Experimental and Computational assessment of thermodynamic stability of fission products in advanced reactor fuels

PI: Elizabeth Sooby, University of Texas at San Antonio

Collaborators: Eunja Kim- University of Texas at El Paso, Xochitl Lopez Lozano – University of Texas at San Antonio, Mark Pederson- University of Texas at El Paso, Patrick Warren- University of Texas at San Antonio, Tiankai Yao-Idaho National Laboratory, and Mira Khair- University of Texas at San Antonio

Program: IRP-2: Grand Challenge Research and Development at Minority Serving Institutions (MSI)

ABSTRACT:

The IRP proposed brings together two minority serving institutions (The Universities of Texas at San Antonio and El Paso) and a leading DOE-NE national laboratory, Idaho National Laboratory, in a collaborative effort to advance the state of knowledge for fission product (FP) behavior in advanced reactors fuels, particularly uranium mononitride (UN). The IRP, if funded, will stimulate NE research at UTSA and UTEP, develop a capacity at UTSA for f-electron computational science, and leverage novel experimental data to bolster computational efforts at both institutions all while providing the training and professional preparation of undergraduate and graduate students in the experimental and computation techniques necessary to advance the field. UN fuel is selected in the present study, as well as proposed for several advanced reactor types, in part for its high thermal conductivity which will result in more efficient heat transfer out of the fuel and a resulting lower thermal gradient in the fuel.

Fission products are expected to play a significant role in the evolution of mechanical and thermal properties in UN fuel based on thermal and mechanical studies carried out in other ceramic fuel systems. Limited FP solubility can result in various effects, such as contributing to fuel swelling by causing the precipitation of solid FPs, and the creation of inert gases bubbles. This, in turn, can lead to mechanical interactions with the metallic cladding, potentially resulting in a failure of the primary safety barrier. Therefore, the assessment of FP behavior is crucial for ensuring the safety of this nuclear fuel.

In a combined experimental and computational effort, this project, if awarded, will investigate the solubility and speciation of FPs and their influence on the thermal and mechanical properties of UN. The team will identify troublesome FPs with increased potential for release, in either monolithic-clad or particle fuel architectures. To achieve this, the project is divided into three complementary and integrated thrust areas described below and in the included Figure.

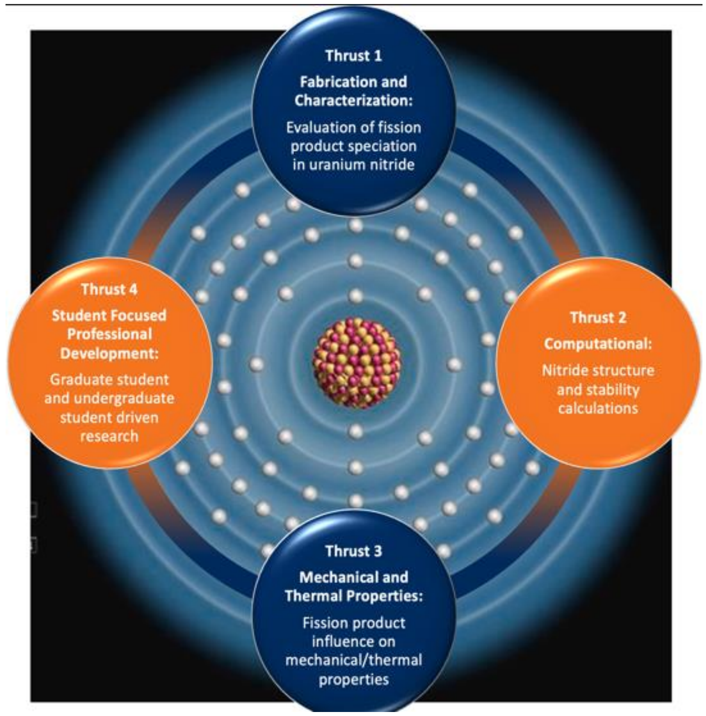
Thrust 1: Fabrication and characterization of simulated fuel monoliths (SIMFUEL) as well as identified FP phases (intermetallics and carbides)

Thrust 2: Computational modeling to inform solubility of FPs in UN as well as FP structures formed to bridge data gaps in thermodynamic properties of carbide and nitride FP systems.

Thrust 3: Mechanical and thermal properties determination of SIMFUEL and segregated FP structures.

Thrust 4: Student Training and Professional Development

The fabrication of UN samples incorporating FPs (Thrust 1), followed by an in-depth examination of the (1) interactions between these FPs and UN, (2) their solubility and speciation within the material, (3) potential formation of intermetallic compounds, and (4) compounding behavior as a nitride, uranium intermetallic, or ternary phase, stands as a pivotal endeavor. This research is instrumental in validating the outcomes of modeling studies. Furthermore, the properties of these materials are intricately linked to the speciation of FPs. Computational efforts (Thrust 2) aim to both guide the solubility and speciation experiments as well as verify resulting structures and phase compositions. Variations in speciation can lead to changes in diffusivity, kinetics, and ultimately influence the release of these elements. Consequently, a comprehensive study of the interaction between UN containing FPs and graphite is underway, with a focus on how this interaction affects thermal and mechanical properties (Thrust 3).



The culmination of these studies will contribute significantly to the existing body of knowledge, bridging the gap in the literature and providing valuable experimental insights. In these three technical thrust areas, four graduate students, three postdoctoral fellows, and >15 undergraduates will be trained in the experimental and computational techniques required to advance the field, and the investigators will work with national laboratory collaborators as well as across academic institutions to prepare these students for careers in nuclear energy science.