ANL/NEAMS-13/2

NEAMS Update

Quarterly report for January – March 2013

Published May 2013

Quarterly Highlights

- Modeling of fuel pellet and cladding interactions was improved by adding frictional slip and release to the contact model in BISON (page 2).
- The mobility of vacancies at Σ5 grain boundaries in oxide fuels was determined with Monte Carlo calculations (page 2).
- The variation in the diffusivity of fission gas atoms in oxide fuels was quantified as a function of UO_2 stoichiometry (page 2).
- Atomistic simulations of fracture behavior in UO_2 were performed (page 2).
- A new model for fuel restructuring by void/pore and grain boundary migration was implemented in MARMOT (page 3).
- The NEAMS neutronics, thermal fluids, and structural mechanics modules were integrated in SHARP to perform high-fidelity, multiphysics simulations of an SFR fuel assembly (page 3).
- Transient multiphysics neutronics, thermal fluids, and reactor kinetics have been simulated for simple fuel assembly geometries in a core with fluctuating total power levels (page 3).
- Collaborations with Russia and Euratom continue to assess models of thermal fluid flows (page 4).
- The PROTEUS neutronics module has been enhanced with models of core kinetics and resonance self-shielding, and alternate methods are being incorporated to model neutron transport (page 4).

The NEAMS Vision

The goal of the NEAMS program is to enhance DOE-NE's research and development portfolio through the development of advanced computational methods. The tools we are developing —the NEAMS ToolKit — will provide insights into the performance and safety of advanced reactor systems that we cannot obtain through experimentation alone. They will also complement experimental work by helping us design experiments that are more complex and informative and then helping us interpret the results of those experiments.

To achieve this, the NEAMS ToolKit will incorporate fundamental descriptions of the underlying physics that govern the critical behaviors we must understand and accommodate in new reactor designs. In other words, we strive to replace the empiricism and correlations typically employed in modeling and simulation tools with mechanistic descriptions that have been validated using experiments targeting each phenomenon in isolation as well as experiments conducted to address the interaction and competition between phenomena.

With this approach, the ToolKit will not only succeed at reproducing the results previously observed, but it will permit designers and analysts to predict performance in regimes beyond the test base, that is, where we have no direct experimental observations.

The NEAMS team hopes this quarterly report of our accomplishments will provide insight into our challenges and achievements.

The quality and utility of the NEAMS ToolKit will only be as good as the guidance we get from stakeholders. Please, reach out to the team if you have advice or ideas to share. Your input is essential to our success.

Fuels Product Line Accomplishments

Engineering Scale (BISON)

A major new model was implemented in BISON during the past quarter: the modeling of contact between independent bodies (e.g., pellet-cladding contact, pellet-pellet contact) was enhanced to include frictional slip. Previously, BISON's only contact modeling options were frictionless or no-slip. Friction modeling is necessary for achieving more accurate representations of pellet-cladding mechanical interactions. For an initial assessment of this capability, the Halden reactor IFA431-Rod3 elongation experiment was simulated. Cladding elongation occurs when the fuel expands (due to heat and fission-product-driven swelling) and contacts the cladding. Once contact is established, friction can bond the fuel and cladding, and the elongating fuel stack can stretch the cladding by inducing a permanent strain along the fuel rod axis. [INL]

The Halden experiment was simulated using two fuel column geometries: (1) a continuous fuel column where all pellets were considered to be a single body and (2) a discrete pellet column in which individual fuel pellets were resolved and treated as independent bodies. In both cases, the friction model provided better comparisons with experimental data than did the frictionless or no-slip models. Of the two friction geometries, the discrete-pellet simulation agreed better with the experimental rod elongation data. The contact model was further modified to allow for contact release, which is vital for accurately modeling a fuel rod during abrupt power changes as part of normal operations as well as off-normal scenarios (e.g., cladding ballooning during a loss-of-coolant accident). [INL]

The fuels team and BISON early users continue to assess BISON simulations using experimental data from a broad class of benchmarks from both the FRAPCON and FUMEX experimental databases. See the Technical Spotlight on page 5 for details of some of these assessments. [INL]

*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).

Subcontinuum Scale (MARMOT and Atomistic Simulations)

Understanding the behavior of fission gases in oxide fuels continues to be one of the highest-priority efforts for subcontinuum phenomena. Within this effort, two major studies were completed: vacancy diffusion at grain boundaries and diffusion of fission gas in stoichiometric UO_2.

