COMSOL Multiphysics® Simulation of 3D Single-Phase Transport in a Random Packed Bed of Spheres

A. Dixon[1]

[1]Department of Chemical Engineering, Worcester Polytechnic Institute, Worcester, MA, USA

Abstract

Packed beds are important in the chemical industries in separations and as catalytic reactors. The standard approach to modeling the complex particle/tube arrangement is to employ an effective medium approach with one-dimensional flow and lumped transport parameters. Simplification of the flow and estimation of the transport quantities is usually by experiment and empiricism. Computational fluid dynamics (CFD) can simulate the detailed flow and scalar transport in packed beds to provide improved understanding and quantitative information.

The aim of the present work is to use COMSOL Multiphysics® software to perform detailed simulations of flow, heat transfer and dispersion in fixed beds of tube-to-particle diameter ratio (N) in the range 3 - 10, commonly used for reactions such as steam reforming where heat effects and pressure drop lead to use of large particles in thin tubes. Specialized finite volume CFD tools have been used for 3D simulations [1 - 5], mainly for flow and heat transfer only, while finite element methods such as COMSOL Multiphysics® software have been restricted to 2D simulations [6, 7] or small structured clusters of spheres [8]. Here we present simulations of single-phase gas flow, conjugate heat transfer and isothermal dispersion of mass in a 3D model of a randomly-packed bed (N = 5.96) of 400 spheres.

Random packs of spheres were generated by a Monte Carlo collective re-arrangement algorithm, and the resulting geometry was imported into COMSOL Multiphysics using the CAD Import Module (Figure 1). Contact points between the spheres were avoided by shrinking the particles by 1% of their diameters. Flow simulations used Laminar and Turbulent flow (k-ε with wall functions) physics; conjugate heat transfer was added using the Heat Transfer Module; dispersion of mass was handled in the Transport of Dilute species interface. The simulations were converged by first running a study for flow alone and using the results to set initial values for flow in the subsequent study of simultaneous flow and heat or mass transfer. The size of the model forced the use of coarse (laminar) and extremely coarse (turbulent) meshes (giving up to 1 million DOF) and the segregated solution algorithm.

Simulations were carried out in both laminar ($50 \le Re \le 400$) and turbulent ($400 \le Re \le 5000$) regimes. A laminar flow (Re = 100) is shown (Figure 2); the regions of fast flow and back flow can be seen on the 3D tube slices and on the mid-plane. Simulations were extended to include conjugate heat transfer where the tube was heated from the wall. Figure 3 shows the developing temperature profile within the gas and the particles. Finally, isothermal simulations were run of a

tracer source at the tube inlet to show the radial dispersion of mass caused by lateral displacement of flow around the packing (Figure 4).

COMSOL Multiphysics was used successfully to simulate flow and transport over a wide range of flow rates in a realistic 3D packed bed of spheres. Future research will look at the inclusion of simultaneous heat and mass transfer and chemical reactions.

Reference

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Figures used in the abstract

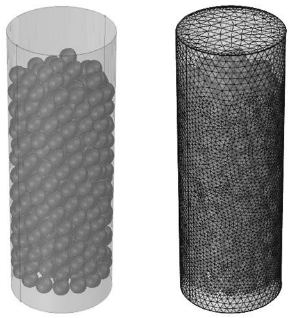

Figure 1: Geometry and mesh for N = 5.96 bed of spheres.

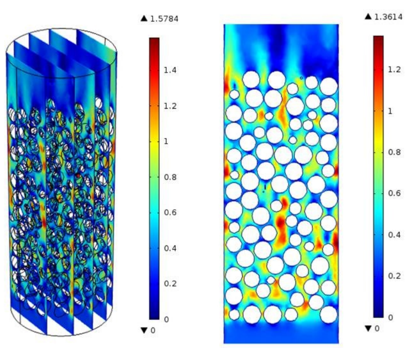

Figure 2: 3D slices and 2D center plane contour plot of axial velocity, Re = 100.

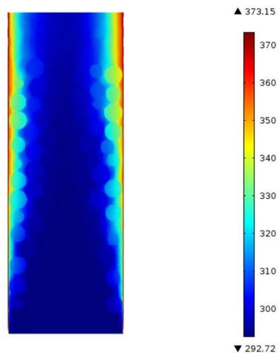

Figure 3: Temperature contours on center plane show development of thermal field, Re = 1000.

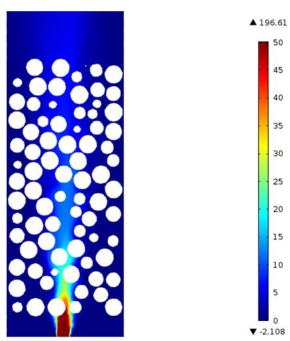

Figure 4: Species contours on center plane show dispersion, Re =200.