Predictive models of temperature distributions in packed beds of lithium ceramics, with applicability beyond initial packing states, are critical for operation of solid breeders in fusion reactors. The importance of accurate and robust predictive capabilities is a result of relatively-narrow operational temperature windows imposed on solid breeders by tritium release concerns. Heat transfer in solid breeder pebble beds is characterized by a complicated coupling between mechanical forces and heat conductance among individual pebbles as well as interaction with slow-moving purge gas. As a consequence, models of heat transfer for solid breeders are significantly more complex than standard material models; many physical phenomena in pebble beds require special treatment.

Due to its inherent complexity, modeling heat transfer has traditionally advanced by treating packed beds as fictitious continua wherein broad brush strokes of empirically-derived correlations mask the intricate pebble-pebble and pebble-fluid interactions. Empirical correlations are often required to be generated for specific combinations of solid and fluid phase materials at relevant packing fractions. Yet the continuum assumption does allow many simple packed-bed engineering situations to be treated in a tractable way with phenomenological models of effective material properties. A parameter often used to relate heat transfer in beds is the packing state, itself a macroscopic reflection of microscopic interactions. However, changes to packing states are expected in solid breeders due to high temperatures and forces in ceramic pebble regions. As a consequence of anticipated packing state changes, limited applicability of empirical correlations, and the requirement for high-accuracy temperature predictions, continuum models are currently insufficient for predicting temperature distributions.

Thus, in the current study, a multi-scale approach is adopted as an alternative to the purely-continuum method. The approach will allow direct modeling of packing structures and temperature distributions and so provide increasingly reliable predictive capabilities for heat transfer in solid breeder blankets. In the development of models, several phenomena are identified as capable of causing alterations to packing structures in solid breeders and thereby heat transfer properties, including: (i) inter-particle sintering, or necking; (ii) creep relaxation; (iii) crushing/cracking of individual pebbles in ensembles. These phenomena, and their specific changes to temperature distributions in pebble beds, will each require individualized attention and modeling efforts. In this study, I focus on heat transfer phenomena relating to, and develop predictive capabilities for, temperature distributions in pebble beds with packing structures solely altered by pebble crushing and fragmentation.

From the microscopic point-of-view, the thermal discrete element method (DEM) is used to track motions of, and heat transfer between, individual pebbles in packed bed assemblies. DEM models provide an opportunity to study transient changes to packing structures and simulate pebble fragmentation and heat transfer. The slow-moving, interstitial helium purge gas is considered by coupling DEM models with two modeling approaches, differentiated by their scale. In the first approach, the fluid is considered with a macroscopic, volume-averaged computational fluid dynamic (CFD) method. Volume-averaged models of helium are computationally efficient and provide an overall view of helium influence on heat transfer in solid breeder pebble beds. To gain insight into the complete fluid flow patterns and heat transfer in packed beds with changing packing states, a second microscopic approach for fluid modeling with the lattice-Boltzmann method (LBM) is also employed. The lattice-Boltzmann method is well-suited to modeling of complex porous structures due to its inherent parallelizability and simple application of solid-fluid interface boundary conditions on structured grids.

DEM, CFD-DEM, and LBM-DEM models are first validated against known heat transfer states with stagnant interstitial gases from experiments. Following validation and benchmark tests, the models are applied toward the study of fusion-relevant conditions in solid breeders. Three main application studies were performed: (i) DEM and CFD-DEM simulations predict effective thermal conductivity responses to solid conductivity reductions due to irradiation damage, (ii) parametric studies with CFD-DEM of heat transfer in ITER-relevant solid breeder volumes as a response to, among other features, pebble crushing and fragmentation, and (iii) LBM-DEM simulations of flow, tortuosity, and transverse dispersive conductivity changes in packed beds with crushed pebble fragments.

From the multi-scale research provided by the models developed in this thesis, several interesting and unintuitive phenomena were uncovered. Demonstrations of the predictive capabilities of the models as useful for solid breeder designers were also given. Lastly, insights provided by the models provided pathways toward future research topics. The following lists several of the achievements.

1. From CFD-DEM models of pebble crushing and fragmentation re-settling in the study of ITER-relevant configurations, when fragments are small compared to the original pebbles (fragments with diameters
2. Horizontal-style configurations of coolant interfaces