Fluid flow simulation in packed bed unit operations in chemical engineering

Christian Jordan, Mario Pichler, Bahram Haddadi-Sisakht, and Michael Harasek

Technische Universität Wien, Institute of Chemical, Environmental and Bioscience Engineering, Getreidemarkt 9/1662, A-1060 Wien

Many chemical engineering processes involve the contact of fluids and solids, e. g. iron making blast furnaces (heat transfer, reaction), coffee making (extraction) or flue gas cleaning (adsorption). For design of such processes besides of mass and energy balances usually empirical lumped parameter models with low resolution are used - they are fast and easy to handle. If more detailed insight for optimizations of e. g. a packed bed adsorption process is required, such models cannot be used. Computational Fluid Dynamics (CFD) can be utilized for in-depth analysis of packings and the fluid flow, heat and mass transfer in there. This involves a sufficiently fine spatial discretization (splitting the computational domain in "finite volumes", small grid cells) and numerical solving mass, energy, species and momentum balances for all cells. This solution process is computationally quite demanding, as a fully resolved lab scale packed bed can have several Millions of grid cells. Creating the computational grid for a random packed bed of particles is a challenge of its own (see Figure 1). First, the packing geometry has to be defined - usually this can be done with specialized Discrete Element Methods (DEM) which can export the geometry as STL files. Next, automated meshing tools like snappyHexMesh (from the open source CFD code OpenFOAM) can be applied. If the task involves only fluid flow and surface interactions, a simple single region grid will be sufficient. However, if heat transfer has to be considered, the particles will also need to be meshed - generating a multi-region mesh (gas and solid phase). To obtain reasonable results for the heat transfer, so called "bridges" are used in the solid region. They are introduced by a CAD tool, e. g. Salome.

This procedure for multi-region meshing has a certain drawback: First, the bridges have to be designed to model the correct intra-particle heat flux, second, they should not influence the void fraction of the packing, otherwise the fluid flow and the pressure drop are compromised. Therefore, various particle packings have been investigated in a lab scale packed bed unit to analyze the pressure drop for different gas flow rates. These lab experiments have been modelled using CFD and the simulation results have been compared. It was shown that typical bridge sizes (0.1 - 0.2 x particle diameter) do not have a significant influence on the pressure drop of the simulated packings and they are safe for use in combined heat-mass-transfer simulations.

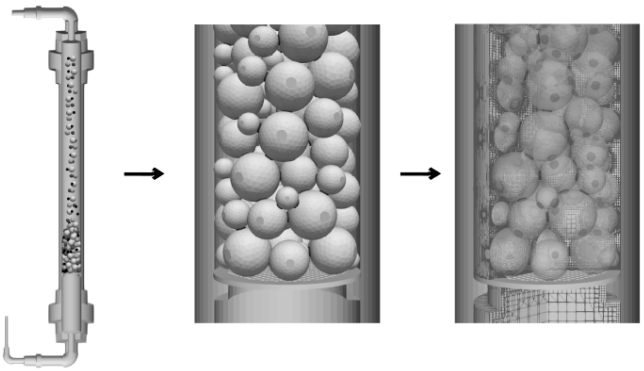

Fig. 1: Geometry creation process for a lab scale packing: DEM packing of the particles, scripted adding of the bridges, automated meshing of the volume regions.

References

[1] Pichler, M., Effect of particle contact point treatment on the heat transfer in packed beds, MSc thesis, TU Wien (2018), http://katalog.ub.tuwien.ac.at/AC14556986.

[2] Haddadi, B., Jordan, C., and Harasek, M., Cost efficient CFD simulations: Proper selection of domain partitioning strategies, Comp. Phys. Comm., 219 (2017), S. 121 - 134, DOI: 10.1016/j.cpc.2017.05.014.