Project Title

Combining Multi-Scale Modeling with Microcapsule Irradiation to Expedite Advanced Fuels Deployment

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Program: Advanced Reactor Technologies

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ABSTRACT:

Scope and Objectives of the Project: The proposed work aims to combine advances made in microstructurally-informed fuel performance modeling and simulation (M&S) tools with a new microcapsule irradiation capability that can substantially reduce the schedule and cost burden associated with qualifying new fuel systems for commercial deployment. This hybrid data/modeling approach, herein referred to as “accelerated fuel qualification” (AFQ), will be applied to investigate the fission gas release (FGR) and swelling behavior of uranium carbide (UC) – a high-performance fuel applicable to a wide range of advanced reactor concepts. The objective is to develop a predictive property model of UC swelling and FGR calibrated through a series of UC microsphere irradiations in the High Flux Isotope Reactor (HFIR). The scope includes fabrication of test samples of UC microspheres, microcapsule irradiation in HFIR and post-irradiation examination (PIE), multi-scale M&S of FGR and swelling behavior, and comparison of test results with model predictions.

Project Description: UC is the preferred fuel for the U.S. and European Gas-cooled Fast Reactor (GFR) programs and is under active consideration for micro-reactors for future space applications. Its advantages over oxide or metal fuel are i) high metal content that compensates for the limitation of low-enriched uranium; ii) high thermal conductivity that allows higher power-density, and iii) high melting point that enables safe high-temperature operation. UC is also the most compatible fuel with silicon-carbide (SiC) composite (SiC-SiC) cladding. The UC fuel and SiC-SiC system is an excellent candidate for long-life cores because of its ability to tolerate high displacement per atom from fast neutrons. Historically, the issues associated with UC include difficulties in fabricating pellets with sufficient stoichiometric and chemical purity, reaction with air, and high swelling. However, GA has developed a new manufacturing technique with a porous UC pellet design that achieves very high purity and has promise to accommodate high swelling. With this accomplishment, it is timely to further advance the understanding of UC irradiation performance for advanced reactors.

The major impact of the proposed work is in the efficient qualification of new fuels/materials that is achieved through the AFQ methodology. The methodology envisioned here consists of designing and executing targeted irradiation experiments with a goal of obtaining data that is of sufficient quality and accuracy to validate theoretical property models developed from first principles. For the nuclear industry to move beyond current light-water reactor technologies, simulations and experiments must be strategically combined to reduce the years of data that would otherwise be required to deploy new fuels/materials. Since nuclear fuels and materials operate in extreme environments that induce complex multi-physics phenomena, their interactions must be experimentally demonstrated to ensure that fuel behavior is accurately described in the simulations. The advanced M&S capabilities developed by the U.S. Department of Energy (DOE) Consortium for the Advanced Simulation of Light Water Reactors (CASL) and Nuclear Energy Advanced Modeling and Simulation (NEAMS) have made impressive progress and are approaching a predictive capability. In parallel, experimental techniques and diagnostics

have reached a new level of sophistication, with ever-increasing precision in measuring critical parameters. With a well-chosen set of experiments, material behavior can be characterized over a broad range of conditions. With multi-scale modeling and powerful finite element analysis, the behavior of small test samples can be extended to full-scale engineering structures subject to a variety of stressing environments. The proposed work will demonstrate the methodology using UC as a test case to validate critical material properties necessary for high-temperature and long life operation of UC.

The innovative concept behind microcapsule irradiation is that it allows multiple test sample variations (e.g. grain size, stoichiometry, impurity level etc.) to be conducted in a single experiment. The test matrix includes two temperatures and two burnup levels. The total irradiation period will be approximately one year. At the end of irradiation, gas release and swelling will be measured during PIE. In parallel with the irradiations, microstructurally-informed, multiscale material models of fission gas evolution in UC will be developed with a focus on xenon and krypton diffusion and bubble accumulation. The modeling effort will leverage and build on the work previously done for uranium oxide (UO_2) fuel under the Scientific Discovery through Advanced Computing (SciDAC), CASL, and NEAMS initiatives funded by DOE. Grounding the multi-scale models with experimental data as a function of burnup and temperature will enable eventual development of non-linear UC property models with incorporation of dependencies on various fabrication parameters such as C/M ratio, impurity, and grain size. The impact of swelling on UC fuel deformation will be evaluated by a finite element method code PISA (or BISON) by updating these codes with the swelling and diffusion models obtained from the multiscale modeling and conducting integral validation tests against measurements obtained from irradiation experiments.

Major Tasks:

- Task 1 – GA will fabricate UC microspheres (~300-450 μm) for the irradiation tests. Characterization tests will measure carbon and oxygen content, bulk density, particle size, and phase determination.
- Task 2 – ORNL will construct the test microcapsules containing the UC microspheres and irradiate them in HFIR at different burnups and temperatures. PIE will be performed to determine the swelling and FGR as a function of temperature and burnup.
- Task 3 – UTK will extend the multi-scale UO_2 modeling approach developed under the SciDAC program to UC swelling and FGR. This will use density functional theory calculations and cluster dynamics fission gas bubble evolution as incorporated in the XOLOTL code. The modeling will be calibrated with the irradiation results.
- Task 4 – GA will incorporate the theoretical/experimental results into engineering-scale fuel performance codes used for fuel design, analysis and licensing.

Impact / Outcome:

The two key outcomes of the project are i) a working model representing two key aspects of fuel performance, i.e. swelling and FGR. The model will be used to inform and advance UC fuel design for a range of advanced reactors; and ii) A cost-effective and accelerated qualification methodology applicable to a range of novel fuels. Notably, the proposed work directly supports innovation and competitiveness of the U.S. nuclear industry because it will help transition the advances made in M&S into useable and affordable engineering tools for the applied industry.

Major Deliverables:

- Fuel samples Quality Assurance report
- Interim report on multi-scale M&S of FGR and swelling UC
- PIE report of target rod #1 containing UC fuel samples subject to three HFIR operating cycles
- PIE report of target rod #2 containing UC fuel samples subject to six HFIR operating cycles
- Final project report