purpose. The three sets experiments are: 1) Power step change transient tests; 2) DHX-DRACS natural circulation tests; and 3) heater frequency response tests. For all tests, steady-state or transient, SAM predicted results show very good agreement with experimental data. The successful validation of SAM against these selected CIET data demonstrates that the computer code is well suited for thermal-hydraulics analysis of FHR designs. The details of the SAM code validation using CIET Test data can be found in another Argonne report (Zou et al. 2019).

6.2 Code Validation using MSRE Test Data

For MSR applications, two new capabilities were recently added in SAM (Zhang and Hu 2018) a precursor drift model and Point Kinetic Equation (PKE) for flowing fuel. Given the continuous interest in MSR technologies, it is important to demonstrate that these new capabilities can accurately predict the transient behaviors in MSRs. To that end, these capabilities are being benchmarked against three transient experiments conducted in MSRE, include the pump start-up and coast-down tests at zero power and a natural convection transient. The pure thermal hydraulic validation using the MSRE water mockup test data and preliminary thermal hydraulic analysis of MSRE during normal operating condition and a postulated loss-of-flow transient were performed in an earlier study [Leandro et al. 2019] using the SAM code. Overall, the results predicted by SAM are in good agreement with the experimental measurements. The details of the SAM code validation using MSRE test data can be found in Fei et al. (2020).

6.3 NSTF benchmark

The Natural Shutdown heat removal Test Facility (NSTF) was an air based natural convection system designed as a half-scale facility of the reactor cavity cooling system (RCCS) of the General Atomic Modular High Temperature Gas-cooled Reactor design. This facility was equipped with a variety of sensors to monitor the system mass flow rates, temperatures, and velocities at various locations. In addition to experimental data, results from RELAP5 simulations of the facility were available (Lisowski et al. 2016). This made the NSTF an ideal facility to benchmark SAM's capability to model gas-cooled systems.

The preliminary SAM validation using the air-based NSTF test data was performed in a previous work (Hollrah et al. 2019). The results of this model were compared with experimental data and a simulation of the same system using RELAP5. SAM predictions were comparable with RELAP5 predictions and with experimental results, as shown in Figure 6-1.

Figure 6-1. SAM and RELAP5 simulations results of mass flow rate, temperature rise, pressure drop, velocity compared to NSTF experimental values, Run 011.

To improve riser duct wall temperature predictions, a 3D-1D coupling method was applied, in which the riser duct walls are explicitly modeled using 3D mesh and the fluid are modeled as 1D channels. This allows for accurate modeling of 3D conduction in the solid structures while removed the needs of computationally expansive CFD simulations of the flow channels, since the flow is dominantly one-dimensional.

SAM 3D-1D coupling analysis of the NSTF was compared to CFD simulations for two steady state cases. The first was a baseline power case with approximately 50 kW heat removed by the fluid while the second was as low power case of approximately 33 kW. The total mass flow rate of the system was 0.61 and 0.58 kg/s for the respective cases. The fluid inlet temperatures were 18.8 and 16.7°C.

Results from the CFD simulations include the radiative heat flux transmitted to each node on the outer surface of the riser ducts. These results were adapted for use as the outer riser boundary conditions in the SAM model. Each riser wall was divided into eight regions as shown in Figure 6-2. A layered average of the CFD heat flux result was taken in each region and applied as the boundary condition in the SAM model.

Figure 6-2. The division of riser wall in 8 regions to allow a distinct heat flux on different riser walls

Figure 6-3 and Figure 6-4 show the layered maximum temperature of SAM and CFD simulations for baseline power and low power simulations respectively. In almost every simulation, a trend is observed where SAM overpredicts the temperature closer to the inlet of the riser, then under-predicts temperature in the upper half of the riser. The exception to this trend is riser 1. An explanation for this exception will be discussed later.

To explain the differences between the SAM and CFD results, it is necessary to examine the heat transfer coefficients (HTCs) calculated by both codes. Figure 6-5 shows the layered average HTC along the entire length of the riser. It can be seen that, near the inlet, SAM calculates a lower HTC compared to the CFD while the opposite is true farther up the riser. A lower HTC means less efficient heat transfer into the fluid and thus, higher riser wall temperatures. The exponential decrease of the CFD HTC explains why the differences between CFD and SAM temperature calculations are largest near the inlet. This large difference is caused by entrance effects that can be modeled by the CFD code but is unaccounted for in SAM's closure models.

Overall, the results of this study showed good agreement with previous CFD analysis. The disagreements that did exist were caused by differences between HTC calculation between the two codes. If different HTC models for the inlet region are available, the differences can be greatly reduced.

