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Interfacial Interactions between Graphite and Molten Fluoride Fuel Salt

PI: Jinsuo Zhang, Virginia Tech

Collaborators: Ju Li – Massachusetts Institute of Technology; Nidia Gallego-Oak Ridge National Laboratory; Dane Wilson-ThorCon US.

Program: Topic Area 1 – Reactor Development and Plant Optimization

ABSTRACT:

Nuclear-grade graphite is used as moderator as well as core structural materials in thermal molten salt reactors (MSRs). Despite its excellent neutronic and thermal properties, due to the harsh environments (e.g., complex molten salt chemistry, high temperature, irradiation) in the core of MSRs, the *microstructure and surface morphology* of nuclear graphite are likely to change during irradiation and exposure to molten halide salt. In turn, this will affect the lifetime of graphite in molten salt-cooled and/or fueled reactors. Although these issues are directly related to safety concerns for MSRs, the graphite degradation by irradiation and exposure to molten halide salts has not been well-studied, thus, exploratory research is needed to investigate the interaction landscape and formulate key hypotheses and test them. This research proposal aims to study graphite degradation, including the micro-chemistry and structure evolution in high-temperature molten fuel salt (UF_4-KF-NaF), by employing an integral approach of experiments, advanced characterization, and atomic scale modeling. The fuel salt will be purified using hydrofluorination and synthesized for this project. For experiments, the impacts of molten fluoride salt exposure with different conditions, fission products, and corrosion products on the salt-graphite interfacial interactions will be considered. Different pressures will be applied for immersion tests of graphite in molten salt fuel to study the infiltration behaviors of salt into graphite. In addition, the molten-salt flow will be simulated on the surface of graphite with different flow velocities to study graphite erosion behaviors. The synergistic effects of irradiation and molten salt chemistry will also be tested by placing graphite specimens in a nuclear reactor. For characterizations, in addition to conventional characterization methods such as SEM and TEM, neutron-computed tomography (N-CT) will also be employed to produce a 3D real space representation to understand the infiltration behaviors and microstructures.

Atomistic simulations based on a recently developed universal interatomic potential (UIP) will be carried out to complement the experiments and provide atomistic insights into various graphite-salt interactions. The atomic-scale focus of this study will be on both chemical interactions (bond formation) and graphite microstructural changes (change of potential sites for bond formation), which will enable us to explore the driving force for graphite degradation under different molten salt chemistries, pressures, flow conditions and irradiations. Careful characterizations and atomic scale simulation will reveal how these atomistic-scale defects cluster and agglomerate to change porosity and pore structure. This project will reveal which graphitic materials best meet the integrated environmental requirements of MSRs, and predict their rates and mechanisms of degradation. Therefore, this research project will produce significant scientific and engineering impacts on the interfacial interaction between graphite and molten fluoride fuel salts in MSRs. This project directly addresses Topic Area 1 - Reactor Development and Plant Optimization, by fundamentally understanding the degradation mechanisms of nuclear-grade graphite by molten salt fuel in the core of MSRs.