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

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Introduction: In the design of radial flow fixed bed reactors, it is important to ensure proper flow distribution through the catalyst bed. Utilizing COMSOL Multiphysics, 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 catalysts, screen sizes and flow direction were simulated.

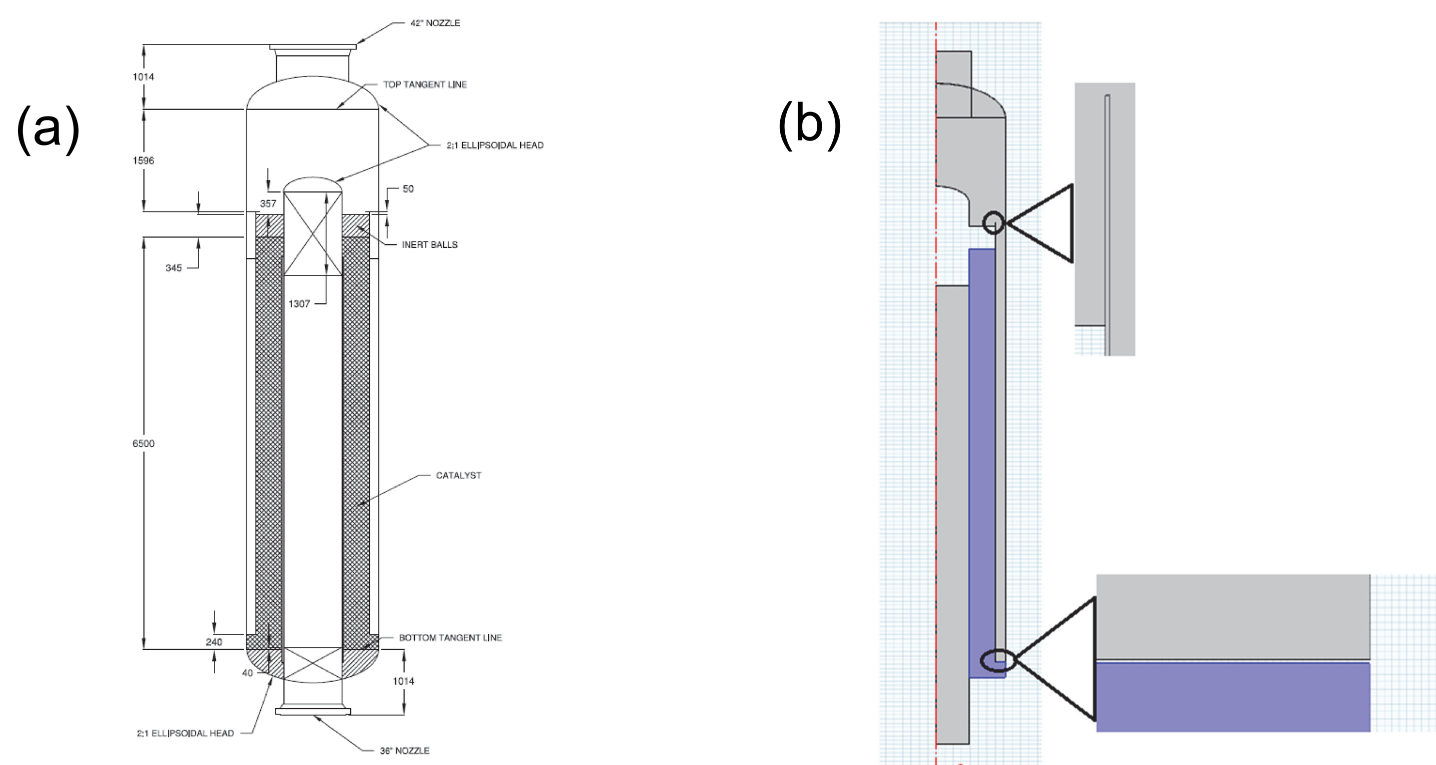

Figure 1. a) Conceptual radial-flow reactor; b) 2D axisymmetric model

Computational Methods: The flow simulations used incompressible Turbulent flow (k-ε with wall functions) physics, in COMSOL Multiphysics 4.3b. The equations for mass and momentum balances are:

$$\rho(\mathrm{u}\cdot\nabla)\mathrm{u} = \nabla\cdot\left[-\rho l + (\mu+\mu_T)(\nabla\mathrm{u}+(\nabla\mathrm{u})^T) - \frac{2}{3}\rho k l\right] + F$$

$$\rho\nabla\cdot\mathrm{u} = 0$$

The term F represents forces acting on the fluid per unit volume. This term was added to the system to provide the resistance in the screens and in the bed.[1,2] The equation for *F* in the catalyst bed was:

$$F = -\frac{\mu}{K} * v - \frac{C2B*\rho}{2} * |v| * \vec{v}$$

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

$$F = -\frac{C2S*\rho}{2} * |v| * \vec{v}$$

Different values for the inertial resistance *C2S* could be used for the inner and outer screens. Values for *K* and *C2B* in the bed 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 ⅛ × $^3/_{16}$ in. (D × L) pellets.

