Modeling of Packed Bed Reactors: Hydrogen Production by the Steam Reforming of Methane and Glycerol

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Introduction: For gas-phase reactions with large mole changes in a packed tube reactor, density and velocity change.[1] We show how to include these in the reactor model, for methane steam reforming (MSR):

$$CH_4 + H_2O \leftrightarrow 3H_2 + CO$$

$$CO + H_2O \leftrightarrow CO_2 + H_2$$

$$CH_4 + 2H_2O \leftrightarrow 4H_2 + CO_2$$

and steam reforming of glycerol (GSR):

$$C_3H_8O_3 + 3H_2O \rightarrow 7H_2 + 3CO_2$$

We solve an isothermal model with a 1-D domain for the reactor tube coupled to a 2-D domain for the single particle[2] in COMSOL.

Computational Methods: The Coefficient PDE feature was used for the pressure drop equation. The equations for diffusion and reaction in the pellet and convective dispersion in the tube were handled by use of the Chemical Reaction Engineering Module; the gas-phase equation was changed[3] to

$$-c_{tot}D_{ea}\frac{d^2y_i}{dz^2} - \frac{y_iG}{M^2}\frac{dM}{dz} + \frac{G}{M}\frac{dy_i}{dz} = a_p(1-\varepsilon_b)k_g\left(C_{pi}^s - c_{tot}y_i\right)$$

$$M = \sum_{i=1}^{N_s} y_iM_i\,, \qquad \frac{dM}{dz} = \sum_{i=1}^{N_s} M_i\frac{dy_i}{dz}$$

The tube and pellet equations used coupling variables to exchange information:

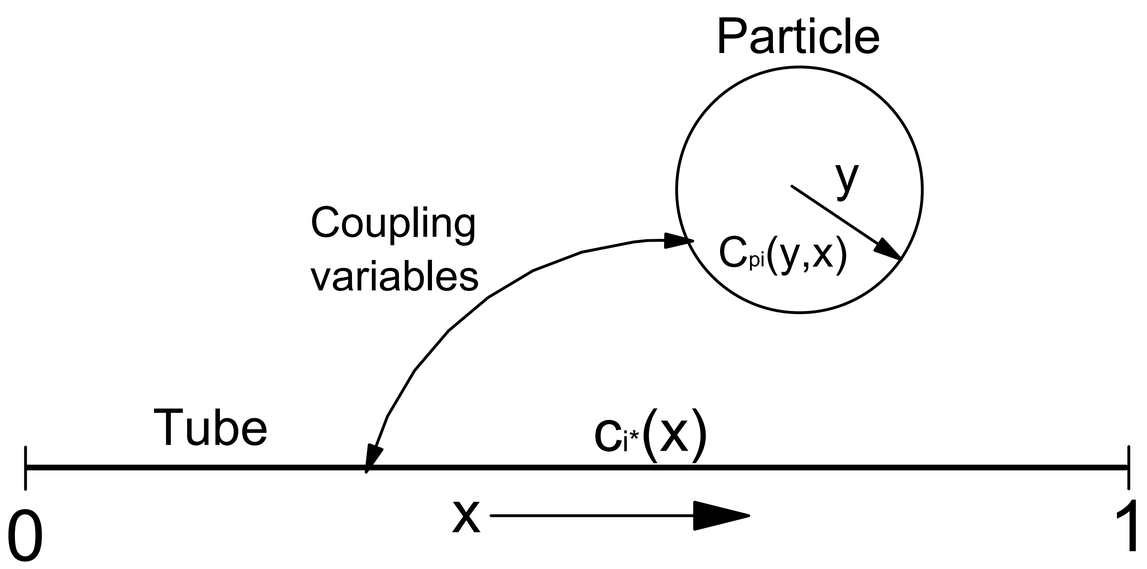

Figure 1. Tube and particle geometry

Results: MSR has higher ΔP and lower reaction mole change. GSR has lower ΔP and high reaction mole change. Effects of both on velocity are accounted for by the model equations.

