Catalytic Oxidative Dehydrogenation Of Propane To Propylene

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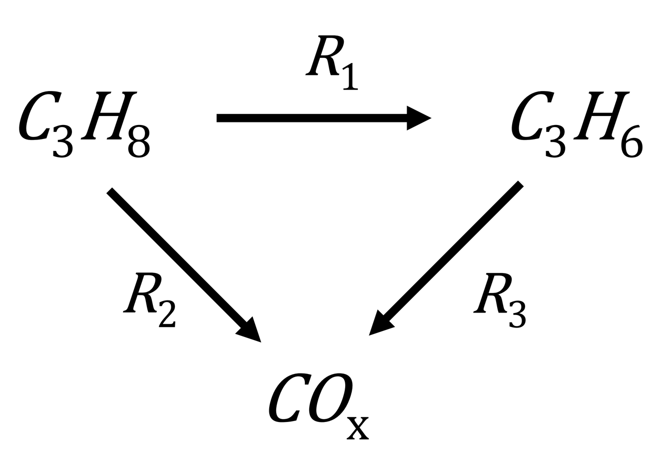
INTRODUCTION

Propylene is the second most important olefin and the second largest volume industrial chemical produced globally. Growth in demand is outpacing supplies from steam cracking and catalytic cracking. To address this supply gap, there is active research on alternative on-purpose propylene technologies. Catalytic oxidative dehydrogenation of propane is a promising alternative technology for propylene production.

COMPUTATIONAL METHODS

Reaction Kinetics

Parallel-series triangular reaction network,[1] where oxidation of propane is with the lattice oxygen of the $VO_x/\gamma\text{-}Al_2O_3$ catalyst,



$$R_1 = k_1 K_{C_3H_8} C_{C_3H_8} f$$

$$R_2 = k_2 K_{C_3H_8} C_{C_3H_8} f$$

$$R_3 = k_3 K_{C_3H_6} C_{C_3H_6} f$$

where,

$$k_i = A_i e^{\frac{-E_i}{R}\left(\frac{1}{T}-\frac{1}{T_m}\right)} \qquad K_i = K_i^0 e^{\frac{-\Delta H_i}{R}\left(\frac{1}{T}-\frac{1}{T_m}\right)} \qquad f = \frac{e^{-\lambda X_{C_3H_8}}}{1 + K_{C_3H_8} + K_{C_3H_6}}$$

Transport Phenomena

Momentum:
$$0 = -\frac{\partial P}{\partial z} + \frac{\mu}{\epsilon}\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial v_z}{\partial r}\right) - \frac{\mu}{\kappa}v_z$$

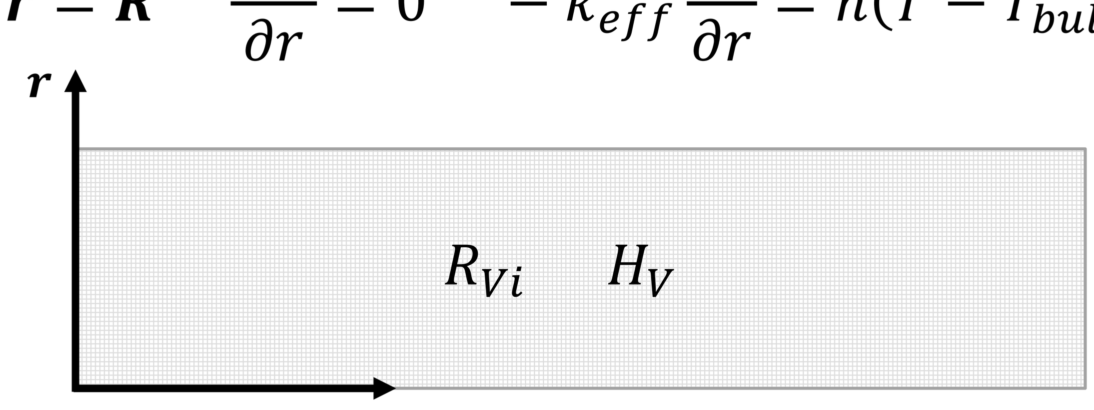
Energy:
$$\rho C_P v_z \frac{\partial T}{\partial z} = k_{eff}\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial T}{\partial r}\right) + \frac{\partial^2 T}{\partial z^2}\right] + H_V$$

