ANL/NEAMS-14/1

NEAMS Update

Quarterly report for October 2013 – December 2013

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Overview

- The mechanistic smeared cracking model was extended from two to three dimensions (page 2).
- Subcontinuum molecular dynamics simulations were used to investigate oxide fuel grain boundary fractures during reactor transients (page 2).
- An improved model of bubble and grain boundary interaction was developed (page 2).
- Improved descriptions of fission-gas/grain boundary interactions and cluster and defect formation are being developed to create new fission gas diffusion models in MARMOT (page 3).
- The SHARP team has integrated structural mechanics feedback into coupled multiphysics dynamic simulations of sodium fast reactor (SFR) cores, with the sponsorship of the Advanced Reactor Concepts program (page 5).
- The coupled simulation effort has driven debugging and other code improvements, as well as advances in mapping dissimilar computational meshes (page 5).
- The MOOSE framework was updated with a robust capability to recover from processing interruptions (page 5).
- The risk analysis capabilities of RAVEN were extended by importing the Boost library and implementing n-dimensional distributions (page 7).
- Industry collaborators help improve the graphical user interface of RELAP-7 (page 7).
- The flow model in the SFR System Module was updated (page 8).

MARMOT Developer Receives Leadership Award

Michael Tonks, staff scientist at Idaho National Laboratory, has been selected as one of seven 2014 professional young leaders by the Minerals, Metals, and Materials Society (TMS).

Tonks is being honored by the Structural Materials Division (SMD) of TMS with the 2014 TMS SMD Young Leader Professional Development Award. The award was created to enhance the professional development of dynamic young people from TMS's five technical divisions. He was presented with the award at the Structural Materials Division luncheon on Feb. 19, 2014, in San Diego during the 143rd TMS annual meeting.

Tonks graduated with a doctorate degree in mechanical engineering from the University of Illinois, Urbana-Champaign, in 2008, with his research focused on stochastic methods for crystal plasticity. He spent the last three years of his doctorate work at Los Alamos National Laboratory as a graduate research assistant. After graduation, he completed a year as a postdoctoral researcher at Idaho National Laboratory developing multiphysics models of microstructure evolution in irradiated materials. Currently, he is the Computational Microstructure Science group leader at Idaho.

During his tenure at INL, Tonks has made several significant contributions. He is the creator and lead developer of the mesoscale MARMOT code, a finite-element-based code that predicts the coevolution of microstructure and properties under applied load, temperature, and radiation damage. MARMOT is the signature mesoscale code for the NEAMS program. He has also helped to pioneer the application of multiscale modeling to develop physics-based materials models of fuel for the NEAMS program.

FPL Accomplishments

Engineering Scale (BISON)

Much of the development effort during the first quarter related to extending the mechanistic smeared cracking model, which was initially implemented in two dimensions (R-Z), to three dimensions. This has involved both extension of the model itself and how it is implemented within BISON. The three-dimensional model is on track to be incorporated into the Fuels Product Line (FPL) next quarter. [INL]

The smeared cracking model is a mechanistic model that treats the effects of cracking at a continuum level. Also under development are discrete cracking models that will enable arbitrary crack initiation and growth using the extended finite element (XFEM) method. Progress during the last quarter included implementation and extensive testing of methods to handle initialization of elements where a crack terminated in the previous time step and allow an arbitrary set of line segments to define an evolving set of cracks. The result is a working model for dynamic crack growth across an arbitrary mesh, and the algorithm is now ready for use in a physics-based crack growth model. [INL]

The FPL team performed another set of sensitivity analyses on the fission gas-release model implemented last year in BISON. The input parameters varied included temperature, grain size, intra-granular diffusion coefficient, resolution, and grain-boundary (GB) diffusion coefficient. These were varied at three levels per input parameter, for a full factorial design at 7 levels of linear heat generation rate (LHGR) from 150 to 450 W/cm and a total of 1,701 automated BISON executions. Main effects analysis was performed for the overall sample as well as the sample of 243 runs at each LHGR level. [SNL]

Overall, the results suggest that the temperature, diffusion coefficient, and resolution are significant in terms of predicting fission gas release at any of the LHGR levels, while fuel grain size and GB coefficient are only occasionally significant in the fission-gas release prediction (depending on the LHGR level).

