Example 11: Fixed bed reactors gas (dynamic)

Partial oxidation of methanol to formaldehyde

CH3OH +1/2 O2 ---> CH2O + H2O

CH2O + 1/2 O2 ---> CO + H2O

The Model

dynamic particle energy balance

$$\frac{d}{d\tau}\theta p(\tau,\eta,z) = \alpha_{Hp}(\omega,\theta,p)\cdot\left[\frac{1}{\eta}\cdot\left(\frac{d}{d\eta}\theta p\right)+\frac{d^2}{d\eta^2}\theta p\right]+\alpha_{PF}(\omega,\theta,p)\cdot(\theta f-\theta p)+\frac{L\cdot\rho_f(\omega,\theta,p)\cdot Qr(\omega,\theta p,p)}{G\cdot\rho_c\cdot Cp_c\cdot T_0}$$

BC: $\frac{d}{d\eta}\theta p(\tau,0,z) = 0$ $\quad -\frac{d}{d\eta}\theta p(\tau,1,z) = Bi_w\cdot\left(\theta p-\theta_w\right)$ $\quad \theta p(\tau,\eta,0) = \theta f(\eta,0)+\frac{L\cdot Qr\left(\omega_0,\theta_0,p_0\right)}{\alpha_{PF}\cdot G\cdot Cp\left(\omega_0,\theta_0\right)\cdot T_0}$

where $\tau = t\cdot\frac{v}{L}$

$$\alpha_{Hp}(\omega,\theta,p) = \frac{k_{es}\cdot\rho_f(\omega,\theta,p)\cdot L}{G\cdot\rho_c\cdot Cp_c\cdot Ri^2}\qquad \alpha_{PF}(\omega,\theta,p) = \frac{h_s\cdot L\cdot\rho_f(\omega,\theta,p)\cdot a_v}{G\cdot\rho_c\cdot Cp_c}$$

steady state fluid energy balance

$$\frac{d}{dz}\theta f(\eta,z) = \alpha_{Hf}\cdot\left[\frac{1}{\eta}\cdot\left(\frac{d}{d\eta}\theta f\right)+\frac{d^2}{d\eta^2}\theta f\right]-\alpha_{FP}\cdot(\theta f-\theta p)$$

BC: $\frac{d}{d\eta}\theta f(0,z) = 0$ $\quad -\frac{d}{d\eta}\theta f(1,z) = Bi_w\cdot\left(\theta f-\theta_w\right)$ $\quad \theta f(\eta,0) = Tf(t)$

where

$$\alpha_{Hf} = \frac{k_{ef} \cdot L}{G \cdot Cp(\omega_0, \theta_0) \cdot Ri^2} \qquad \alpha_{FP} = \frac{h_s \cdot a_v \cdot L}{G \cdot Cp(\omega_0, \theta_0)}$$

steady state mass balance (1D)

$$\frac{d}{dz}\omega_i(z) = \frac{L}{G} \cdot \left[Rxn(\omega, \theta p_{ave}, p)\right]_i \qquad \omega(0) = \omega_0$$

where θp_{ave} = radial average of particle temperatures

Much of the input for this example is a repeat of Examples 5 and 7, so that information is included in the collapsed area below.

Dynamic forcing functions

Functions are defined below to allow the feed and wall temperature to change with time. For this example, only the change in feed temperature will be simulated.

cubic transition function used to provide smooth transitions between one state and another

$$SR(vx, x1, y1, x2, y2) := if\left[vx \le x1, y1, if\left[vx > x2, y2, y1 + \left[3 \cdot \left(\frac{vx - x1}{x2 - x1}\right)^2 - 2 \cdot \left(\frac{vx - x1}{x2 - x1}\right)^3\right] \cdot (y2 - y1)\right]\right]$$

feed temperature

$$temp := \frac{530 \cdot K}{T_0}$$

$$Tin := \begin{pmatrix} temp \\ temp - \frac{15\Delta°C}{T_0} \end{pmatrix}$$ feed temperature

