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

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Introduction: Computational fluid dynamics (CFD) can be used to simulate the detailed flow and scalar transport in packed beds to provide improved understanding and quantitative information. Simulations of flow, heat transfer and dispersion of mass were made in a 400-sphere random fixed bed of tube-to-particle diameter ratio N = 5.96.

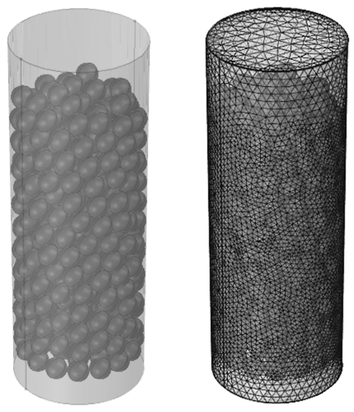

Figure 1. 400-sphere N = 5.96 column and mesh

Computational Methods: A random pack of spheres was generated by a Monte Carlo collective re-arrangement algorithm and validated,[1] and the geometry was imported into COMSOL Multiphysics 4.3b using the CAD Import Module.

The flow simulations used Laminar and Turbulent flow (k-ε with wall functions) physics. The conjugate heat transfer problem used the Heat Transfer Module where the Heat Transfer in Fluids model was first set up then the Heat Transfer in Solids model was added to it, which ensured that the two models coupled temperature and flux correctly across the fluid-solid interface. Dispersion of mass was handled in the Transport of Dilute species model.

Contact points between the spheres were avoided by shrinking the particles by 1% of their diameters. The simulations were converged by using the segregated solution algorithm.

Results: Representative results of fluid flow, heat transfer and mass dispersion are shown in the figures. Extensive results were obtained for nine values of flow rate, both laminar and turbulent.

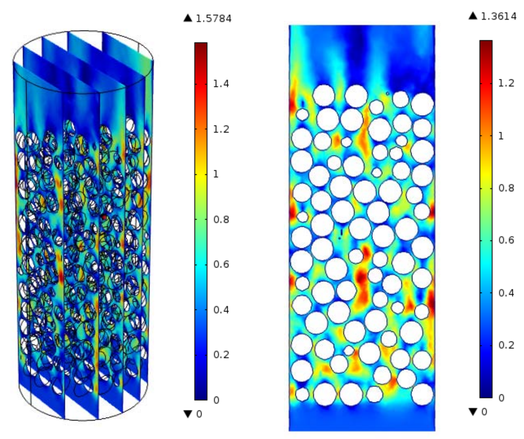

Figure 2. Velocity field Re = 100

Re	$-\frac{\Delta P}{L}$ (Pa/m) calculated	$-\frac{\Delta P}{L}$ (Pa/m) Reference [2]
50	0.811	0.8025
100	2.305	2.219
200	7.009	6.894
400 (lam.)	22.476	23.611
400 (turb.)	27.037	23.611
600	52.179	50.152
800	84.636	86.516
1000	124.27	132.703
2000	427.34	510.99
5000	2340.2	3119.35

Table 1. ΔP comparison to literature

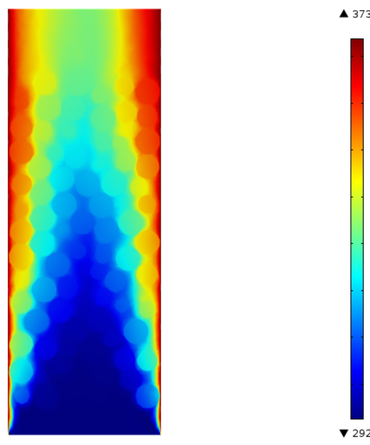

Figure 3. T contours, Re = 100

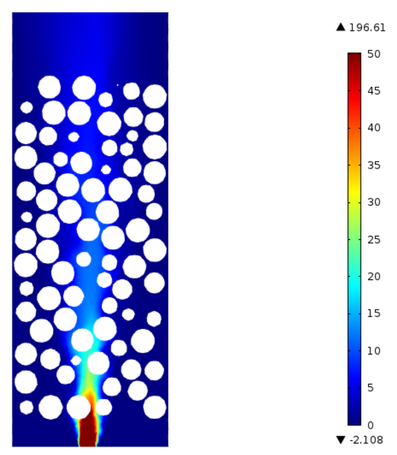

Figure 4. C contours, Re = 200

Conclusions: Flow and transport were simulated 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.

References:

1. Behnam, M., Dixon, A. G., Nijemeisland, M., Stitt, E. H., A new approach to fixed bed radial heat transfer modeling using velocity fields from computational fluid dynamics simulations, *Ind. Eng. Chem. Res.*, **52**, 15244-15261 (2013)
2. Eisfeld, B.; Schnitzlein, K., The influence of containing walls on the pressure drop in packed beds, *Chem. Eng. Sci.*, **56**, 4321-4329 (2001)