Future output metrics to be examined are fuel swelling at the middle, inner, and outer regions of fuel cross-section. [SNL]

Considerable work on BISON validation took place during the past quarter, and the BISON validation plan is on track for completion during the next quarter. A list of new assessment cases for the upcoming year has been developed and prioritized, and development of the needed input files is underway. [INL]

Finally, a BISON training workshop was held at INL on December 5-6. It was well-attended by both current users/developers and interested new users. [INL]

Subcontinuum Scale (MARMOT and Atomistic Simulations)

Due to the importance of correctly treating fuel cracking, mechanistic modeling is also occurring at the subcontinuum scale for this phenomenon. Molecular dynamics (MD) simulations have been used to investigate the GB fracture mechanism that occurs in oxide fuel during reactor transients. The simulations indicate that GB fracture occurs due to weakening of the GB by the gas bubbles that have nucleated on it and that the event is independent of the bubble pressure. A rate-independent crack growth model has been implemented in MARMOT. While the optimal solution approach is still being determined, this model will be a critical part of the task to develop an advanced fracture model for BISON. [INL]

An improved model of bubble and GB interaction that accounts for the diffusion direction of surface and GB diffusion has been developed. Additionally, MD simulations have been used over the last several months to determine GB mobility in UO_2 using various approaches. These simulations are now complete, allowing for a comparison between the various approaches, which showed that they are in good agreement. These combined efforts are being used to investigate GB and bubble interaction in three dimensions within oxide fuels and improve the average grain size model in BISON. [INL]

Three-dimensional mesoscale simulations have been performed with the pore/GB interaction model in MARMOT to inform the development of a mechanistic model for migration of GBs laden with gas bubbles. The MARMOT results were first compared with MD simulations to verify the model. Zener pinning

*The organizations that performed the work are listed in brackets at the end of each topic. The national laboratories performing NEAMS work are Argonne (ANL), Idaho (INL), Lawrence Livermore (LLNL), Los Alamos (LANL), Oak Ridge (ORNL), Pacific Northwest (PNNL), and Sandia (SNL).

theory was then adapted to represent the GB behavior. For a given number of bubbles resident on the GB, the analytical model compares extremely well with the results from the MARMOT simulations. [INL]

Work is proceeding on implementing new fission gas diffusion models into MARMOT. The latest accomplishments include an improved description of fission-gas/GB interactions and formation of various clusters and defects via rate theory reactions within the phase-field framework. A methodology to extract effective diffusivities for different thermodynamic and irradiation conditions has been implemented. [LANL]

Atomistic simulations are being performed to understand equilibrium gas bubble geometries and locations in oxide fuels. Using the Kawasaki Dynamics Canonical Monte Carlo code, simulations of Xe-loaded UO_2 samples containing GBs were performed. A significant reduction in total system energy was observed as a result of Monte Carlo moves redistributing the Xe gas towards the GBs and depleting the bulk UO_2. Further efforts are in progress to accelerate the equilibration process by lowering the switching energy barriers for complex Monte Carlo moves. [LANL]

Work continues on refining the model for UO_2 thermal conductivity degradation under irradiation. Analysis of existing simulation data has provided new understanding of the impact of localized magnetic moments on uranium ions and the associated structural distortion on reduction of UO_2 thermal conductivity, as well as surprising anisotropy observed both in simulations and single-crystal experiments. MD simulations of the reduction of UO_2 thermal conductivity due to fission products are continuing. In addition, the correlation between the atomic displacements and the anisotropic thermal conductivity in UO_2 obtained from MD simulations has been investigated using the direct method and Buckingham potentials (Basak potential). The local lattice constant at different sampling regions in the supercell has small variations due to the applied thermal gradient, signifying anisotropic local distortions. [LANL]