Results: Flow results are shown in Fig. 2 for boundary conditions of inlet velocity and outlet pressure, under baseline conditions. Normal flow direction was downwards as in (a) and (b). High flow resistance gave larger ΔP and good flow distribution.

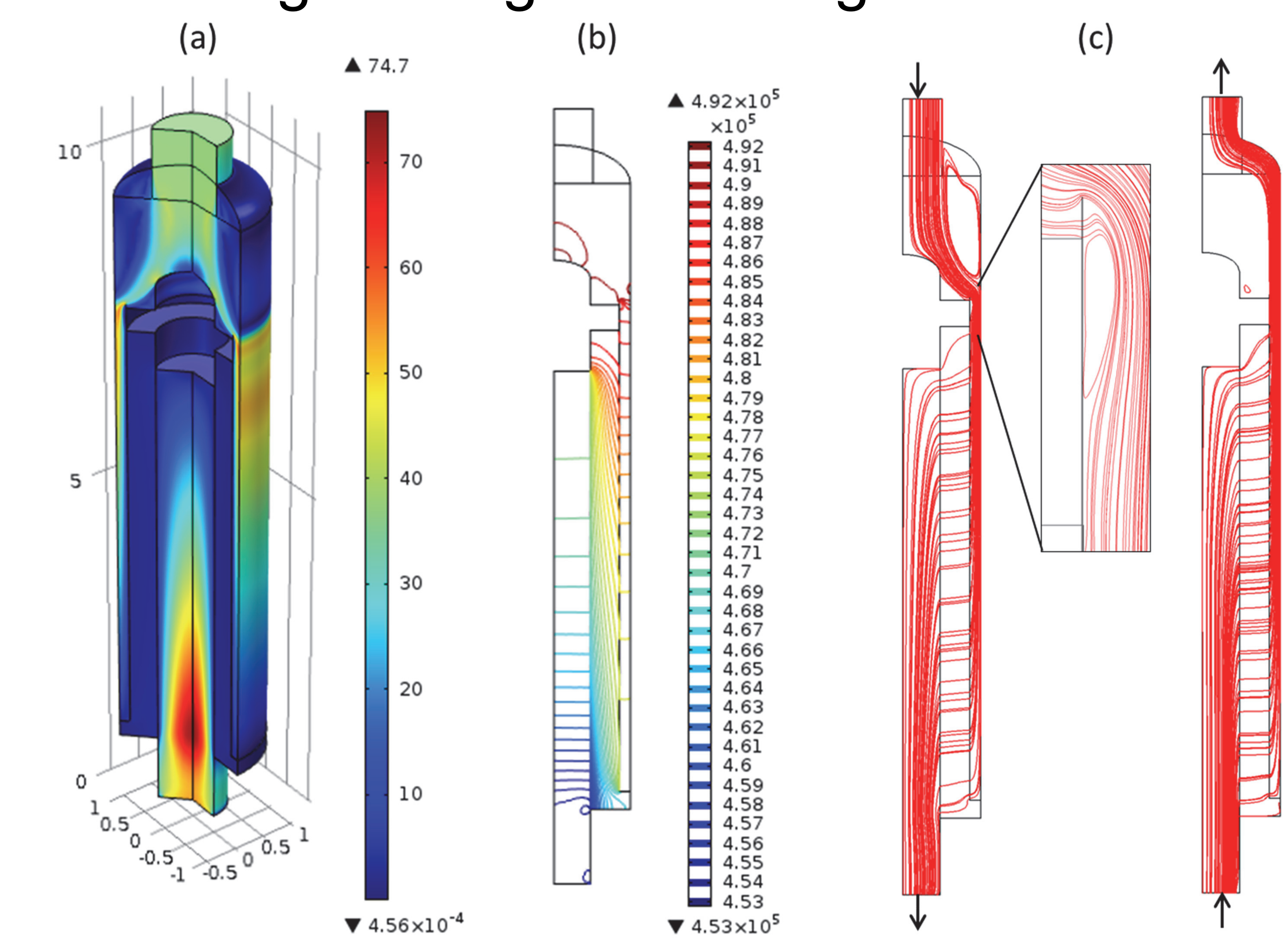

Figure 2. (a) 3D contours of |v|; (b) contours of pressure; (c) streamlines for normal and reverse flow

Fig. 3 shows more details of flow, while Fig. 4 gives the effect of changing bed and screen resistance.

