Proposal 09-822

NUCLEAR ENERGY UNIVERSITY PROGRAMS

Microscale Heat Conduction Models and Doppler Feedback

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Abstract

The objective of this project is to establish an approach for predicting the magnitude and time-dependence of the Doppler feedback mechanism in very high-temperature reactors. This mechanism is the foremost contributor to the passive safety of gas-cooled reactors that use tristructural-isotropic (TRISO) coated fuel particles. Since the effect is directly dependent on the actual temperature reached by the fuel during transients, the underlying phenomena of heat deposition, heat transfer, and temperature rise must be correctly predicted. To achieve the above objective, this project will devise a computational approach that accounts for lattice effects as well as local temperature variations and the correct definition of temperature and related local effects.

The approach is to devise molecular dynamic models to define the fuel temperature in the immediate vicinity of the zone where fission energy is deposited by the fission products. The temperature thus defined is then used to quantify the Doppler broadening effect. The project team will develop potentials for the fuel and will carry out molecular dynamics (MD) simulation of the energy deposition from fission events in order to derive local temperature definitions, giving special consideration to lattice effects that may be important to low-energy neutrons. The research team will model energy transport within the fuel kernel and subsequent layers of the TRISO particle in detail , including wave effects, and will apply the results to determination of the background and the local temperature distribution and to its time evolution. These temperatures will be used to compute the effect of Doppler broadening on the various resonant effects, starting with absorption. Resonance integrals will initially be computed with the usual assumption of a Maxwell-Boltzman velocity distribution (albeit using an MD-derived temperature corrected for lattice effects – i.e, Debye or Einstein). Integration will later be attempted with velocity distributions that incorporate directly the effects of the specific material lattice under consideration and as derived from MD simulations.