To further understand the local distortions, an MD-calculated position profile of an oxygen ion was analyzed in various simulation settings. The shape of the distribution is an ellipsoid with the short axis along the [001] direction rather than a sphere, as would be expected for a cubic or isotropic system. This observation suggests that UO_2 thermal conductivity may be anisotropic. [LANL]

In the area of mechanistic modeling of creep in oxide fuel, results from density functional theory calculations of uranium vacancy diffusion have been implemented in a kinetic Monte Carlo code that accounts for strain fields. This has enabled the simulation of how diffusion rates are influenced by strain fields, which is an important step in understanding interactions with dislocations. It has also been extended to study charged uranium vacancies – the predominant defect in stoichiometric UO_2. [LANL]

Technical Spotlight: Using BISON to Understand Failure Propagation

Background

The Advanced Test Reactor (ATR) is used to study the effects of long-term irradiation on fuels and materials. One of the on-going programs at the ATR is the testing of advanced fuel cycle (AFC) fuels and components. Tests AFC-2A and 2B used sodium-bonded metallic fuels doped with minor actinides and lanthanide fission products to study their transmutation behavior in a reactor core. Each experimental test train inserted into the ATR for irradiation was made of 6 short fuel rods (rodlets) stacked inside a stainless steel capsule for containment.

Post-irradiation examination of the rodlets (***Fig. 1***) revealed breaches in the rodlet cladding and fuel melting. The large-scale damage was attributed to the release of the fission gas into the helium gap between the rodlet cladding and the outer capsule. This release was not unexpected, and the double-encapsulation provided by the stainless steel capsule was for the purpose of providing protection from the ATR coolant in such an instance.

During nominal (low-power) operation, the fuel and cladding temperatures remained within the capsule design limits, but these limits were exceeded during short periods when the reactor power was raised. Rodlet 4 was found to have operated at the

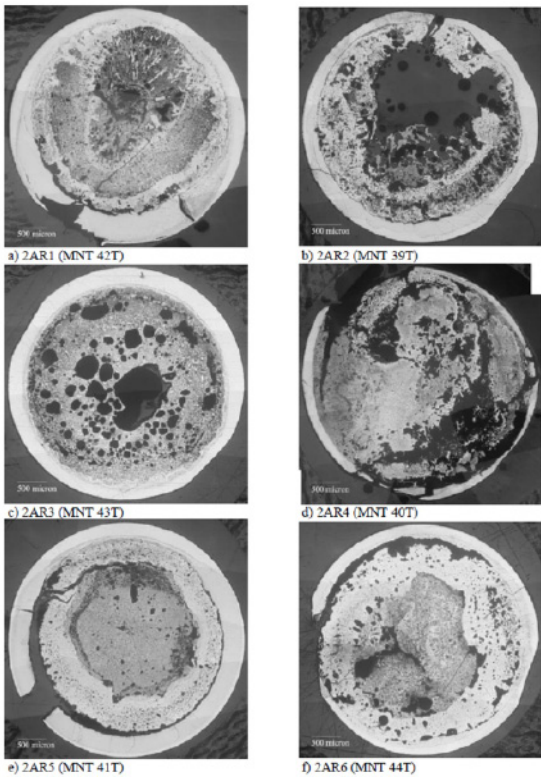

Fig. 1. Post-irradiation examination images of AFC-2A rodlet cross-sections.

highest temperature and is assumed to have been the first one to breach, but it was not clear how the first breach led to breaches in every rodlet. It was decided to explore the subsequent rodlet breaches with BISON.