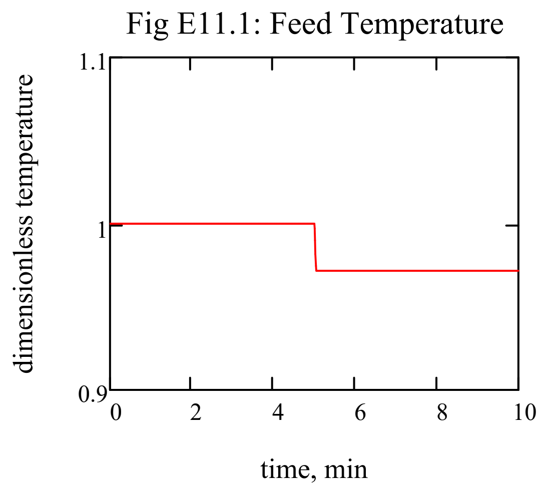
wall temperature

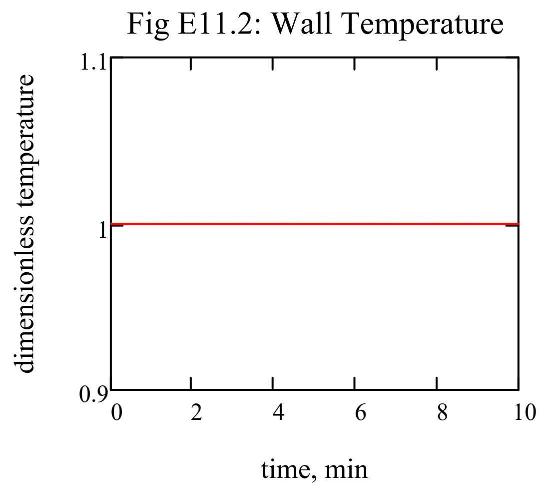
$$Twall := \frac{530 \cdot K}{T_0}$$

$$Tj := \begin{pmatrix} Twall \\ Twall \end{pmatrix}$$ wall temperature is constant in Examples 11 and 12

$$Tf(t) := SR(t, 5 \cdot min, Tin_0, 5.05 \cdot min, Tin_1)$$

$$Tw(t) := SR(t, 20 \cdot min, Tj_0, 25 \cdot min, Tj_1)$$





Parameter groups used in the model equations

The effects of density changes will be included in the parameter groups. Other parameters will be assumed constant based on feed or reference conditions.

fluid radial energy dispersion

$$\alpha_{Hf} := \frac{k_{ef} \cdot L}{G \cdot Cp(\omega_0, \theta_0) \cdot Ri^2}$$

$$\alpha_{Hf} = 25.271$$

particle radial energy dispersion

$$\alpha_{Hp}(\omega, \theta, p) := \frac{k_{es} \cdot \rho_f(\omega, \theta, p) \cdot L}{G \cdot \rho_c \cdot Cp_c \cdot Ri^2}$$

$$\alpha_{Hp}(\omega_0, \theta_0, p_0) = 0.018$$

fluid to particle heat transfer

$$\alpha_{FP} := \frac{h_s \cdot L \cdot a_v}{G \cdot Cp(\omega_0, \theta_0)}$$

$$\alpha_{FP} = 293.45$$

particle to fluid heat transfer

$$\alpha_{PF}(\omega, \theta, p) := \frac{h_s \cdot L \cdot \rho_f(\omega, \theta, p) \cdot a_v}{G \cdot \rho_c \cdot Cp_c}$$

$$\alpha_{PF}(\omega_0, \theta_0, p_0) = 1.248$$

Numerical difference functions

Formulas have been divided into sub functions to fit to page. This probably increases the computation time, so Mathcad users may wish to re-write the final function as one long expression which they can hide for a report.

Inlet particle energy

implicit interphase term, approximate. reaction term uses fluid temperature instead of particle temperature

$$Ix0pt\_0(\omega, \theta f, p, x, kx, ky, Ac) := \frac{L \cdot \rho_f(\omega_0, \theta f_{x,0}, p_0) \cdot Qr(\omega_0, \theta f_{x,0}, p_0, Ac_{x,0})}{G \cdot \rho_c \cdot Cp_c \cdot T_0}$$

$$Ix0pt(\omega, \theta f, p, x, kx, ky, Ac) := \frac{\alpha_{PF}(\omega_0, \theta f_{x,0}, p_0) \cdot \theta f_{x,0} + Ix0pt\_0(\omega, \theta f, p, x, kx, ky, Ac)}{\alpha_{PF}(\omega_0, \theta f_{x,0}, p_0)}$$