The first study looked at uranium vacancy diffusion in the presence of a Σ5 symmetric tilt and a Σ5 twist grain boundaries. These boundary types were selected as a starting point because they are the simplest of the boundaries considered in previous work on segregation. A combination of molecular statics and kinetic Monte Carlo calculations were used to determine that the mobility of vacancies significantly increases at Σ5 grain boundaries. Given that the diffusion of Xe and other fission gases are intimately tied to the mobility of uranium vacancies, these results give important insight into how grain boundary geometries and fission gas mobility are connected. [LANL]

The second study quantified the variation in the diffusivity of fission gas atoms in UO_2 as a function of stoichiometry (the degree to which the relative quantities of O and U vary from a 2:1 ratio, i.e., $UO_{2\pm x}$), both with and without irradiation effects. Unlike the first study, this one focused on bulk diffusion and the calculations were performed using both density functional theory and empirical potentials. The fission gas diffusivity was found to depend strongly on both the $UO_{2\pm x}$ stoichiometry and irradiation conditions (which govern the concentration of uranium vacancies). The results were shown to compare well to available experimental data. These understandings have been incorporated into a new model for fission gas behavior that is being implemented in BISON. [LANL]

The development of models to account for cracking in oxide fuels is also an important effort due to the major influence cracking has on thermal and gas transport, as well as fuel-cladding mechanical interaction. Atomistic simulations of fracture behavior in UO_2 were performed with seven different embedded-atom-method potentials, which elucidated the role of metastable phase transformations (i.e., Rutile phase evolution) at the onset of fracture. This information is used to inform mesoscale, finite-element simulations, as shown in Figure 1. [INL]

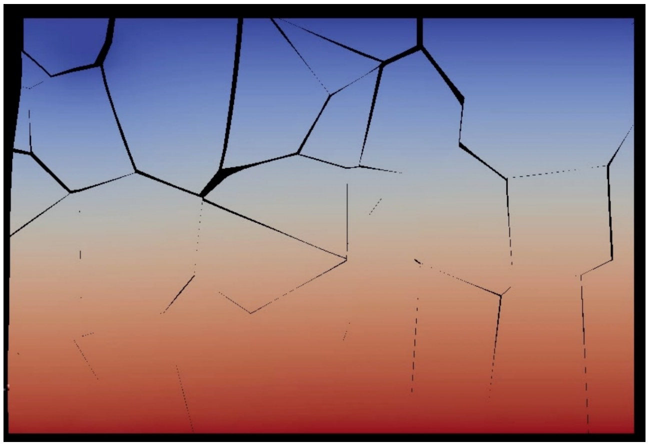

Fig. 1. Mesoscale simulation of fractures in UO_2 fuel.

Another phenomenon that strongly influences thermal and gas transport in oxide fuels operated at higher temperatures (i.e., peak rods in LWRs and nominal rods in SFRs) is restructuring, which leads to formation of a central hole; this tends to increase the thermal conductivity of the fuel in the restructured zone (due to reduction of porosity) and greatly increase fission gas release. A new model that allows simulation of restructuring by both void/pore and grain boundary migration under a thermal gradient was implemented in MARMOT.

Simulations using the new model have shown that fast-moving pores drag grain boundaries: as the pores migrate to the hot center of the pellet, they leave elongated grains in their wake. Thus, it has been shown that diffusion along grain boundaries provides a rapid vacancy transport path, allowing a central void to grow by Ostwald ripening (i.e., it grows at the expense of smaller voids in the periphery). [INL]

In late January, PNNL hosted the first training workshop for MARMOT developers from PNNL and Washington State University. The developers are collaborating on a crystal plasticity model for MARMOT. The base model has been implemented and is being tested and assessed against an existing solid-mechanics-based model. [PNNL]

Finally, progress continues in development of the THERMOCHIMICA code, which will supply thermochemical property information within BISON and MARMOT. Current efforts are expanding its thermochemical database and integrating it with BISON and MARMOT. [ORNL]

Supporting Tools

The sensitivity analyses of the new fission gas release model recently scaled up to BISON is nearing completion. To date, these analyses have used DAKOTA to assess the effects of linear heat rate, diffusion coefficient, porosity, and other uncertain inputs on calculated fuel centerline temperature and magnitude of fission gas release. [SNL]