Mass:
$$v_z \frac{\partial C_i}{\partial z} = D_{eff}\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial C_i}{\partial r}\right) + \frac{\partial^2 C_i}{\partial z^2}\right] + R_{Vi}$$

Boundary Conditions:

$$\boldsymbol{r = R} \qquad \frac{\partial C_i}{\partial r} = 0 \qquad -k_{eff}\frac{\partial T}{\partial r} = h(T - T_{bulk})$$

$\boldsymbol{z = 0}$: $v_z = v_{in}$, $T = T_{in}$, $C_{C_3H_8} = C_{C_3H_8}^{in}$



$\boldsymbol{z = L}$: $\partial T/\partial z = 0$, $\partial C_i/\partial z = 0$

$$\boldsymbol{r = 0} \qquad \frac{\partial T}{\partial r} = 0 \qquad \frac{\partial C_i}{\partial r} = 0$$

RESULTS

Table 1. Reactor dimensions and process conditions.

L (m)	D (mm)	D_p (mm)	P_{in} (atm)	T_{in} (°C)	T_{bulk} (°C)	V_{in} (Nm^3/h)
3	500	5	3	200	400	50

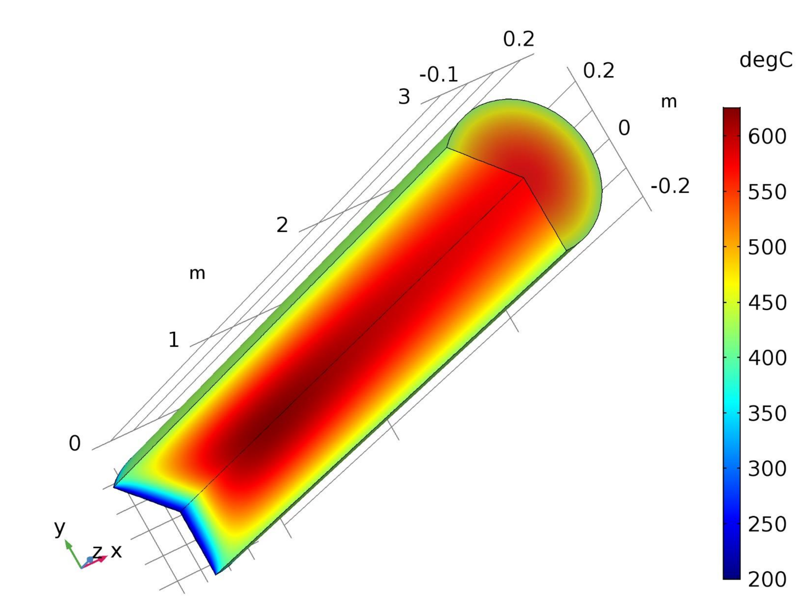


Figure 1. Surface revolution plot of reactor temperature as function of radial and axial coordinates.