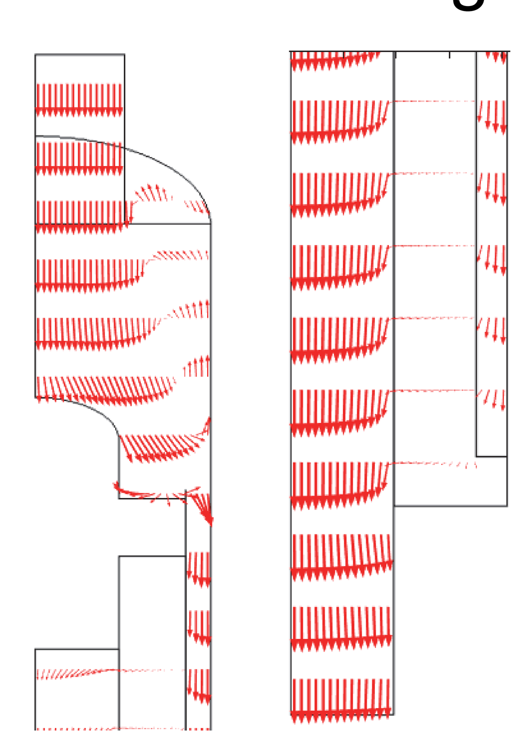

Figure 3. Velocity vectors at top & bottom of bed

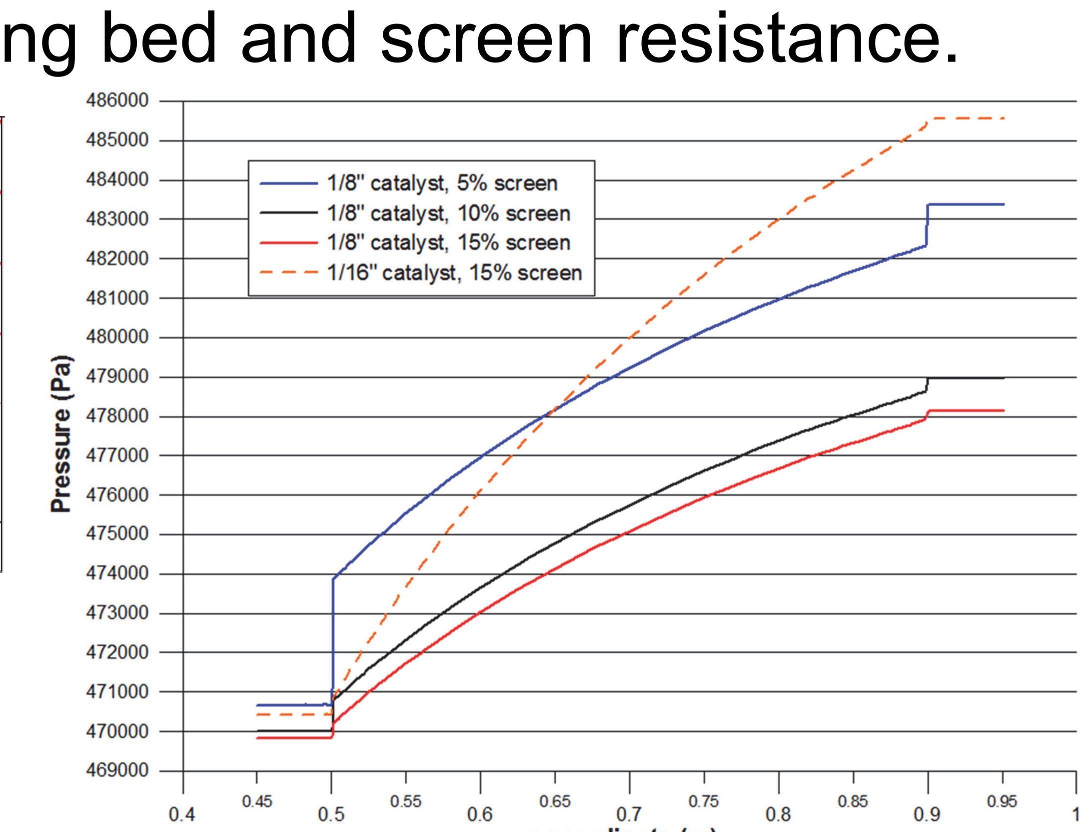

Figure 4. Effect of pellet size & screen opening on pressure drop

Conclusions: Resistance to flow can be 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.

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References:

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., Zughbi, H. D., and Al-Ali, H. H. (2006). Simulation of flow distribution in radial flow reactors. *Ind. Eng. Chem. Res., 45*(8), 2862-2874.