Work was initiated to extend the capabilities of VisIt, the NEAMS tool to be used for visualization and analysis. The extension will allow the inclusion of Exodus global variables in queries and query-over-time scenarios needed by BISON and MARMOT. [LLNL]

Reactors Product Line Accomplishments

Code Integration (SHARP)

For the first time, the NEAMS neutronics, thermal fluids, and structural mechanics modules were integrated in SHARP to perform high-fidelity, multiphysics simulations of an SFR fuel assembly. The simulations attempted to duplicate measurements from the XX09 instrumented assembly used in the shutdown heat removal tests (SHRTs) completed in the Experimental Breeder Reactor II (EBR-II). The initial series of simulations approximated both steady-state conditions and simple transients (Fig. 2). The simulations will be expanded soon to include adjacent

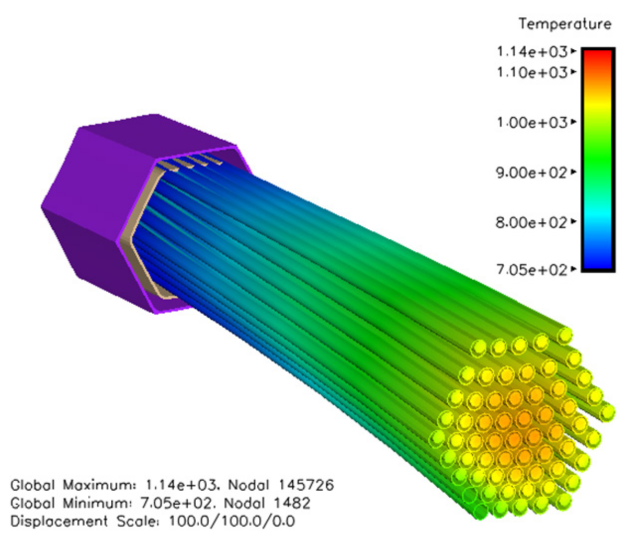

Fig. 2. Predicted deformations in the EBR-II XX09 assembly during an SHRT pseudo-transient simulation. Displacements are exaggerated 100-fold.

assemblies on the path to full-core multiphysics validation simulations of the EBR-II SHRT experiments. [ANL, LLNL]

The second quarter also marked the first use of SHARP to model transient phenomena. Until now, all simulations were performed with the total core power held constant, which limited the demonstrations to steady or pseudo-steady states. Transient multiphysics neutronics, thermal fluids, and reactor kinetics have been simulated for simple fuel assembly geometries in a core with fluctuating total power levels. Further development of the transient capabilities of SHARP will be a significant focus for the remainder of the fiscal year. [ANL, LLNL]

The structural mechanics module (Diablo) has now been integrated into the framework modules and can receive data from the neutronics and thermal fluids modules to evaluate structural stress, strain, and deformation. The mesh deformation capability needed to predict structural deformation feedback effects will be developed when funding is available. [ANL, LLNL]

Thermal Fluids (Nek5000)

A low-fidelity turbulence model based on the Unsteady Reynolds-Averaged Navier-Stokes (URANS) methodology has been initiated within the Nek5000 computational fluid dynamics (CFD) module. This capability will enable NEAMS simulations of increasingly larger power plant segments, reduce computational time when needed, and enable the NEAMS ToolKit to run on desktop and cluster computers. The initial implementation provides a small library of two-equation URANS model options and is being developed in collaboration with selected members of the Nek5000 user community. [ANL]

The thermal fluids collaboration with Russia continues to validate CFD simulations based on experiments completed in the Russian SIBERIA subchannel flow blockage facility. Recent efforts have used Nek5000, CONV3D, and CABARET to quantify the sensitivity of the simulations to mesh resolution and inlet boundary conditions (Fig. 3). Specifications have been prepared for upcoming validation exercises based on the isothermal jet mixing experiments completed in the MAX facility. Future experiments will focus on natural convection phenomena, which may be the basis of validation exercises. [ANL]

