

Slim Fixed Bed Reactor Tubes

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A catalytic fixed bed reactor is a cylindrical tube, randomly filled with catalyst particles, which may be spheres or cylindrical pellets. During operation, a gas or liquid (or both) flows through the tube and over the catalyst particles, and reactions take place.

For many reactions, the heat effects are moderate, and large-diameter reactor tubes are used, with many catalyst particles across a tube diameter (large N). For more exo- or endothermic reactions where efficient heat transfer is required through the tube wall, such as steam reforming of methane, the number of particles across a tube diameter must be reduced (small N).

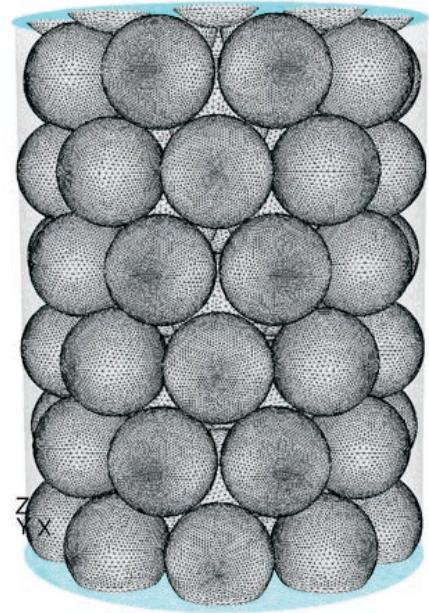
A precise description of the interstitial flow through a packed tube has long been considered impossible, and fixed bed reactor models have relied on a continuum approach that uses averaged fluid and solid properties, plug flow, and empirical parameters for heat and mass transfer. The correlations for heat and mass transfer in the literature are contradictory and relatively inaccurate. This causes reactor models to be unreliable, since reaction rates are strongly dependent on local temperature and concentrations in the tube.

With the recent increases in computing power, and the availability of unstructured CFD codes such as FLUENT, it has become possible to perform detailed calculations of fluid flow and heat transfer for slim fixed bed tubes¹, where the ordered arrangement of

particles near the tube wall allows a representative model to be built. In a recent project carried out at Worcester Polytechnic Institute (WPI), the influence of the complex fixed bed flow field on heat transfer at the wall was investigated, to provide insight for improved catalyst particle design.

Two fixed bed models were developed. First, an axially periodic section of a full bed packed with spheres, corresponding to $N = 4$, was created. Flow and heat transfer solutions were obtained, and mesh refinement studies were carried out. In a previous study CFD simulations for fluid flow and heat transfer in a similar fixed bed with $N = 2$ had been validated against experimental data, giving confidence that the CFD simulations were realistic.²

To include conjugate heat transfer, the particle internals needed to be meshed as well. To cut back on the number of cells required for this phase of the project, a representative segment of the full bed was identified. This second model consisted of a 120-degree section with two axial layers of spheres, symmetry boundary conditions on the sides, translational periodic boundary conditions on the top and bottom, and a constant temperature boundary condition on the cylindrical tube wall. Because constant properties were used, the steady-state flow solution was performed first, and was validated against the simulations from the full bed model. The energy solution was performed next, and the results were analyzed to give temperature fields and a surface heat



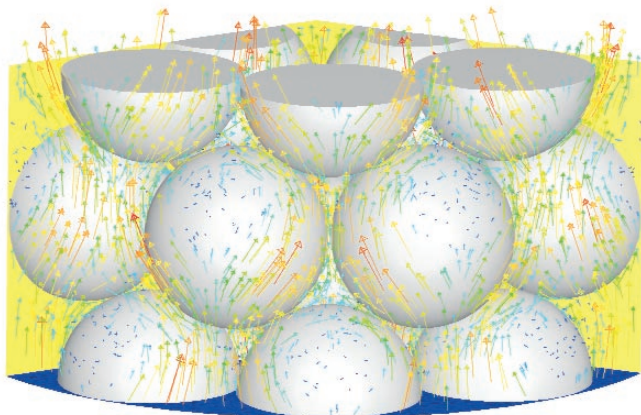
Periodic section of six particles depth of the $N = 4$ full bed model

flux map for the cylindrical tube wall. The map showed that the wall heat flux pattern is the result of the flow features in the bed and the packing structure of the particles near the wall.

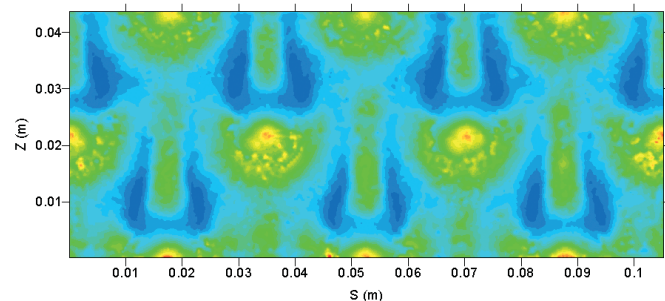
By extending the research into the detailed modeling of flow and heat transfer in heterogeneous chemical reactor systems, it will be possible in the future to effectively optimize and understand the intricate processes at play in these reactors. Using techniques such as CFD on a large scale in the chemical industry, may make it possible to reduce the need for much more expensive empirical experimentation. ■

references:

1. A.G. Dixon and M. Nijemeisland, *Industrial and Engineering Chemistry Research*, **40**, p. 5246-5254, 2001.
2. M. Nijemeisland and A.G. Dixon, *Chemical Engineering Journal*, **82**, p. 231-246, 2001.



Wall-segment geometry with velocity vectors, showing areas of recirculating flow and "jet-like" flow



Map of local heat flux (W/m^2) on the cylindrical tube wall

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