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Dynamic Nonisothermal Trickle Bed Reactor with both Internal Diffusion and Heat Conduction Sugar Hydrogenation as a Case Study

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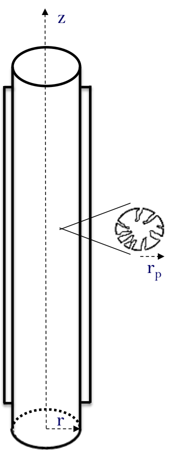
Merits of gPROMS ModelBuilder

- Fast! • No need to think step-by-step!
- User friendly equation typing!
- Local phenomena solved simultaneously.
- Process flow sheet modelling.
- Everything as program code.
- Parameter estimation & statistics.
- Steady-state and dynamic.

Fixed Bed Reactor

- Gas-liquid-solid.
- Heat & mass transfer.
- Conduction, dispersion(axial and radial)
- Kinetics: known/unknown.
- Particles: Internal heat & mass transfer.

Mass and energy balances for three phases



Gas phase

Accumulation G-L Mass transfer Convection Axial Dispersion

$$\varepsilon_G \cdot \frac{\partial C_{i,G}(t,z,r)}{\partial t} = -k_{i,L} a_L \cdot (C^*_{i,L} - C_{i,L}) - \frac{\partial (u_G(z,r) \cdot C_{i,G}(t,z,r))}{\partial z} + \varepsilon_G \cdot D_{z,G}(z,r) \cdot \frac{\partial^2 C_{i,G}(t,z,r)}{\partial z^2} +$$

Radial Dispersion

$$+\varepsilon_G \cdot D_{r,G(z,r)} \cdot \left(\frac{\partial^2 C_{i,G}(t,z,r)}{\partial r^2} + \frac{1}{r} \cdot \frac{\partial C_{i,G}(t,z,r)}{\partial r} \right)$$

Liquid phase

Accumulation G-L Mass transfer Convection Axial Dispersion

$$\varepsilon_L \cdot \frac{\partial C_{i,L}(t,z,r)}{\partial t} = +k_{i,L} a_L \cdot (C^*_{i,L} - C_{i,L}) - u_L \cdot \frac{\partial C_{i,L}(t,z,r)}{\partial z} + \varepsilon_L \cdot D_{z,L} \cdot \frac{\partial^2 C_{i,L}(t,z,r)}{\partial z^2} +$$

Radial Dispersion Mass transfer from the solid

$$+\varepsilon_L \cdot D_{r,L} \cdot \left(\frac{\partial^2 C_{i,L}(t,z,r)}{\partial r^2} + \frac{1}{r} \cdot \frac{\partial C_{i,L}(t,z,r)}{\partial r} \right) - \frac{D_{eff,i} \cdot s}{R_p} \cdot \left. \frac{\partial C_{i,s}(t,z,r,r_p)}{\partial r_p} \right|_{r_p=R_p}$$

Solid phase

Accumulation Internal diffusion with shape factor Reactions

$$\frac{\partial C_{i,s}(t,z,r,r_p)}{\partial t} = \frac{D_{eff,i}}{\varepsilon_p} \cdot \left(\frac{\partial^2 C_{i,s}(t,z,r,r_p)}{\partial r_p{}^2} + \frac{s}{r_p} \cdot \frac{\partial C_{i,s}(t,z,r,r_p)}{\partial r_p} \right) + \rho_s \cdot \sum \left(\nu_i \cdot r_{xn}(t,z,r,r_p) \cdot \frac{\varepsilon_L}{\varepsilon_p} \right)$$

Gas phase

Accumulation Convection Axial conduction

$$\varepsilon_G \cdot \rho_G(z,r) \cdot c_{p,L} \cdot \frac{\partial T_G(t,z,r)}{\partial t} = -\varepsilon_G \cdot c_{p,G} \cdot \frac{\partial (\rho_G(z,r) \cdot u_G(z,r) \cdot T_G(t,z,r))}{\partial z} + k_{z,G} \cdot \frac{\partial^2 T_G(t,z,r)}{\partial z^2} +$$