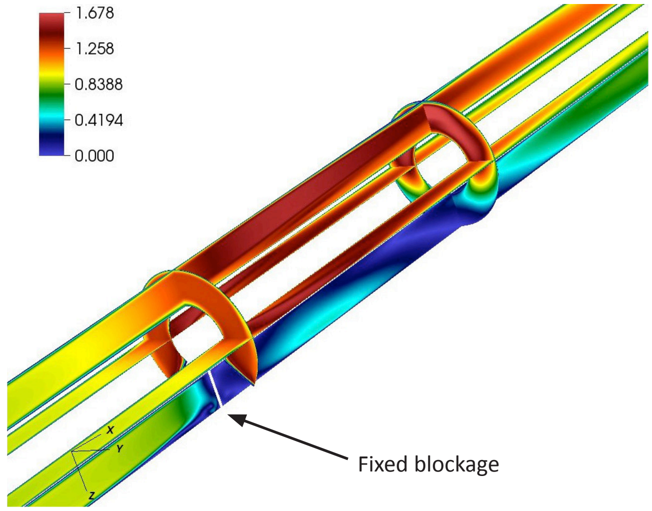

Fig. 3. Flow velocity contours from high-fidelity Nek5000 simulations of flow through the annular test section of the SIBERIA flow blockage experiment.

The collaboration with Euratom is focusing on experiments developed to support the MYRRAH fast spectrum research reactor. An initial benchmark dataset has been extracted from existing hydraulics simulations of a seven-rod SFR fuel assembly, and specifications for flow conditions have been provided to Euratom collaborators. The Euratom team has provided specifications for a pebble bed hydraulics benchmark exercise, and the U.S. team has begun high-fidelity simulations. [ANL]

Neutronics (PROTEUS)

The PROTEUS-SN (discrete ordinates) module is being prepared for release to outside users later this year with capabilities for forward, adjoint, and quasistatic neutronics calculations. The PROTEUS team is working to finalize documentation, streamline user input, and simplify interfaces to required external libraries. [ANL]

A quasi-static kinetics capability has been implemented in PROTEUS-SN using the SN2ND solver. However, the master driver time step for multiphysics simulations is large compared to the prompt neutron lifetime, so SN2ND uses much shorter time steps in the core kinetics simulation. Simply applying a step reactivity change in the first neutronics time step after the multiphysics data exchange does not accurately capture the effects of the reactivity insertion. The use of ramp schemes over the several inner neutronics iterations is being investigated. [ANL]

An improved resonance self-shielding method has been implemented within the MC²-3 cross-section library generation module to extend the current methodology to the whole core. In this method, the resonance interference effects are accounted for through the NR approximation or slowing-down calculations for specific compositions, and the heterogeneity effect is accounted for by the use of isotopic escape cross-sections. The isotopic escape cross-sections are estimated from fixed-source transport calculations for the whole problem domain. [ANL]

The NEAMS neutronics team continues to develop a subgroup cross-section library and interface to increase the use of the subgroup method, which can reduce the computational burden while keeping the loss of accuracy manageable. Of the methods considered, the resonance integral table method appears to offer some advantages for fast-reactor applications. Initial functional routines have been implemented for a subgroup method interface that can be used by many different neutron transport codes. Appropriate subgroup cross-section data libraries are also being developed. [ANL, ORNL]

System Simulation (RELAP-7)

The new 7-equation two-phase flow model in RELAP-7 was demonstrated for selected BWR components, including a pipe, core, and separator/dryer. A recently published RELAP-7 development plan (INL/MIS-13-28183) will guide future development. [INL]

Technical Spotlight: BISON Fuel Benchmarks

As part of the NEAMS ToolKit development, BISON has been used to simulate 21 well-known nuclear fuel benchmark experiments. These benchmarks are listed in Table 1, and results from selected Halden and Risø benchmark cases are presented here.

Beginning of life (BOL) fuel centerline temperatures were simulated for 6 fuel rods from the Halden research reactor in Norway. The fuel rods were part of two instrumented fuel assemblies (IFAs 431 and 432) equipped with thermocouples at the top and bottom of each rod (with the exception of one rod), for a total of 11 measurement points. The measured BOL fuel centerline temperatures are plotted against the BISON-predicted temperatures in Fig. 4.

Table 1: BISON benchmark simulations performed to date.

Reactor, Experiment, or Program	Rods	FCT BOL	FCT TL	FCT Ramp	FGR	Elon-gation	PCMI
FUMEX-II	27(1),(2a), (2b),(2c)				X		
IFA-431	1, 2, 3	X					
IFA-431 (3D)	4	X					
IFA-432	1, 2, 3	X					
IFA-513	1, 6	X	X				
IFA-515.10	A1	X	X	X			
IFA-597.3	7			X		X	
IFA-597.3	8						
OSIRIS	J12						X
REGATE	–						X
Risø-3	AN3, AN4			X	X		
Risø-3	GE7						X

Key: BOL = beginning of life, FCT = fuel centerline temperature, TL = through life, FGR = fission gas release, and PCMI = pellet-cladding mechanical interactions.