Figure 6-3. A comparison of maximum riser wall temperature along riser axis between SAM and CFD results for the baseline power simulation

Figure 6-4. A comparison of maximum riser wall temperature along riser axis between SAM and CFD results for the low power simulation

Figure 6-5. Comparison between SAM and the layered average CFD calculated HTC

6.4 Minnesota Natural Circulation Loop Benchmark

In an effort to aid the development of these cartridge loops for the Versatile Test Reactor (VTR), experiments conducted at the University of Minnesota observing the transient behavior of single-phase natural circulation water loops was used for validation of the CARLITA code. The same test data were then used for SAM code validation, which can be also used as code-to-code verification of CARLITA code. This study also increased the awareness of the SAM code in the VTR Experimental Program.

Two experimental loops were designed and tested at the University of Minnesota in an effort to study the transient behavior of single-phase natural circulation water loop systems. Data for a total of three experimental tests were available in the literature (Alstad et al. 1956). A few experimental conditions for these tests were not specified, such as the secondary side flow rate for the first experimental loop, so a few assumptions were made when defining the secondary side of the heat exchangers. The data includes measurements of the loop flow rate as well as temperatures at locations *T1*, *T3*, and *T4*. Tests 2 and 3 were conducted on the first experimental loop, while test 4 was conducted on the second experimental loop. A summary of the experimental conditions is shown below in Table 6-1.

Table 6-1. Experimental conditions for the three tests provided.

Test	Loop	Heater Conditions	Coolant Inlet Temp.	Initial Fluid Temp.
2	1	Abrupt heat input to all 4 heaters (24.75 kW total)	3.1 °C	Uniform 50 °C
3	1	Bottom heater turned on (6.39 kW) until steady-state, then abrupt heat input to top three heaters (24.88 kW total)	2.5 °C	62.2 °C at T1 25.3 °C at T4
4	2	Abrupt heat input to top three heaters (19.17 kW total)	4.4 °C	Uniform 42.8 °C

Based on the initial benchmark simulation results, it was suspected that the heat exchanger design used in the first experimental loop was likely operating at a reduced efficiency or different secondary side flow rate than the second experimental loop. For this reason, results from another computational code CARLITA were compared to results from both SAM and the experimental tests. CARLITA was used in a similar validation study against the experimental tests done at the University of Minnesota in an effort to aid the VTR cartridge loop development. Results from CARLITA showed that a 100% heat exchanger efficiency at a secondary coolant flow rate of 10 GPM for test 2 compared very similar to results found from SAM simulations. Both simulations under predicted the loop temperatures but matched the loop mass flow rate well with the experimental data.

The CARLITA validation study found that using a heat exchanger efficiency of 65% best matched the experimental results for tests 2 and 3. For a qualitative comparison, SAM simulations were re-run with a heat exchanger efficiency of 65%. Plots of the loop temperatures and flow rates between SAM, CARLITA, and experimental data for tests 2 and 3 are shown below in Figure 6-6 and Figure 6-7, respectively. Qualitatively, the results from SAM and CARLITA are in good agreement with the experimental data for the two tests, and SAM and CARLITA were shown to often converge to similar steady-state values.

Figure 6-6. Plots of loop temperatures and flow rates of CARLITA and SAM results with a heat exchanger efficiency of 65% against experimental data for test 2.

Figure 6-7. Plots of loop temperatures and flow rates of CARLITA and SAM results with a heat exchanger efficiency of 65% against experimental data for test 3.

The second experimental loop was used for test 4, where only the top section of the loop was changed. An initial flow rate of zero and a uniform temperature of 42.8 °C was assumed at the start of the transient. The secondary side flow rate was set to 10 gpm at an inlet temperature of 4.4 °C. One of the bottom heaters and two of the top heaters were then turned on to initiate the transient,

resulting in a total power input of 19.17 kW. Data was then collected until steady-state conditions were achieved at a time of approximately 400 seconds. Steady-state for the SAM simulation reached a steady-state at a slightly later time of 500 seconds. Plots of the experimental data and SAM results are shown below in Figure 6-8 and Figure 6-9.

The results in general show a good comparison to the experimental data. Hot leg temperatures in the early stages of the transient were over predicted by about 5 °C that later leveled off to under predict the temperature by about 3 °C as the loop approached steady-state. The cold leg temperature follows the early transient trend of the experimental data well until deviating around 200 seconds where the temperature then remains under predicted by about 3 °C, similar to the hot leg temperatures. Loop flow rates are reasonably predicted in the early stages of the transient, but the final steady-state flow rate is then under predicted with a percent difference of around 3%.

Figure 6-8. Plot of loop temperatures from experimental data and SAM results for test 4.

Figure 6-9. Plot of loop flow rates from experimental data and SAM results for test 4.

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