Average of X

$$Ave(X, y, kx, NR) := 2 \cdot kx^2 \cdot \sum_{i=1}^{NR} \frac{\left[X_{i,y} \cdot i + X_{i-1,y} \cdot (i-1)\right]}{2}$$

Formulas for explicit steps

interior

steady state fluid energy balance

$$Exyf(\omega, \theta f, p, \theta p2, x, y, kx, ky) := \theta f_{x,y-1} - ky \cdot \alpha_{FP} \cdot \left(\theta f_{x,y-1} - \theta p2_{x,y-1}\right) \ldots + ky \cdot \alpha_{Hf} \cdot \left(\frac{\theta f_{x,y-1} - \theta f_{x-1,y-1}}{kx^2 \cdot x} + \frac{\theta f_{x+1,y-1} - 2 \cdot \theta f_{x,y-1} + \theta f_{x-1,y-1}}{kx^2}\right)$$

steady state mass balance (1D)

$$E0yn(\omega, \theta f, p, \theta p2, y, n, kx, ky, Ac, NR) := \left(\omega_{y-1}\right)_n + ky \cdot \left(\frac{L}{G} \cdot Mw_n \cdot Rxn\left(\omega_{y-1}, Ave(\theta p2, y-1, kx, NR), p_{y-1}, Ave(Ac, y-1, kx, NR)\right)_n\right)$$

steady state pressure equation (1D)

$$E0yp(\omega, \theta f, p, y, kx, ky) := p_{y-1} - ky \cdot \left[\frac{f_k \cdot G^2 \cdot L}{d_p \cdot \rho_f\left(\omega_{y-1}, \theta f_{0,y-1}, p_{y-1}\right) \cdot Ptot} \cdot \left(\frac{1-\varepsilon}{\varepsilon^3}\right)\right]$$

dynamic particle energy balance, solving for $\theta p2$ (new time step) at x and y with θp from previous step

$$Exypt\_0(\omega, \theta f, p, \theta p, x, y, h, kx, ky, Ac) := h \cdot \alpha_{Hp}\left(\omega_y, \theta f_{x,y}, p_y\right) \cdot \left(\frac{\theta p_{x,y} - \theta p_{x-1,y}}{kx^2 \cdot x} + \frac{\theta p_{x+1,y} - 2 \cdot \theta p_{x,y} + \theta p_{x-1,y}}{kx^2}\right)$$

$$Exypt\_1(\omega, \theta f, p, \theta p, x, y, h, kx, ky, Ac) := h \cdot \alpha_{PF}\left(\omega_y, \theta f_{x,y}, p_y\right) \cdot \left(\theta f_{x,y} - \theta p_{x,y}\right)$$

$$Exypt\_2(\omega, \theta f, p, \theta p, x, y, h, kx, ky, Ac) := \frac{h \cdot L \cdot \rho_f\left(\omega_y, \theta f_{x,y}, p_y\right)}{G \cdot \rho_c \cdot Cp_c} \cdot \frac{Qr\left(\omega_y, \theta p_{x,y}, p_y, Ac_{x,y}\right)}{T_0}$$

$$Exypt(\omega,\theta f,p,\theta p,x,y,h,kx,ky,Ac) := \theta p_{x,y} + Exypt\_0(\omega,\theta f,p,\theta p,x,y,h,kx,ky,Ac) \ldots$$
$$+ Exypt\_1(\omega,\theta f,p,\theta p,x,y,h,kx,ky,Ac) \ldots$$
$$+ Exypt\_2(\omega,\theta f,p,\theta p,x,y,h,kx,ky,Ac)$$

Centerline

steady state fluid energy balance

$$E0yf(\omega,\theta f,p,\theta p,y,kx,ky) := \theta f_{0,y-1} - ky \cdot \alpha_{FP} \cdot \left(\theta f_{0,y-1} - \theta p_{0,y-1}\right)$$

dynamic particle energy balance

$$E0ypt(\omega,\theta f,p,\theta p,y,h,kx,ky,Ac) := \theta p_{0,y} \ldots$$
$$+ h \cdot \alpha_{PF}\left(\omega_y,\theta f_{0,y},p_y\right) \cdot \left(\theta f_{0,y} - \theta p_{0,y}\right) \ldots$$
$$+ \frac{h \cdot L \cdot \rho_f\left(\omega_y,\theta f_{0,y},p_y\right)}{G \cdot \rho_c \cdot Cp_c} \cdot \frac{Qr\left(\omega_y,\theta p_{0,y},p_y,Ac_{0,y}\right)}{T_0}$$

