

Fully-coupled Engineering and Mesoscale Simulations of Thermal Conductivity in UO₂ Fuel Using an Implicit Multiscale Approach

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Though the thermal conductivity of solid UO₂ is well characterized, its value is sensitive to microstructural changes. In this study, we capture the microstructural dependence of the thermal conductivity in a UO₂ fuel pellet using a two-way coupling of a mesoscale phase field irradiation model to an engineering-scale, finite element calculation. To achieve this, the engineering scale thermomechanics system is solved in a parallel, fully-coupled, fully-implicit manner using the preconditioned Jacobian-free Newton Krylov (JFNK) method. Within the JFNK function evaluation phase of the calculation, the microstructure-influenced thermal conductivity is calculated by the mesoscale model and passed back to the engineering-scale calculation. The coupled model demonstrates quadratic nonlinear convergence and good parallel scalability. The calculated mesoscopic microstructure shows strong radial dependence, with large pores forming in the center of the pellet and no porosity on the outer circumference. The resultant radial variation in the thermal conductivity causes distinct temperature distributions in irradiated and unirradiated fuel pellets.