Investigation with BISON

The primary objective of the work reported here was to simulate the fuel and cladding temperature history during irradiation of experiments AFC-2A and 2B. To accomplish the investigation, a BISON model was developed to simulate fission gas mixing within a capsule consisting of six individually clad fuel rodlets. The model included the following behaviors:

- Mechanistic fuel swelling based on the gas bubble force balance
- Fission gas release based on a gas bubble interconnection criterion
- Burnup-dependent thermal conductivity degradation that accounts for the effects of gas-induced porosity and initial fuel composition
- Fuel creep based on on the fuel temperature, stress, and porosity

Irradiation simulation with an initial condition of a single breached rodlet demonstrated that cladding temperature rise due to breach in a single rodlet is sufficient to cause breaches in the other rodlets. The most drastic impact of the breach on the fuel and cladding temperature is predicted when the fission gas bubbles in the rodlet 4 fuel interconnect and begin releasing fission gas into the fuel/cladding plenum and builds internal pressure that can be released into the capsule if a cladding breach occurs.

As the fission gas escaping from rodlet 4 contaminates the capsule fill gas, the cladding-capsule gap conductance decreases, resulting in an increase of the fuel and cladding temperature beyond its design limit of 650°C (see ***Figs. 2 and 3***). By the end of irradiation, the cladding temperature in most of the rodlets exceeds the Fe-U eutectic temperature of 720°C. Based on this finding, the investigation concluded that the amount of fission gas released into a capsule during a breach of a single rodlet is sufficient to increase the cladding temperature in the remaining rodlets beyond the design limit and cause their failure.

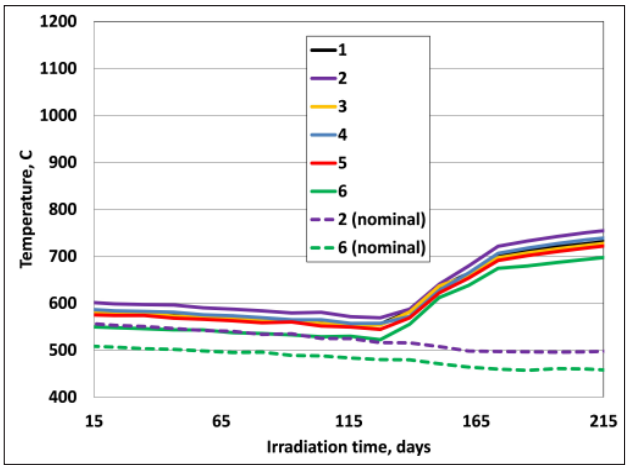

Fig. 2. Rodlet cladding temperatures during irradiation of AFC-2A.

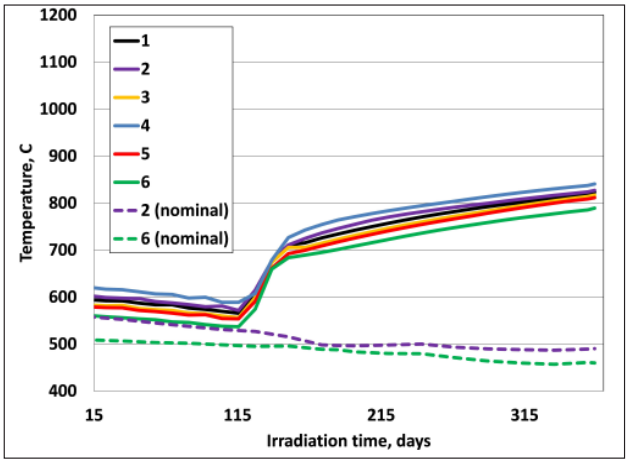

Fig. 3. Rodlet cladding temperatures during irradiation of AFC-2B.

Additional simulations were run with initial conditions of multiple breached rodlets. It was determined that as a result of the temperature increase associated with the fission gas release from breached rodlets into the capsule, the cladding temperatures ranged from 928°C to 983°C (AFC-2A) and 1,000°C to 1,040°C (AFC-2B). Peak fuel temperatures ranged from 1,144°C to 1,235°C (AFC-2A) and 1,201°C to 1,286°C (AFC-2B).