Wall

steady state fluid energy balance

$$ERyf(\omega,\theta f,p,\theta p,NR,y,kx,ky) := \theta f_{NR,y-1} - ky \cdot \alpha_{FP} \cdot \left(\theta f_{NR,y-1} - \theta p_{NR,y-1}\right)$$

dynamic particle energy balance

$$ERypt(\omega,\theta f,p,\theta p,NR,y,h,kx,ky,Ac) := \theta p_{NR,y} \ldots$$
$$+ h \cdot \alpha_{PF}\left(\omega_y,\theta f_{NR,y},p_y\right) \cdot \left(\theta f_{NR,y} - \theta p_{NR,y}\right) \ldots$$
$$+ \frac{h \cdot L \cdot \rho_f\left(\omega_y,\theta f_{NR,y},p_y\right) \cdot Qr\left(\omega_y,\theta p_{NR,y},p_y,Ac_{NR,y}\right)}{G \cdot \rho_c \cdot Cp_c \cdot T_0}$$

Formulas for implicit steps

Interior

steady state fluid energy balance

$$Ixyf(\omega, \theta f, p, \theta p2, x, y, kx, ky) := \frac{\theta f_{x,y-1} + \frac{ky \cdot \alpha_{Hf}}{kx^2} \cdot \theta f_{x+1,y} + \alpha_{Hf} \cdot \left(\frac{ky}{kx^2} - \frac{ky}{kx^2 \cdot x}\right) \cdot \theta f_{x-1,y} + ky \cdot \alpha_{FP} \cdot \theta p2_{x,y}}{1 - \frac{ky \cdot \alpha_{Hf}}{kx^2 \cdot x} + 2 \cdot \frac{ky \cdot \alpha_{Hf}}{kx^2} + ky \cdot \alpha_{FP}}$$

dynamic particle energy balance

$$Ixypt\_0(\theta p2, \omega, \theta f, p, x, y, h, kx, ky, Ac) := h \cdot \alpha_{Hp}\left(\omega_y, \theta f_{x,y}, p_y\right) \cdot \left(\frac{\theta p2_{x+1,y}}{kx^2} + \frac{\theta p2_{x-1,y}}{kx^2} - \frac{\theta p2_{x-1,y}}{kx^2 \cdot x}\right)$$

$$Ixypt\_1(\theta p2, \omega, \theta f, p, x, y, h, kx, ky, Ac) := h \cdot \alpha_{PF}\left(\omega_y, \theta f_{x,y}, p_y\right) \cdot \theta f_{x,y}$$

$$Ixypt\_2a(\theta p2, \omega, \theta f, p, x, y, h, kx, ky, Ac) := \frac{h \cdot L \cdot \rho_f\left(\omega_y, \frac{\theta f_{x+1,y} + \theta f_{x-1,y}}{2}, p_y\right)}{G \cdot \rho_c \cdot Cp_c \cdot T_0}$$

$$Ixypt\_2b(\theta p2, \omega, \theta f, p, x, y, h, kx, ky, Ac) := Qr\left(\omega_y, \frac{\theta p2_{x+1,y} + \theta p2_{x-1,y}}{2}, p_y, \frac{Ac_{x+1,y} + Ac_{x-1,y}}{2}\right)$$

$$Ixypt\_2(\theta p2, \omega, \theta f, p, x, y, h, kx, ky, Ac) := Ixypt\_2a(\theta p2, \omega, \theta f, p, x, y, h, kx, ky, Ac) \cdot Ixypt\_2b(\theta p2, \omega, \theta f, p, x, y, h, kx, ky, Ac)$$

$$\begin{aligned} Ixypt\_N(\theta p2, \omega, \theta f, \theta p, p, x, y, h, kx, ky, Ac) := {} & \theta p_{x,y} + Ixypt\_0(\theta p2, \omega, \theta f, p, x, y, h, kx, ky, Ac) \ldots \\ & + Ixypt\_1(\theta p2, \omega, \theta f, p, x, y, h, kx, ky, Ac) \ldots \\ & + Ixypt\_2(\theta p2, \omega, \theta f, p, x, y, h, kx, ky, Ac) \end{aligned}$$