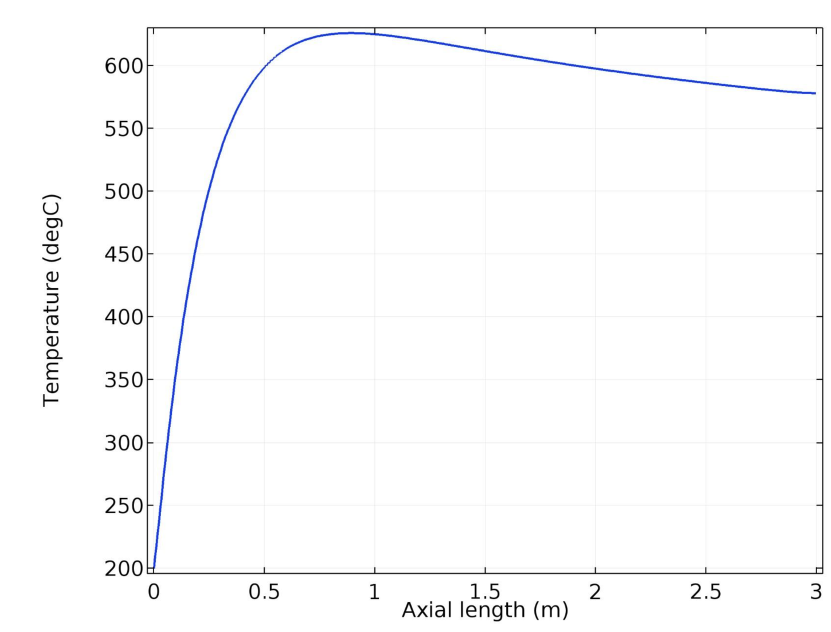


Figure 2. Temperature at center-line of reactor as function of axial coordinate.

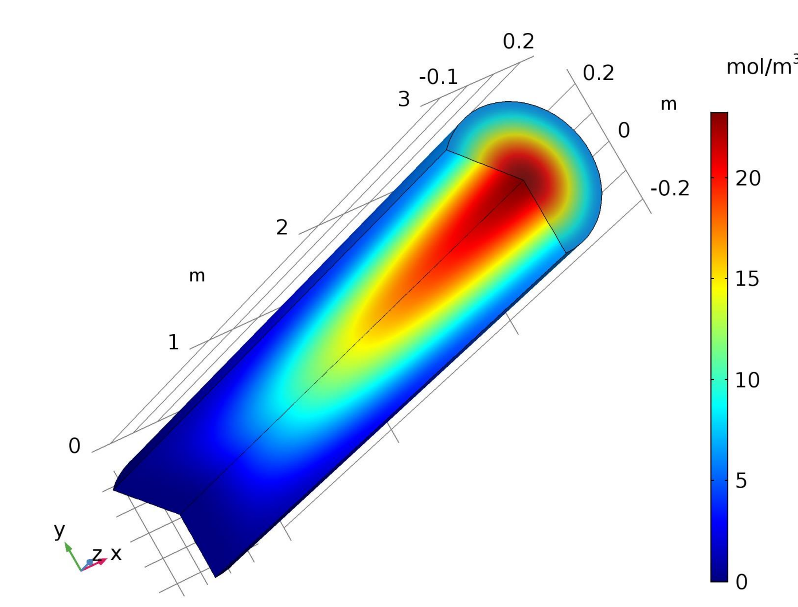


Figure 3. Surface revolution plot of propylene concentration as function of radial and axial coordinates.

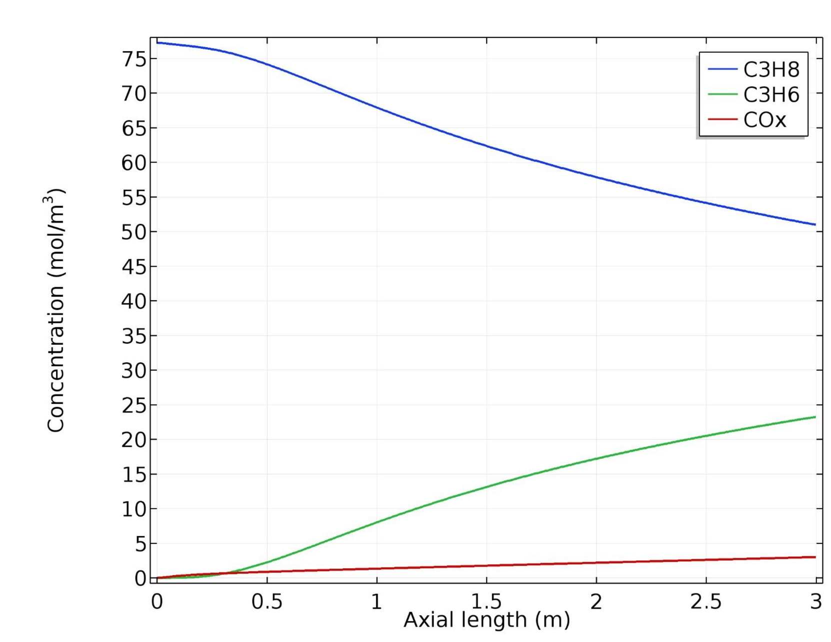


Figure 4. Species concentrations at reactor center-line as functions of axial coordinate.