The results of the investigation with BISON have led to design changes that will prevent failure propagation in future AFC experiments.

Pavel G. Medvedev, INL

RPL Accomplishments

Module Integration (SHARP)

The SHARP coupled simulation team has focused on integrating structural mechanics feedback into the dynamic simulations for sodium fast reactors (SFRs). The integration of the structural mechanics code Diablo into SHARP is being demonstrated on the partially homogenized full core of the Advanced Burner Test Reactor (ABTR). The first fully coupled, fully three-dimensional iteration of the three physics has been demonstrated on a 7-assembly mini-core based on the ABTR geometry. [ANL, LLNL]

In the ABTR model, the ducts, load pads, core restraint rings, and bypass sodium are explicitly modeled; the interior of each ducted assembly is homogenized both in the neutronics and thermal-hydraulics models. The objective of this effort is to give advanced reactors programs an affordable next-generation tool for the prediction of radial core expansion, which is one of the most significant reactivity feedback mechanisms in liquid metal reactors. See the Structural Mechanics section for further discussion. [ANL, LLNL]

Overall, this intensive coupled simulation effort is driving development and debugging for the Reactors Product Line (RPL). CouPE and MeshKit were significantly improved to include components beyond the fuel assemblies and to account for structural deformation effects. Several bugs have been fixed, especially in memory management. [ANL, LLNL]

Integrated Frameworks

Development of the RPL frameworks is driven by the challenge associated with mapping deformations of the computational mesh in one physics model, e.g., structural mechanics, to the meshes used by other physics models. In most prior multiphysics integration efforts, the separate physics codes have been required to use meshes that are identical or substantially similar. Ultimately, this approach means that the computational elements are incorrectly distributed for some, if not all, of the individual physics models. The NEAMS frameworks allow each code to use its optimal mesh and provides tools for mapping not only scalar data but also deformations on module-specific meshes across the physics codes. [ANL]

Code to account for structural mechanics deformations in coupled simulations has been developed for MOAB and demonstrated on meshes and deformation data used for the ABTR multiphysics benchmark model. See the next section for further discussion. [ANL]

Another challenge is to provide a reliable, easy-to-use recovery from unexpected interruptions, which are all too common in multiphysics modeling. The MOOSE framework was updated to establish a reliable and pervasive restart capability, which stores state data across all integrated applications at user-selected restart points. The high degree of variability across the broad scope of MOOSE applications made this important feature difficult to implement. [INL]

Structural Mechanics (Diablo)

This quarter saw considerable effort toward a SHARP multiphysics demonstration funded by the Advanced Reactor Concepts (ARC) program. The core configuration targeted is the ABTR with the goal of coupled thermal-hydraulic and neutronic simulations informed by successive deformed geometries computed by the structural mechanics module Diablo. A model problem was formulated using a 7-assembly mini-core (***Fig. 4***), which provides a much more modest computational workload for exploring modeling strategies and data paths between the physics modules. [LLNL]

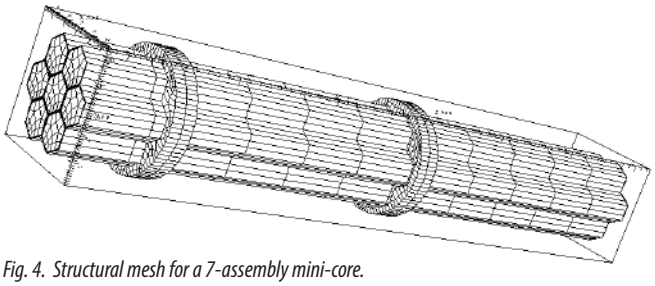

Fig. 4. Structural mesh for a 7-assembly mini-core.