$$Ixypt\_D(\theta p2,\omega,\theta f,p,x,y,h,kx,ky,Ac) := 1 + h\cdot\alpha_{PF}\left(\omega_y,\theta f_{x,y},p_y\right) \dots$$
$$+ h\cdot\alpha_{Hp}\left(\omega_y,\theta f_{x,y},p_y\right)\left(\frac{2}{kx^2}-\frac{1}{kx^2\cdot x}\right)$$

$$Ixypt(\theta p2,\omega,\theta f,\theta p,p,x,y,h,kx,ky,Ac) := \frac{Ixypt\_N(\theta p2,\omega,\theta f,\theta p,p,x,y,h,kx,ky,Ac)}{Ixypt\_D(\theta p2,\omega,\theta f,p,x,y,h,kx,ky,Ac)}$$

Centerline

$$I0yf(\theta f,y,kx,ky) := \theta f_{1,y}$$ fluid energy boundary condition

$$I0ypt(\theta p2,y,h,kx,ky) := \theta p2_{1,y}$$ dynamic particle energy boundary condition

Wall

$$IRyf(\theta f,NR,y,kx,ky,Tw) := \frac{\theta f_{NR-1,y} + kx\cdot Biw\cdot Tw}{1 + kx\cdot Biw}$$ fluid energy boundary condition

$$IRypt(\theta p2,NR,y,h,kx,Tw) := \frac{\theta p2_{NR-1,y} + kx\cdot Biw\cdot Tw}{1 + kx\cdot Biw}$$ dynamic particle energy boundary condition

$Dyn\_g(Cf, Tf, IT, IM, Tw, Ac, NR, NY, v, tf) :=$

"Dynamics of a 2D Reactor"

$brk \leftarrow 0$

"Tmax is the maximum dimensionless temperature allowed"

$Tmax \leftarrow 10$

"NR and NY must be even integers"

$$kx \leftarrow \frac{1}{NR}$$

$$ky \leftarrow \frac{1}{NY}$$

$$h \leftarrow ky \cdot \frac{\rho_c \cdot Cp_c}{\rho_f(Cf, Tf(0), 1) \cdot Cp(Cf, Tf(0))}$$

"compute the number of time steps between each save"

$$NSave \leftarrow max\left(trunc\left(\frac{4 \cdot tf}{h \cdot NY}\right), 1\right)$$

$$NSave \leftarrow NSave \quad if \quad trunc\left(\frac{NSave}{2}\right) \cdot 2 = NSave$$

$$NSave \leftarrow NSave + 1 \quad otherwise$$

"initial conditions"

$for \quad y \in 0 .. NY$

- $\omega_y \leftarrow IM$
- $for \quad x \in 0, 1 .. NR$
  - $\theta f_{x,y} \leftarrow IT$
  - $\theta p_{x,y} \leftarrow IT$

$p_0 \leftarrow 1$

$for \quad y \in 1 .. NY$

- $p_y \leftarrow E0yp(\omega, \theta f, p, y, kx, ky)$

""

$\theta p2 \leftarrow \theta p$

"initialize the output matrices"

$\Omega_0 \leftarrow \omega$

$\Theta f_0 \leftarrow \theta f$

$\Theta p_0 \leftarrow \theta p$

$P_0 \leftarrow p$

"r is the time step number for the heat balance"

$r \leftarrow 0$

$tv_0 \leftarrow 0$

$t \leftarrow 0$

$k \leftarrow 0$

$while\ \ t < tf$

"Solve the heat balance for one time step"

$for\ \ n \in 0 .. NC - 1$

$\left(\omega_0\right)_n \leftarrow Cf_n$

$for\ \ x \in 0, 1 .. NR$

$\theta f_{x,0} \leftarrow Tf\left(t \cdot \frac{L}{v}\right)$

$\theta p2_{x,0} \leftarrow \theta f_{x,0}$

"Use simi-implicit step at inlet for particle temperature"

$for\ \ x \in 0 .. NR$

$\theta p2_{x,0} \leftarrow Ix0pt(\omega, \theta f, p, x, kx, ky, Ac)$

"βh is the even-odd indicator for the heat balance step"

$\beta h \leftarrow if\left(trunc\left(\frac{r}{2}\right) \cdot 2 = r, 1, 0\right)$

""

$if\ \ \beta h = 1$

"Because of the inlet condition, the y index will start at 1."

