CFD-DEM predictions of heat transfer in packed beds using commercial and open source codes

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ABSTRACT

Correct prediction of gas-particle momentum, heat and mass transfer is vital in the modelling of packed bed reactors commonly employed throughout the chemical process industry. Even though a wide array of experimentally derived correlations and models are available, further work is required in cases involving complex particle shapes, particle size distributions and real process operating conditions (e.g., high temperature and pressure). It should also be noted that various sources of experimental error can influence the accuracy of experimentally derived correlations.

CFD-DEM approaches offer an attractive platform to fundamentally study the transfer phenomena between the gas, particles and walls in fully controlled simulation experiments. This methodology can simulate any combination of particle and gas properties order to improve understanding and derive closure models for large scale simulations. In general, DEM is employed to attain a realistic packing of particles, after which CFD is used to solve the transport equations within the resulting packing structure.

The objective of this paper is to evaluate CFD-DEM approaches available in the commercial software, ANSYS FLUENT, and the open source software, CFDEM Coupling, which couples the established open source simulation tools, LIGGGHTS and OpenFoam. A small geometry filled with spherical particles will be used as the test case where both the inlet gas and particle temperatures are fixed to facilitate heat transfer.

The different software packages will be evaluated in terms of accuracy via comparisons to established correlations for heat transfer coefficient and pressure drop, as well as computational speed and ease of use. Even though the CFD-DEM methodologies employed with the different tools show subtle differences, a reliable comparison will be ensured by closely following best practice guidelines provided by the respective support/development teams.

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