The multiphysics model required the SHARP team to reconcile the modeling needs of three physics modules, which interact primarily at the so-called "load pads" between assemblies at axial positions corresponding to the restraint rings. The structural mesh must capture "contact" between neighboring bowing assemblies without pinching the inter-assembly sodium domain, which would create zero-volume elements (***Fig. 5***). The solution was to doubly mesh the minor volumes displaced by the load pads and thereby maintain a continuous sodium domain even when adjacent load pads close in. The approximation is acceptable, as the coolant flow through the inter-assembly passages is very small and the sodium there was already modeled as only a zero-velocity conducting layer. [LLNL]

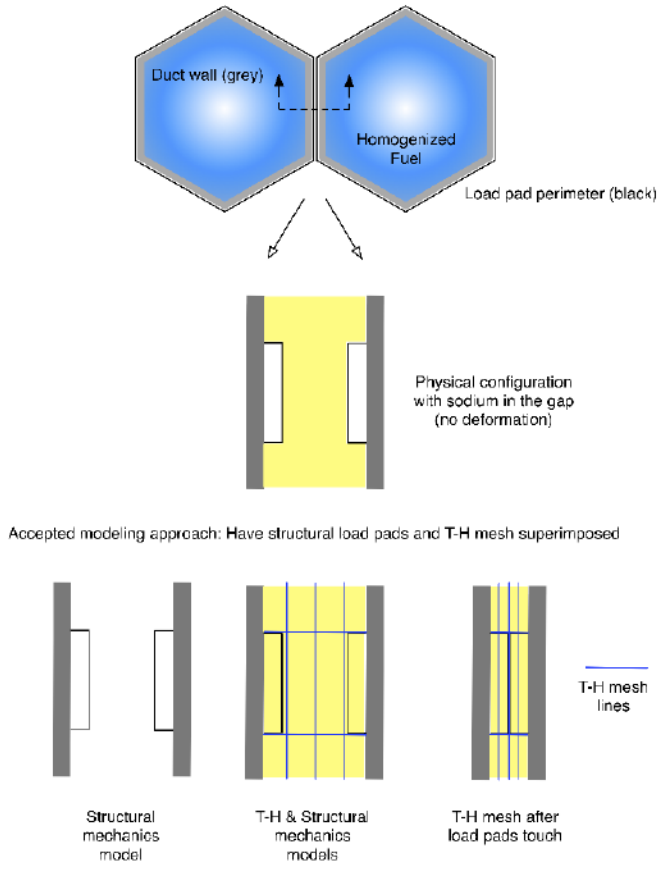

Fig. 5. Meshing approach used to couple fluid and structural components in the mini-core model.

Neutronics (PROTEUS)

To make the RPL broadly applicable to various reactor types, a unique suite of cross-section libraries and library generation capabilities are being implemented. Verification tests for the generalized cross-section libraries have been performed for heterogeneous (pin cells and lattices) problems from various reactor types. For the heterogeneous problems, group libraries comprising less than 300 groups were used, which were condensed from the base ultrafine group (2,158 groups) cross-section library using the group condensation optimization algorithm.

While PROTEUS-SN with a cross-section application interface (API) was under development, a heterogeneous-geometry-based, whole-core neutron transport code (DeCART) was utilized to test the new cross-section libraries. Verification tests will be extended to include 2D and 3D core problems. [ANL]

The cross-section API was also implemented in PROTEUS-SN. The conventional subgroup cross sections were initially tested with the cross-section API, which was found to work correctly for homogeneous problems. The code will be tested for heterogeneous problems during the next quarter. [ANL]

As part of the multiphysics demonstrations for the ABTR reactor discussed above, neutronics models were developed for (1) a 7-fuel assembly "mini-core" (***Fig. 6***) and (2) the full 199-assembly ABTR core (***Fig. 7***). These models were created using finite element meshes generated with the Reactor Geometry Generator and homogenized 9-group cross sections generated using the MC^2-3 code. A python script was written to auto-generate the material assignment file for the various ABTR assembly types. Vacuum boundary conditions were applied on all external surfaces.

