Predicting temperature distributions in packed beds of lithium ceramics beyond initial packing conditions is critical for operations 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 complicated couplings 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 breeder pebble beds 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. A drawback is that 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 in calculations of heat transfer properties of 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 to 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 experimental measurements of known heat transfer conditions of packed beds with stagnant interstitial gases. 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 complete helium flow field, tortuosity, conjugate heat transfer, and transverse dispersive conductivity changes in packed beds with crushed pebble fragments.

Demonstrations of the predictive capabilities of the models as useful for solid breeder designers are given in this thesis. Throughout the studies, the multi-scale nature of models developed for this thesis made possible the uncovering of several critical and consequential phenomena. The following lists several of the main achievements of current modeling efforts:

* Temperature profiles were predicted for pebble beds with irradiation damage in solid pebbles, as modeled by reductions in thermal conductivity. In the case of stagnant interstitial fluid, an example case was shown where a 50% reduction in solid conductivity would permit a solid breeder to operate within a 10% margin on maximum mid-line temperature.
* Fully-dynamic CFD-DEM simulations revealed the impact of packing structure alterations on heat transfer in ITER-relevant packed beds and, as such, the importance of their modeling. Mass re-distribution following crush events, dependent on the size and extent of fragmentation, was shown to induce subtle changes to local packing fractions yet result in macroscopically important changes to temperature distributions with volumetric heating. In the worst case of small fragments (diameters 20% of the original pebbles) and wide-spread pebble damage (5% crushed pebbles in the ensemble), maximum bed temperatures increased by approximately 14% (under a nuclear heating rate of 8 MW/m3)
* Horizontal-style configurations of coolant interfaces (such as in the proposed European Union design of solid breeder for ITER) were shown to be much more tolerant to pebble fragmentation than previously considered. The configuration’s orientation relative to the gravity vector resulted in slight `broadening’ of temperature profiles, and even slightly lower peak-to-average temperatures than vertical-style configurations, as packing structures evolved due to fragmentation.
* LBM models validated the accuracy of the volume-averaged approach of fluid flow and energy interaction between solid and fluid phases, as adopted in CFD-DEM models. The maximum difference between temperature profiles predicted with CFD-DEM and LBM-DEM models was only 6%, while CFD-DEM simulations were run in considerably less time than the full models of LBM-DEM (hours compared to days). The contribution of transverse dispersive conductivity, a heat transfer mechanism not accounted for in CFD-DEM, was shown to be not significant for the range of Reynolds/Peclet numbers of interest for purge gas in solid breeders and the failure percentages in the packed bed configurations considered; the dispersive component of conductivity, even in beds with fragments and higher tortuosity, was only 0.5% of the total effective thermal conductivity

Finally, insights provided by the models were used to shed light on possible future paths of solid breeder research. Briefly, the causes of packing alterations studied here should be complemented with other factors, such as creep and sintering; a framework was demonstrated for including effects of irradiation damage in models of heat transfer in packed beds, the models can be used in conjunction with models of packing structure alteration toward even more precise predictive capabilities for temperature distributions; and lastly, it was shown that heat-spreading due to dispersive conductivity in poly-disperse packed beds may offer significant benefits to lowering maximum temperature distributions in pebble beds that the negative effects on pressure drop may be acceptable, the competing effects should be studied in detail.