Axial dispersion Radial conduction

$$+\varepsilon_G \cdot c_{p,G} \cdot D_{z,G} \cdot \frac{\partial (\rho_G(z,r) \cdot T_G(t,z,r))}{\partial z} + k_{r,G} \cdot \frac{1}{r} \cdot \frac{\partial (\cdot T_G(t,z,r))}{\partial r} + k_{r,G} \cdot \frac{\partial^2 T_G(t,z,r)}{\partial r^2} +$$

Radial dispersion G-L Heat transfer

$$+\varepsilon_G \cdot c_{p,G} \cdot D_{r,G} \cdot \frac{1}{r} \cdot \frac{\partial (\rho_G(z,r) \cdot T_G(t,z,r))}{\partial r} + \varepsilon_G \cdot c_{p,G} \cdot D_{r,G} \cdot \frac{\partial^2 (\rho_G(z,r) \cdot T_G(t,z,r))}{\partial r^2} - h_G a \cdot (T_G(z,r) - T_L(z,r))$$

Liquid phase

Accumulation G-L Heat transfer Convection Conduction and axial dispersion

$$\frac{\partial T_L(t,z,r)}{\partial t} = +\frac{h_G a \cdot (T_G(z,r) - T_L(z,r))}{\varepsilon_L \cdot \rho_L \cdot c_{p,L}} - u_L \cdot \frac{\partial T_L(t,z,r)}{\partial z} + \left(\frac{k_z}{\varepsilon_L \cdot \rho_L \cdot c_{p,L}} + D_z \right) \cdot \frac{\partial^2 T_L(t,z,r)}{\partial z^2} +$$

Radial conduction and dispersion Heat transfer from the solid

$$+\left(\frac{k_r}{\varepsilon_L \cdot \rho_L \cdot c_{p,L}} + D_r \right) \cdot \frac{1}{r} \cdot \frac{\partial T_L(t,z,r)}{\partial r} + \left(\frac{k_r}{\varepsilon_L \cdot \rho_L \cdot c_{p,L}} + D_r \right) \cdot \frac{\partial^2 T_L(t,z,r)}{\partial r^2} - \frac{\lambda_p \cdot s}{R_p \cdot \varepsilon_L \cdot \rho_L \cdot c_{p,L}} \cdot \left. \frac{\partial T_s(t,z,r,r_p)}{\partial r_p} \right|_{r_p=R_p}$$

Solid phase

Accumulation Internal diffusion with a shape factor Reactions

$$\frac{\partial T_s(t,z,r,r_p)}{\partial t} = \frac{\lambda_p}{\rho_s \cdot c_{p,s}} \cdot \left(\frac{\partial^2 T_s(t,z,r,r_p)}{\partial r_p{}^2} + \frac{s}{r_p} \cdot \frac{\partial T_s(t,z,r,r_p)}{\partial r_p} \right) + \frac{1}{c_{p,s}} \cdot \frac{\varepsilon_L}{\varepsilon_p} \cdot \left(\sum r_{xn}(t,z,r,r_p) \cdot (-\Delta H_r) \right)$$

Boundary conditions

Gas phase

Entrance:
$$C_{i,G}(t,r)\big|_{z=0} = C_{i,G}{}^{IN} \qquad T_G(t,r)\big|_{z=0} = T_G{}^{IN}$$

Outlet:
$$\left. \frac{\partial C_{i,G}(t,r)}{\partial z} \right|_{z=L} = 0 \qquad \left. \frac{\partial T_G(t,r)}{\partial z} \right|_{z=L} = 0$$

Center:
$$\left. \frac{\partial C_{i,G}(t,z)}{\partial r} \right|_{r=0} = 0 \qquad \left. \frac{\partial T_G(t,z)}{\partial r} \right|_{r=0} = 0$$