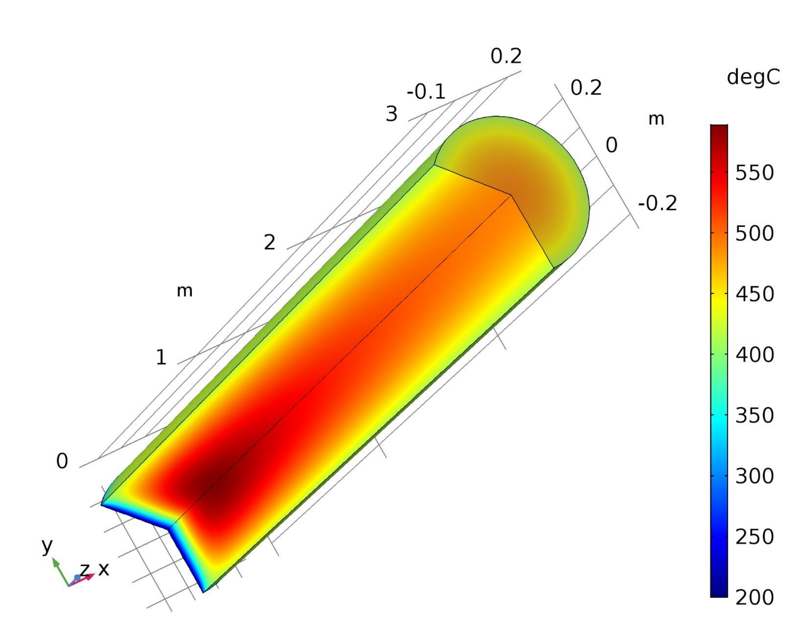


Figure 5. Surface revolution plot of reactor temperature as function of radial and axial coordinates with V_{in} = 10 Nm^3/h.

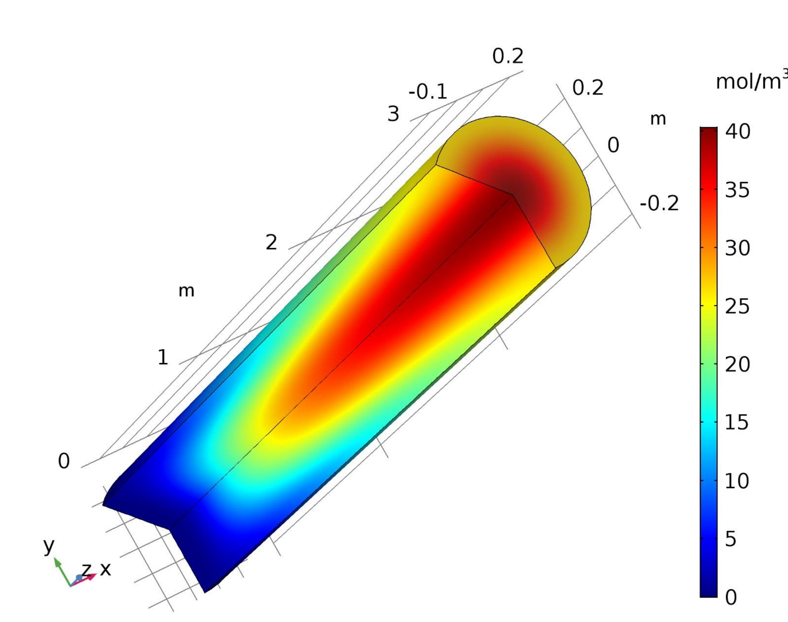


Figure 6. Surface revolution plot of propylene concentration as function of radial and axial coordinates with V_{in} = 10 Nm^3/h.

CONCLUSIONS

Propylene production sensitive to inlet volumetric feed rate. Further simulations forthcoming to examine sensitivity to other process parameters.

REFERENCES:

1. S. Al-Ghamdi, J. Moreira, and H. de Lasa, Kinetic Modeling of Propane Oxidative Dehydrogenation over $VO_x/\gamma\text{-}Al_2O_3$ Catalysts in the Chemical Reactor Engineering Center Riser Reactor Simulator, Ind. Eng. Chem. Res., 53, 15317-15332 (2014)