"explicit step: (odd y +odd x) and (even y + even x)"

$for\ \ y \in 1, 3 .. NY - 1$

$for\ \ x \in 1, 3 .. NR - 1$

$\theta p2_{x,y} \leftarrow Exypt(\omega, \theta f, p, \theta p, x, y, h, kx, ky, Ac)$

$for\ \ y \in 2, 4 .. NY$

$\theta p2_{0,y} \leftarrow E0ypt(\omega, \theta f, p, \theta p, y, h, kx, ky, Ac)$

$for\ \ x \in 2, 4 .. NR - 2$

$\theta p2_{x,y} \leftarrow Exypt(\omega, \theta f, p, \theta p, x, y, h, kx, ky, Ac)$

$\theta p2_{NR,y} \leftarrow ERypt(\omega, \theta f, p, \theta p, NR, y, h, kx, ky, Ac)$

"implicit step: (odd y + even x) and (even y + odd x)"

$for\ \ y \in 1, 3 .. NY - 1$

$\theta p2_{0,y} \leftarrow I0ypt(\theta p2, y, h, kx, ky)$

$for\ \ x \in 2, 4 .. NR - 2$

$\theta p2_{x,y} \leftarrow Ixypt(\theta p2, \omega, \theta f, \theta p, p, x, y, h, kx, ky, Ac)$

"page break"

$\theta p2_{NR,y} \leftarrow IRypt\left(\theta p2, NR, y, h, kx, Tw\left(t \cdot \frac{L}{v}\right)\right)$

$for\ \ y \in 2, 4 .. NY$

$for\ \ x \in 1, 3 .. NR - 1$

$\theta p2_{x,y} \leftarrow Ixypt(\theta p2, \omega, \theta f, \theta p, p, x, y, h, kx, ky, Ac)$

$if\ \ \beta h = 0$

"explicit step: (odd y + even x) and (even y + odd x)"

$for\ \ y \in 1, 3 .. NY - 1$

$\theta p2_{0,y} \leftarrow E0ypt(\omega, \theta f, p, \theta p, y, h, kx, ky, Ac)$

$for\ x \in 2, 4 .. NR - 2$

$\theta p2_{x,y} \leftarrow Exypt(\omega, \theta f, p, \theta p, x, y, h, kx, ky, Ac)$

$\theta p2_{NR,y} \leftarrow ERypt(\omega, \theta f, p, \theta p, NR, y, h, kx, ky, Ac)$

$for\ y \in 2, 4 .. NY$

$for\ x \in 1, 3 .. NR - 1$

$\theta p2_{x,y} \leftarrow Exypt(\omega, \theta f, p, \theta p, x, y, h, kx, ky, Ac)$

"implicit step: (odd y + odd x) and (even y + even x)"

$for\ y \in 1, 3 .. NY - 1$

$for\ x \in 1, 3 .. NR - 1$

$\theta p2_{x,y} \leftarrow Ixypt(\theta p2, \omega, \theta f, \theta p, p, x, y, h, kx, ky, Ac)$

$for\ y \in 2, 4 .. NY$

$\theta p2_{0,y} \leftarrow I0ypt(\theta p2, y, h, kx, ky)$

$for\ x \in 2, 4 .. NR - 2$

$\theta p2_{x,y} \leftarrow Ixypt(\theta p2, \omega, \theta f, \theta p, p, x, y, h, kx, ky, Ac)$

"page break"

$$\theta p2_{NR,y} \leftarrow IRypt\left(\theta p2, NR, y, h, kx, Tw\left(t \cdot \frac{L}{v}\right)\right)$$

"Solve fluid balances (mass and energy) at the new time step"

"a 2D cylinder at steadystate for temperature and 1D steadystate for mass"

$for\ y \in 1 .. NY$

$p_y \leftarrow E0yp(\omega, \theta f, p, y, kx, ky)$

$for\ n \in 0 .. NC - 1$

$\left(\omega_y\right)_n \leftarrow E0yn(\omega, \theta f, p, \theta p2, y, n, kx, ky, Ac, NR)$

"βm is the even-odd indicator for the steady state steps"

$$\beta m \leftarrow if\left(trunc\left(\frac{y}{2}\right) \cdot 2 = y, 1, 0\right)$$

$if\ \ \beta m = 1$

"explicit step for even locations"