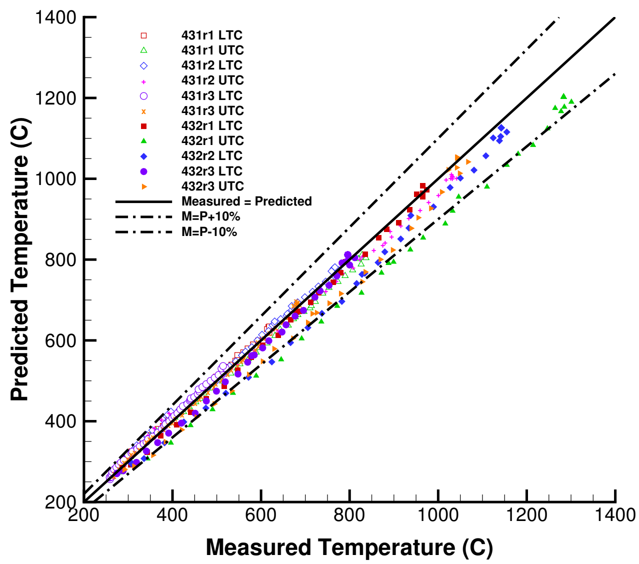

Fig. 4. Comparison of BISON predictions with actual measurements of BOL temperatures in IFAs 431 and 432. (The solid line is where modeled and measured values are equal.)

BISON predicted the BOL fuel centerline temperature as well as results from the fuel performance code FRAPCON.

BISON modeled fuel centerline temperature and fission gas release during power ramps in the Risø reactor (Denmark) AN3 test, which used IFAs equipped with thermocouples and pressure transducers. Fig. 5 compares the benchmark

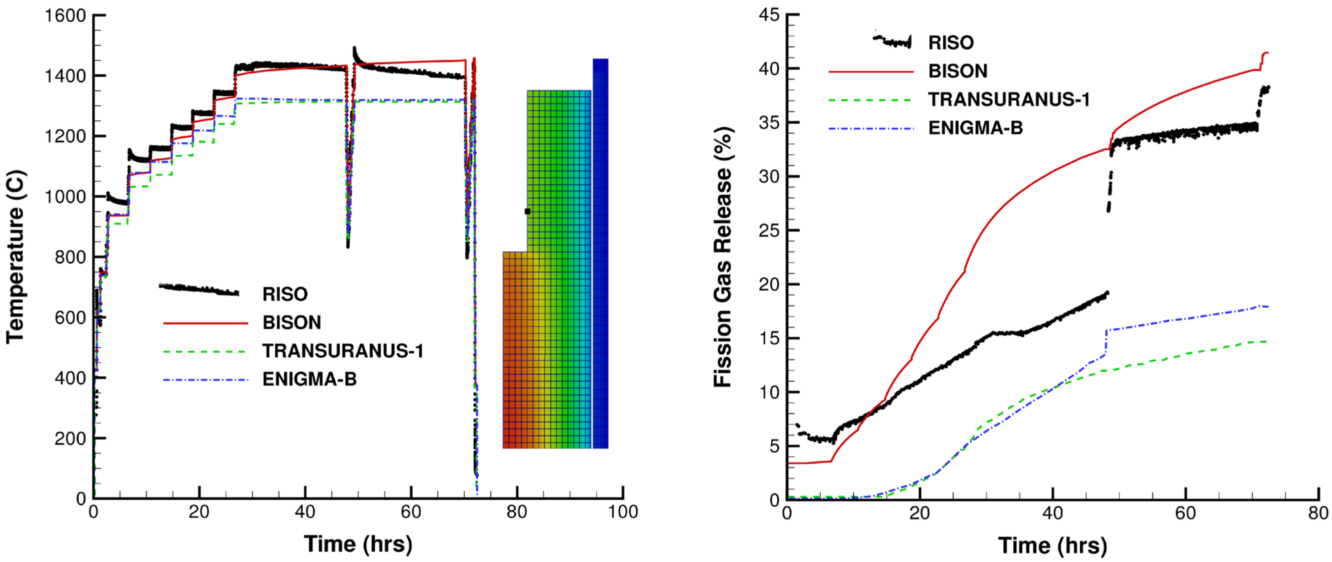

Fig. 5. Simulation of power ramp test results for the Risø AN3 experiment: (left) fuel centerline temperatures and (right) total fission gas release.

to calculations from BISON and two other fuel performance codes, TRANSURANUS and ENIGMA. The comparison between BISON calculations and measurements is favorable.

