

346b Using Discrete Element Method to Predict a Priori Particle Void Fractions for Use in CFD Simulations of Packed Beds

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Randomly packed fixed bed reactors are widely used in commercial chemical processes. Accurate prediction of packing structure is critical to modeling the overall transport characteristics of the bed. Traditionally, fixed bed design is based on a pseudo-homogeneous model with averaged semi-empirical correlations to predict heat and mass transport. At low tube-to-particle ratios, $dt/dp = 2-5$, prediction of transport properties such as inside heat transfer coefficients requires the use of estimated relationships between void fraction and radial position or simplification to 1d models. This presentation builds on previous work showing how the Discrete Element Method, (DEM) Software package, PFC3D, by ITASCA can be used to accurately predict overall as well as local void fractions over a wide range of dt/dp ratios. The resulting packing structures can then be imported into a commercial CFD package, FLUENT, to accurately predict reactor transport properties. Current work has focused on using experimentally measured friction parameters of both alumina spheres and carbon steel pipes in DEM simulations to predict a priori particle packing arrangements. Results are compared against experimental measurements for various dt/dp ratios.