DOE-ID NEPA CX DETERMINATION

CX Posting No.: DOE-ID-19-073

SECTION A. Project Title: Validated, Multi-scale Molecular Dynamics Simulations to Predict the Thermophysical Properties of Molten Salts Containing Fuel, Fission and Corrosion Products – Brigham Young University

SECTION B. Project Description

Brigham Young University (BYU) proposes to study the thermophysical properties of molten salts containing fuel as well as fission and corrosion products in molten salt reactors (MSRs). Using first principle molecular dynamics (FPMD) coupled with classical molecular dynamics (CMD) allows predicted properties to be compared for four salt systems (FLiNaK, FMgNaK, FLiBe and LiCl-KCl) and eight impurities (Uranium [U], Thorium [Th], Zirconium [Zr], Neodymium [Nd], Molybdenum [Mo], Cesium [Ce], Chromium [Cr], and Iron [Fe]) to represent the most likely combinations expected during MSR operation. Experimental measurements of density, heat capacity, viscosity, and thermal conductivity will be collected and compared to the FPMD/CMD predictions. The tasks associated with this project are: 1) Structure/speciation predictions from FPMD; 2) Development of CMD potentials; 3) Physical experiments and model validation; 4) Properties predicted by extended CMD; and 5) Property correlation development. Existing equipment and laboratory facilities will be used.

SECTION C. Environmental Aspects / Potential Sources of Impact

Chemical Use/Storage, Chemical Waste Disposal, and Hazardous Waste Generation – This project will use several kilograms of fluoride molten salts including FLiBe and FLiNaK. These salts will be analyzed both and pure components and as solvents for non-radioactive fission product simulants. These salts must be kept in an anhydrous, anaerobic glove box. One of these salts contains Beryllium, which requires special handling procedures when being loaded into and removed from the glove box. The storage, use, and disposal of these compounds will be done in accordance with BYU Risk Management policies, procedures, and licenses.

SECTION D. Determine the Level of Environmental Review (or Documentation) and Reference(s): Identify the applicable categorical exclusion from 10 CFR 1021, Appendix B, give the appropriate justification, and the approval date.

Note: For Categorical Exclusions (CXs) the proposed action must not: 1) threaten a violation of applicable statutory, regulatory, or permit requirements for environmental, safety, and health, including requirements of DOE orders; 2) require siting and construction or major expansion of waste storage, disposal, recovery, or treatment facilities; 3) disturb hazardous substances, pollutants, contaminants, or CERCLA-excluded petroleum and natural gas products that pre-exist in the environment such that there would be uncontrolled or unpermitted releases; 4) adversely affect environmentally sensitive resources. In addition, no extraordinary circumstances related to the proposal exist which would affect the significance of the action, and the action is not "connected" nor "related" (40 CFR 1508.25(a)(1) and (2), respectively) to other actions with potentially or cumulatively significant impacts.

References: B3.6 Siting, construction, modification, operation, and decommissioning of facilities for small-scale research and development projects; conventional laboratory operations (such as preparation of chemical standards and sample analysis); and small-scale pilot projects (generally less than 2 years) frequently conducted to verify a concept before demonstration actions, provided that construction or modification would be within or contiguous to a previously disturbed or developed area (where active utilities and currently used roads are readily accessible). Not included in this category are demonstration actions, meaning actions that are undertaken at a scale to show whether a technology would be viable on a larger scale and suitable for commercial development.

Justification: The activity consists of research activities to investigate the thermophysical properties of molten salts containing impurities for MSR applications.

Is the project funded by the American Recovery and Reinvestment Act of 2009 (Recovery Act) ☐ Yes ☒ No

Approved by Jason Sturm, DOE-ID NEPA Compliance Officer on 09/16/2019