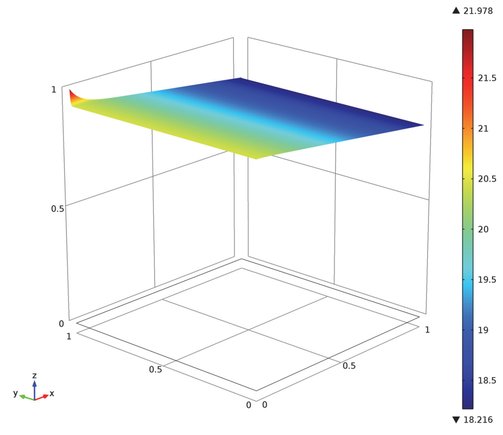

Figure 2. Methane pellet conc.

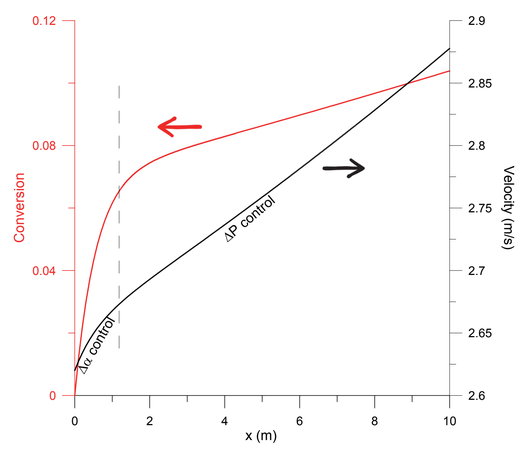

Figure 3. MSR: Conv. and v

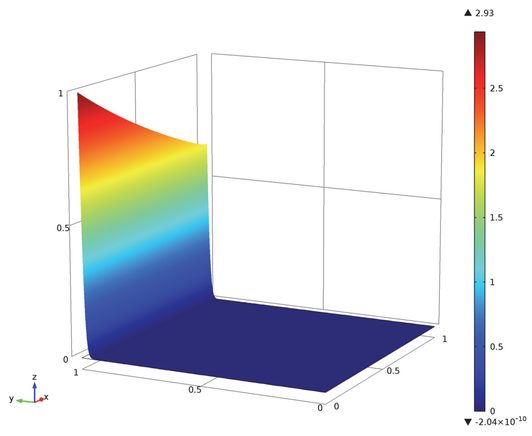

Figure 4. Glycerol pellet conc.

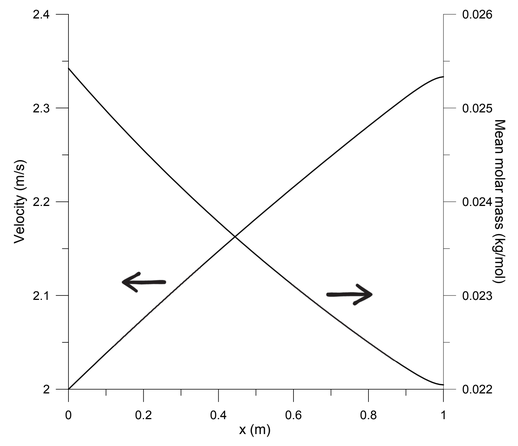

Figure 5. GSR: M and v

Conclusions: Effects of mole increases on the gas velocity and conversion for MSR and GSR were simulated using the mean molar mass. Results are given for isothermal 1-D calculations; future work will extend to 2-D non-isothermal cases.

References:

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2. Petera, J.; Nowicki, L.; Ledakowicz, S., New numerical algorithm for solving multidimensional heterogeneous model of the fixed bed reactor, *Chem. Eng. J.* **214**, 237-246 (2013)
3. Cropley, J. B.; Burgess, L. M.; Loke, R. A., The optimal design of a reactor for the hydrogenation of butyraldehyde to butanol, *ACS Symp. Ser.*, **237**, 255-270 (1984)