BISON's ability to predict pellet-cladding mechanical interactions (PCMI) is being assessed using the Risø GE7 benchmark, which documented dimensional changes of uninstrumented fuel rods after a "ramp and hold" regime. Measurements from the Risø GE7 experiment are compared to BISON and ENIGMA calculations in Figure 6. BISON slightly underpredicted total rod deformation, the "bamboo" shape that irradiated fuel rods take on due to the interaction of cladding with "hour-glass" shaped fuel pellets, but the overall comparison with ENIGMA is good.

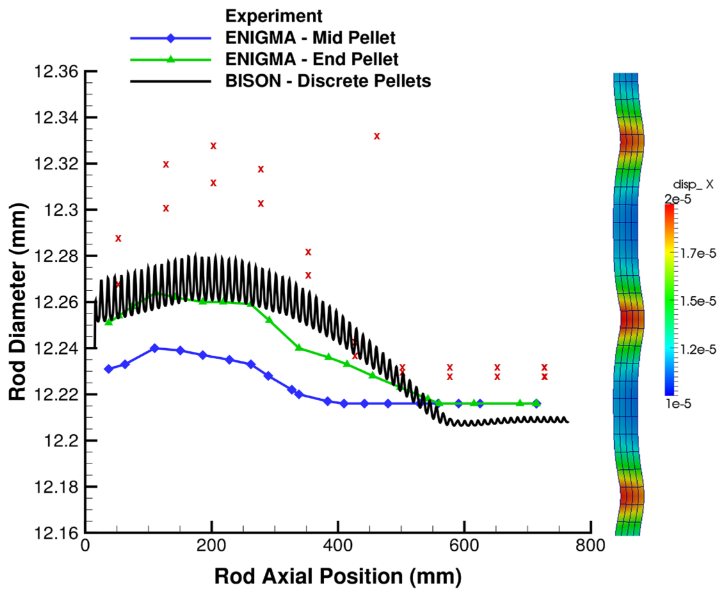

Fig. 6. Simulation of PCMI results from the Risø GE7 experiment: (left) cladding diameter after power ramp (rod position is with respect to the rod bottom) and (right) section of simulated cladding exaggerated to show the "bamboo" effect.

The following papers and reports provide details on the benchmarks discussed here:

Geelhood, K.J., et al., "FRAPCON-3.4: integral assessment," report NUREG/CR-7002, Vol. 2, 2011.

Hann, C.R., et al., "Data report for the NRC/PNL Halden assembly IFA-432," report NUREG/CR-0560, 1978.

Killeen, J., et al., "FUMEX-III: A new IAEA coordinated research project of fuel modeling at extended burnup," paper 2176 in Proceedings of Top Fuel 2009 (Paris), Sept. 6-10, 2009.

Killeen, J., et al., "Fuel modelling at extended burnup: IAEA coordinated research project FUMEX-II," paper 1102 in Proceedings of the 2007 International LWR Fuel Performance Meeting (San Francisco), Sept. 30 – Oct. 3, 2007.

"The third Risø fission gas project: bump test AN3 (CB8-2R)," tech. rep. RISOE-FGP3-AN3, Risø, Denmark, Sept. 1990.

"The third Risø fission gas project: bump test GE7 (ZX115)," tech. rep. RISOE-FGP3-GE7, Risø, Denmark, Sept. 1990.

Williamson, R., et al., "Multidimensional multiphysics simulation of nuclear fuel behavior," J. Nucl. Mater., 423, pp. 149-163, 2012.

Program Spotlight: NE-KAMS

To be useful, the NEAMS ToolKit must be demonstrated to be accurate and reliable for a broad spectrum of physical phenomena and conditions. The demonstration depends on practices for simulation verification and validation (V&V), data quality assessment (QA), and uncertainty quantification (UQ). Despite their importance, these "acceptance" activities are still largely conducted in an ad hoc, sometimes disorderly, manner across the AMS community. Further, reliable data and information sources for V&V are often scarce, incomplete, scattered, or inaccessible. This has led to concerns about the accuracy of AMS results. NEAMS will need better acceptance tools before it can produce results that will be used for critical decision-making.