Wall:
$$\left. \frac{\partial C_{i,G}(t,z)}{\partial r} \right|_{r=R} = 0 \qquad \left. \frac{\partial T_G(t,z)}{\partial r} \right|_{r=R} = 0$$

Liquid phase

Entrance:
$$C_{i,L}(t,r)\big|_{z=0} = C_{i,L}{}^{IN} \qquad T_L(t,r)\big|_{z=0} = T_L{}^{IN}$$

Outlet:
$$\left. \frac{\partial C_{i,L}(t,r)}{\partial z} \right|_{z=L} = 0 \qquad \left. \frac{\partial T_L(t,r)}{\partial z} \right|_{z=L} = 0$$

Center:
$$\left. \frac{\partial C_{i,L}(t,z)}{\partial r} \right|_{r=0} = 0 \qquad \left. \frac{\partial T_L(t,z)}{\partial r} \right|_{r=0} = 0$$

Wall:
$$\left. \frac{\partial C_{i,L}(t,z)}{\partial r} \right|_{r=R} = 0 \qquad -k_r \cdot \left. \frac{\partial T_L(t,z)}{\partial r} \right|_{r=R} = h_w \cdot (T_L(t,z)\big|_{r=R} - T_w)$$

Solid phase

Entrance:
$$C_{i,s}(t,r,r_p)\big|_{z=0} = C_{i,s}{}^{IN} \qquad T_s(t,r,r_p)\big|_{z=0} = T_s{}^{IN}$$

Outlet:
$$\left. \frac{\partial C_{i,s}(t,r,r_p)}{\partial z} \right|_{z=L} = 0 \qquad \left. \frac{\partial T_s(t,r,r_p)}{\partial z} \right|_{z=L} = 0$$

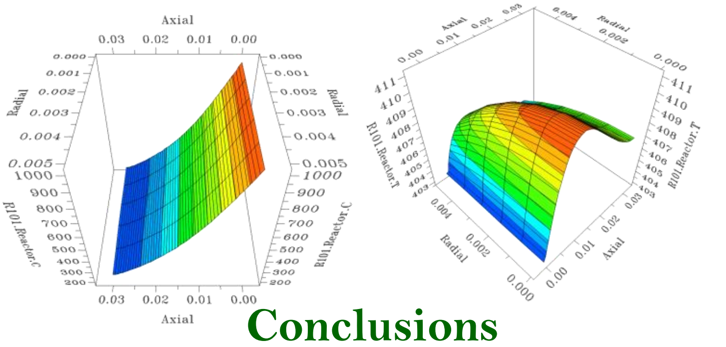
Center:
$$\left. \frac{\partial C_{i,s}(t,z,r_p)}{\partial r} \right|_{r=0} = 0 \qquad \left. \frac{\partial T_s(t,z,r_p)}{\partial r} \right|_{r=0} = 0$$

Wall:
$$\left. \frac{\partial C_{i,s}(t,z,r_p)}{\partial r} \right|_{r=R} = 0 \qquad -k_r \cdot \left. \frac{\partial T_s(t,z,r_p)}{\partial r} \right|_{r=R} = h_w \cdot (T_s(t,z,r_p)\big|_{r=R} - T_w)$$

Particle center:
$$\left. \frac{\partial C_{i,s}(t,z,r)}{\partial r_p} \right|_{r_p=0} = 0 \qquad \left. \frac{\partial T_s(t,z,r)}{\partial r_p} \right|_{r_p=0} = 0$$

Particle surface:
$$C_{i,s}(t,z,r)\big|_{r_p=R_p} = C_{i,L}(t,z,r) \qquad T_s(t,z,r)\big|_{r_p=R_p} = T_L(t,z,r)$$

Results



Conclusions

- Success depends on how well system is defined. (zero degrees of freedom).
- Numerical strategy: ModelBuilder does it itself.
- Program surprisingly fast running and reliable.
- Simultaneous dynamic solution of mass & heat balances for Gas-Liquid-Solid reaction system in three different dimensions (axial, radial, within particles).

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