Angular convergence studies were performed using PROTEUS, and both problems were determined to converge with L5T7 cubature (96 discrete angles in 3D). In standalone mode (no temperature or density feedback and no time dependence), the PROTEUS-calculated eigenvalue for the full core was 1.00269. [ANL]

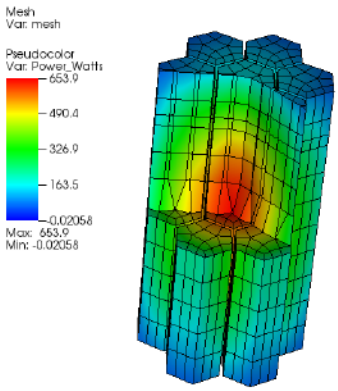

Fig. 6. Power distribution in the active region of a 7-assembly mini-core.

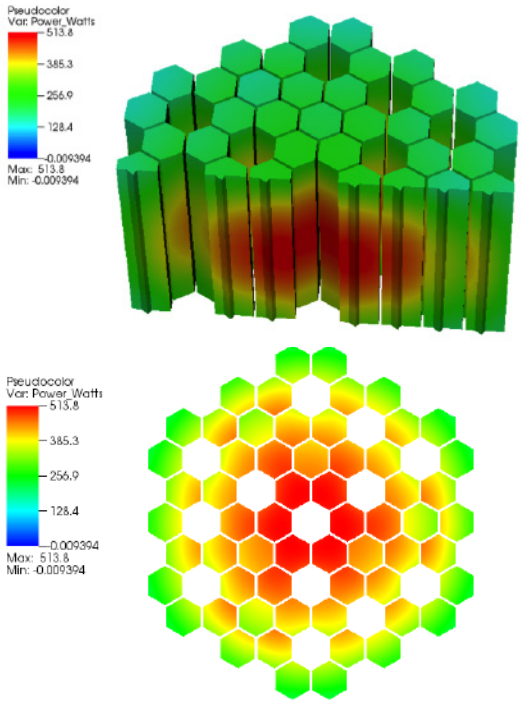

Fig. 7. Two views of power distribution in the ABTR core.

Probabilistic Risk Assessment (RAVEN)

The risk analysis capabilities of RAVEN have been extended by importing the entire distribution package from the Boost library and implementing n-dimensional (i.e., multivariate) distributions (***Fig. 8***). In particular, the probability values for these distributions are provided through files either on Cartesian grids or sparse nonstructured grids. This last capability is needed when probabilities are built out of experimental databases that are often very unstructured and lacking regularity. [INL]

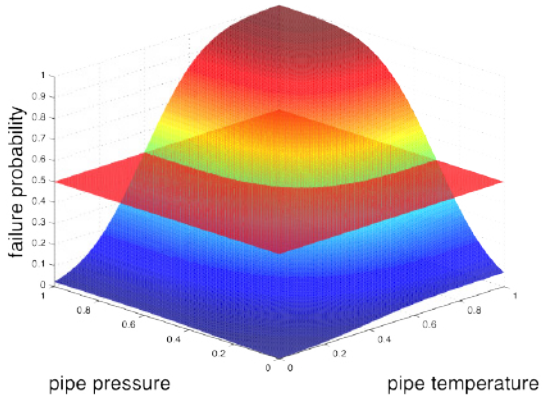

Fig. 8. An n-dimensional cumulative distribution of failure probability as a function of pressure and temperature.

