

COMSOL Multiphysics® Simulation of Flow in a Radial Flow Fixed Bed Reactor (RFBR)

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Abstract

Introduction: In the design of radial flow fixed bed reactors, it is important to ensure uniform flow distribution through the catalyst bed. A 2D axisymmetric model of a conceptual radial-flow reactor design was developed (Fig. 1) and was used to evaluate flow maldistribution through the catalyst bed and the pressure drop through the reactor for the specified flow rate. Effects of different catalyst pellet sizes, screen open area fractions and flow direction were simulated.

Use of COMSOL MULTIPHYSICS®: The flow simulations used the CFD Module to implement incompressible turbulent flow (k-ε with wall functions). The equations for mass and momentum balances are:

$$\rho(\mathbf{u} \cdot \nabla)\mathbf{u} = \nabla \cdot [-\rho \mathbf{I} + (\mu + \mu_T)(\nabla \mathbf{u} + (\nabla \mathbf{u})^T) - \frac{2}{3} \rho \mathbf{kl}] + \mathbf{F}$$
$$\rho \nabla \cdot \mathbf{u} = 0$$

The term \mathbf{F} represents forces acting on the fluid per unit volume. This term provides the resistance in the screens and in the bed (1,2). The equation for \mathbf{F} in the catalyst bed was

$$\mathbf{F} = -\frac{\mu}{K} \mathbf{v} - \frac{C2B \cdot \rho}{2} |\mathbf{v}| \mathbf{v}$$

This is the Darcy-Forchheimer law which describes single-phase laminar flow through a porous medium, including a term for inertial resistance. The resistance in the screens was given by the porous jump model as

$$\mathbf{F} = -\frac{C2S \cdot \rho}{2} |\mathbf{v}| \mathbf{v}$$

Different values for the inertial resistance $C2S$ could be used for the inner and outer screens.

Values for K and $C2B$ were obtained from the Ergun equation for pressure drop in a packed bed, which depends on the particle size and bed void fraction. Values for $C2S$ were determined from the equation of flow through square-edged holes on an equilateral triangular spacing (2). The flow resistance could be adjusted by changing the open area fraction of the screens and/or the catalyst particle diameter. Baseline conditions were for 10% open screens and $\frac{1}{8} \times \frac{3}{16}$ in. ($D \times L$) pellets.

Results: Flow and pressure contours are shown in Fig. 2 for specified inlet velocity and outlet pressure, under baseline conditions. Normal flow direction was downwards in Fig. 2(a) and 2(b). This case gave a quite large ΔP and reasonably uniform distribution of flow. A large contribution to the overall ΔP was caused by the flow constriction into the outer annulus and at the bed exit where the radial and axial flows merged. Flow in the reverse direction was investigated (Fig. 2c) and gave lower ΔP at the cost of much worse flow distribution. Fig. 3 shows the flow field and re-circulation regions for normal flow associated with higher

resistance to flow, which suggests where re-design of the reactor could be beneficial to reduce the pressure drop. Fig. 4 shows changes in catalyst bed ΔP due to bed and screen resistance. Higher open area and larger pellets reduce ΔP but also increase by-passing flow in the bed, giving catalyst underutilization and/or non-uniform deactivation. The screen flow resistance is small for open area fractions above 10%.

Conclusions: Resistance to flow was decreased by larger catalyst particles or more open screens, but this may lead to more severe flow maldistribution. Normal flow was found to give better flow distribution in this configuration than reverse flow.

Reference

1. Ranade, V. V. (2002). Computational flow modeling for chemical reaction engineering, Ch. 5 (pp. 403-423). San Diego, CA: Academic Press.
2. Kareeri, A. A. et al. (2006). Simulation of flow distribution in radial flow reactors. Ind. Eng. Chem. Res., 45(8), 2862-2874.

Figures used in the abstract

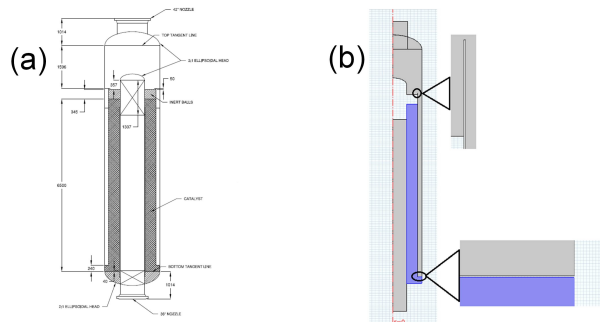


Figure 1: a) Conceptual radial-flow reactor; b) 2D axisymmetric model

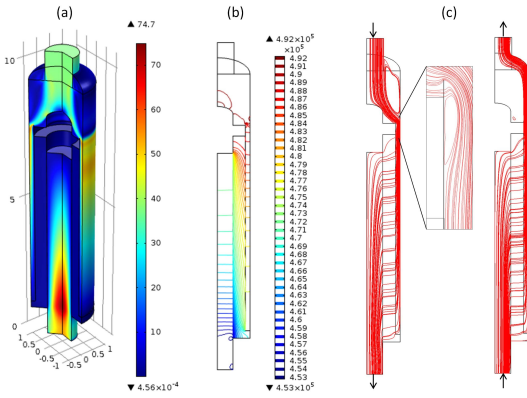


Figure 2: (a) 3D contours of $|v|$; (b) contours of pressure;

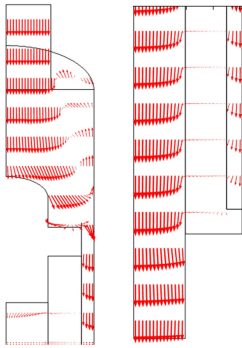


Figure 3: Velocity vectors at

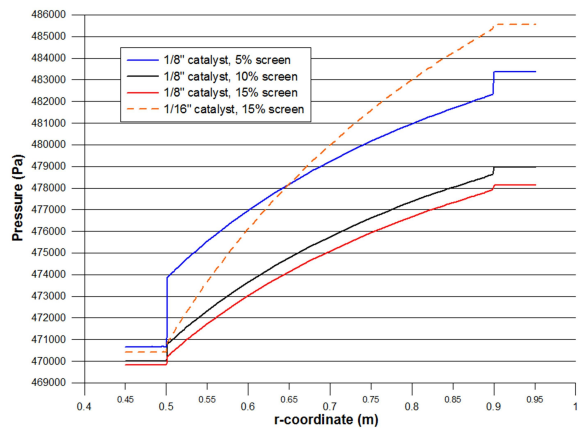


Figure 4: Effect of pellet size & screen