The Nuclear Energy Knowledge-base for Advanced Modeling and Simulation (NE-KAMS) is developing a comprehensive and web-accessible knowledge base that will provide reference data for nuclear energy sciences and engineering. This knowledge base will be an important resource for technical exchange and collaboration. Because it will be implemented on the web, it can also serve academia and eventually the nuclear industry and its regulators. For acceptance activities, NE-KAMS will provide guidance for progressive levels of V&V completeness, tools for UQ and assessment of V&V benchmarks, and information on best practices and computational methods.

NE-KAMS will:

- Establish accepted standards, requirements, and best practices for evaluating computational models and simulations;
- Establish accepted standards and procedures for qualifying and classifying experimental and numerical benchmark data;
- Provide easy access to benchmark databases;
- Maintain an on-line software evaluation library; and
- Develop web applications for search and retrieval tools, V&V and UQ tasks, and the other activities listed here.

Currently, NE-KAMS consists of two major components: the data warehouse and the digital relational database. The warehouse provides a virtual dock-and-storage point for collecting data in various types of electronic files. To make uploading easy, efficient, and secure, the warehouse requires minimal file preparation by the user, and it performs QA as files are uploaded. The digital relational database manages digital data that are processed from the warehouse data sources and provides powerful cataloging tools for managing and processing the data as well as the relationships between the data.

NE-KAMS allows users to easily:

- Identify and extract desired data from the warehouse,
- Reorganize and reformat data for passing it between analytical modules,
- Export data to external AMS software,
- Import data from external sources for cataloging and preservation,
- Generate plots and reports for presentations, and
- Trace data origins through hyperlinks to the original source documents.

V&V and UQ are the primary means to assess the accuracy and reliability of AMS and, hence, to establish confidence in it. Though other industries are establishing standards and developing accepted processes for V&V and UQ, at present, the nuclear industry has no standards and limited processes for these tasks. Although the nuclear industry is beginning to recognize that more rigorous V&V and UQ standards and processes are needed, substantial resources and expertise will be required to develop them. In fact, no single organization, whether a commercial company or government laboratory, has the resources and expertise required to organize, implement, and maintain a robust V&V and UQ program.

Such a program needs to be established at a national or even international level, with a consortium of partners from government, academia, and industry. Participation in the NEAMS program is helping NE-KAMS develop the collaborations needed to create the improved AMS acceptance tools that industry needs.

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Recent and Upcoming Level 1 and 2 Milestones

Completed during this Quarter (January – March 2013)			
Milestone ID	**Description**	**Due Date**	**Finish Date**
M2MS-12LL06031213	Report final results of seismic gap analysis workshop for SHARP	3/31/2013	5/11/2013
M2MS-13AN0603021	Issue NEAMS integrated framework development plan (includes deliverable from milestone M2MS-13IN0603031)	3/31/2013	3/30/2013
M2MS-13AN06030241	Complete experimental measurement of detailed inlet boundary conditions	1/31/2013	2/1/2013
M2MS-13IN0603031	Complete INL portion of NEAMS integrated framework development plan	3/1/2013	2/1/2013
M2MS-13AN06030219	Complete multi-physics simulation using NEAMS structural mechanics, thermal fluids, and neutronics modules	3/29/2013	3/29/2013
M2MS-13AN06030235	Provide MAX isothermal test specifications as part of Russian Federation collaboration	3/31/2013	3/31/2013

Coming Due Next Quarter (April – June 2013)			
Milestone ID	**Description**	**Due Date**	**Status**
M2MS-13LA06020410	Deliver atomistic data for fission gas (Xe and Kr) diffusion and release in UO_2 fuel	4/3/2013	Completed 4/3/2013
M2MS-13IN0602032	Implement improved thermal conductivity model in BISON	4/30/2013	On schedule
M2MS-13IN0602033	Implement improved fission gas release model in BISON	4/30/2013	On schedule
M2MS-13IN0603038	Demonstrate probabilistic risk assessment on PWR reactor	6/30/2013	On schedule

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About Argonne National Laboratory
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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