System Simulation (RELAP-7)

NEAMS continues to develop an advanced reactor system simulation capability that leverages the investments in RELAP-7 made by both the NEAMS and LWRS programs. Based on input from industry collaborators, several small but significant changes have been implemented in the RELAP-7 graphical user interface to improve its usability. For example, users can now change component connections directly from the plant graphical layout (***Fig. 9***). [INL]

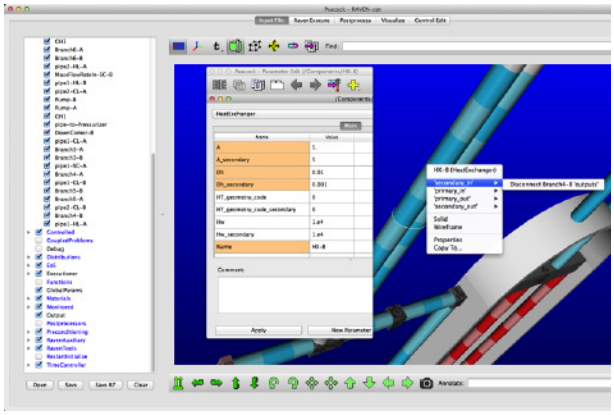

Fig. 9. Detail of the RELAP-7 user interface.

In order to resolve differences between the SFR System Simulation Module and SAS4A/SASSYS-1 simulations of the ABTR loss-of-flow transient, several modeling effects have been examined, including the friction modeling of the wire wrap in the core channels, the multivolume model of the cold pool, and the pump resistance after full stop. It was found that the differences in pump modeling contributed most to the differences in the long-term natural circulation flow rate between the two simulations. [ANL]

The development of the SFR System Module has been shifted to the primitive variable-based formulation for the flow model. Major updates of the flow

model have been made, including physics kernels, boundary conditions, equations of state, and stabilization schemes. The improved performance of the updated finite-element flow model has been confirmed for a wide range of test problems:

- Density wave propagation where numerical instability and numerical diffusion are eliminated by its second-order numerical accuracy in both space and time (***Fig. 10***),
- Steep gradient problems where steep gradient can be modeled and only slightly smoothed, and
- Discharges between tanks where flow reversal and a wide range of flow conditions (convection dominant or not) are modeled. [ANL]

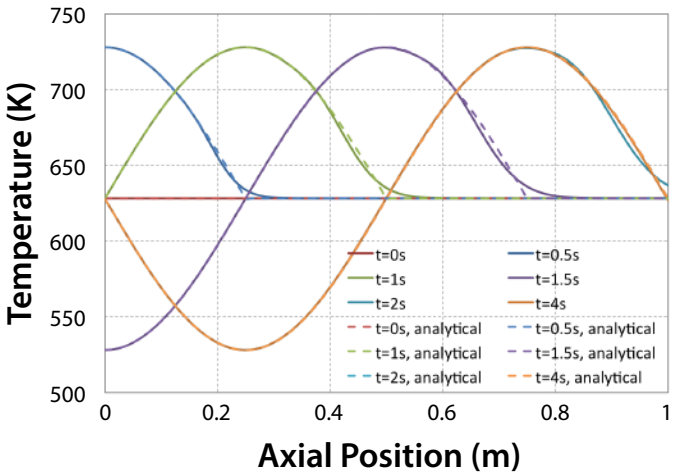

Fig. 10. Pipe transient temperature responses under continuous inlet temperature oscillation.

Upcoming Level 1 and 2 Milestones

Milestone ID	Description	Due Date
M2MS-14IN0603054	Deliver a "pervasive" restart capability that works for every feature in MOOSE through a sophisticated back-end "datastore"	1/31/2014
M2MS-14AN0603039	Provide update on testing and development of Nek5000 thermohydraulic capability	3/28/2014
M2MS-14OR06030628	Implement and demonstrate downloadable SHARP installer	3/31/2014
M2MS-14IN0602021	Issue BISON validation plan	3/31/2014

Note: No milestones were due in the first quarter of FY2014.

Availability of This Report
Online Access: U.S. Department of Energy (DOE) reports produced after 1991 and a growing number of pre-1991 documents are available free via DOE's SciTech Connect (http://osti.gov/scitech/).

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Argonne National Laboratory is a U.S. Department of Energy laboratory managed by UChicago Argonne, LLC. The Laboratory's main facility is outside Chicago, at 9700 South Cass Avenue, Argonne, Illinois 60439. For information about Argonne, see www.anl.gov.

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