$\theta f_{0,y} \leftarrow E0yf(\omega, \theta f, p, \theta p2, y, kx, ky)$

$\theta f_{NR,y} \leftarrow ERyf(\omega, \theta f, p, \theta p2, NR, y, kx, ky)$

$for\ \ x \in 2, 4 .. NR - 2$

$\quad \theta f_{x,y} \leftarrow Exyf(\omega, \theta f, p, \theta p2, x, y, kx, ky)$

"implicit step for odd locations"

$for\ \ x \in 1, 3 .. NR - 1$

$\quad$ "page break"

$\quad \theta f_{x,y} \leftarrow Ixyf(\omega, \theta f, p, \theta p2, x, y, kx, ky)$

$if\ \ \beta m = 0$

"explicit step for odds"

$for\ \ x \in 1, 3 .. NR - 1$

$\quad \theta f_{x,y} \leftarrow Exyf(\omega, \theta f, p, \theta p2, x, y, kx, ky)$

"implicit step for evens"

$\theta f_{0,y} \leftarrow I0yf(\theta f, y, kx, ky)$

$$\theta f_{NR,y} \leftarrow IRyf\left(\theta f, NR, y, kx, ky, Tw\left(t \cdot \frac{L}{v}\right)\right)$$

$for\ \ x \in 2, 4 .. NR - 2$

$\quad \theta f_{x,y} \leftarrow Ixyf(\omega, \theta f, p, \theta p2, x, y, kx, ky)$

$\theta p \leftarrow \theta p2$

$t \leftarrow t + h$

$$if\ \ trunc\left(\frac{r}{NSave}\right) \cdot NSave = r$$

$k \leftarrow k + 1$

$\Omega_k \leftarrow \omega$

""

$\Theta f_k \leftarrow \theta f$

$\Theta p_k \leftarrow \theta p$

$P_k \leftarrow p$

$tv_k \leftarrow t$

$for\ \ y \in 1..NY$

$brk \leftarrow 1\ \ if\ \ \theta f_{0,y} \geq Tmax$

$break\ \ if\ \ brk = 1$

$r \leftarrow r + 1$

$(\Omega\ \ \Theta f\ \ \Theta p\ \ P\ \ h\ \ tv\ \ brk)$

$NR := 6$ last radial position for tubular reactor, must be even number

$n := 0..NC - 1$

$NZ := 1000$ last axial position, must be even number
NZ may need to be increased if results are unstable or error occurs
use the NR and NZ used with *Rxt_2D_ss* if it has been used for your problem

$kx := \frac{1}{NR}$ $ky := \frac{1}{NZ}$

Integration of the model

Initial conditions

$IT := Tw(0)$ temperatures are set to jacket (wall) temperature

$$IM := \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

initial mass fractions in reactor

$$\sum IM = 1$$

radial range index

$i := 0 .. NR$

axial range index

$j := 0 .. NZ$

$Ac_{i,j} := 1$ activity profile

$v_0 := v\left(\omega_0, Tf(0), p_0\right)$ velocity at inlet

$$\frac{L}{v_0} \cdot \frac{\rho_c \cdot Cp_c}{\rho_f\left(\omega_0, Tf(0), p_0\right) \cdot Cp\left(\omega_0, Tf(0)\right)} = 3.683 \cdot min$$

time to steady state affected by catalyst heat capacity and advection rate of energy

$tend := 10 \cdot min$ simulation end time

$\tau_f := tend \cdot \dfrac{v_0}{L}$ dimensionless end time

$time1 := time(0)$ monitor computation time

$$(\Omega \;\; \Theta f \;\; \Theta p \;\; P \;\; h \;\; tv \;\; break) := Dyn\_g\left(\omega_0, Tf, IT, IM, Tw, Ac, NR, NZ, v_0, \tau_f\right)$$

$time2 := time(0)$

$calc\_time := time2 - time1$

$calc\_time = 871.339$ seconds $h = 0.235$ dimensionless time step used

$break = 0$

Results

$NT := rows(\Omega) - 1$ $NT = 272$

$k := 0 .. NT$ time range index

$r_i := \frac{i}{NR}$ radial fraction $z_j := \frac{j}{NZ}$ axial fraction $t_k := tv_k \cdot \frac{L}{v_0}$ time

$comp := 0$ selected component number for plots

$vel(i, j, k) := v\left[\left(\Omega_k\right)_j, \left(\Theta f_k\right)_{i,j}, \left(P_k\right)_j\right]$ velocity

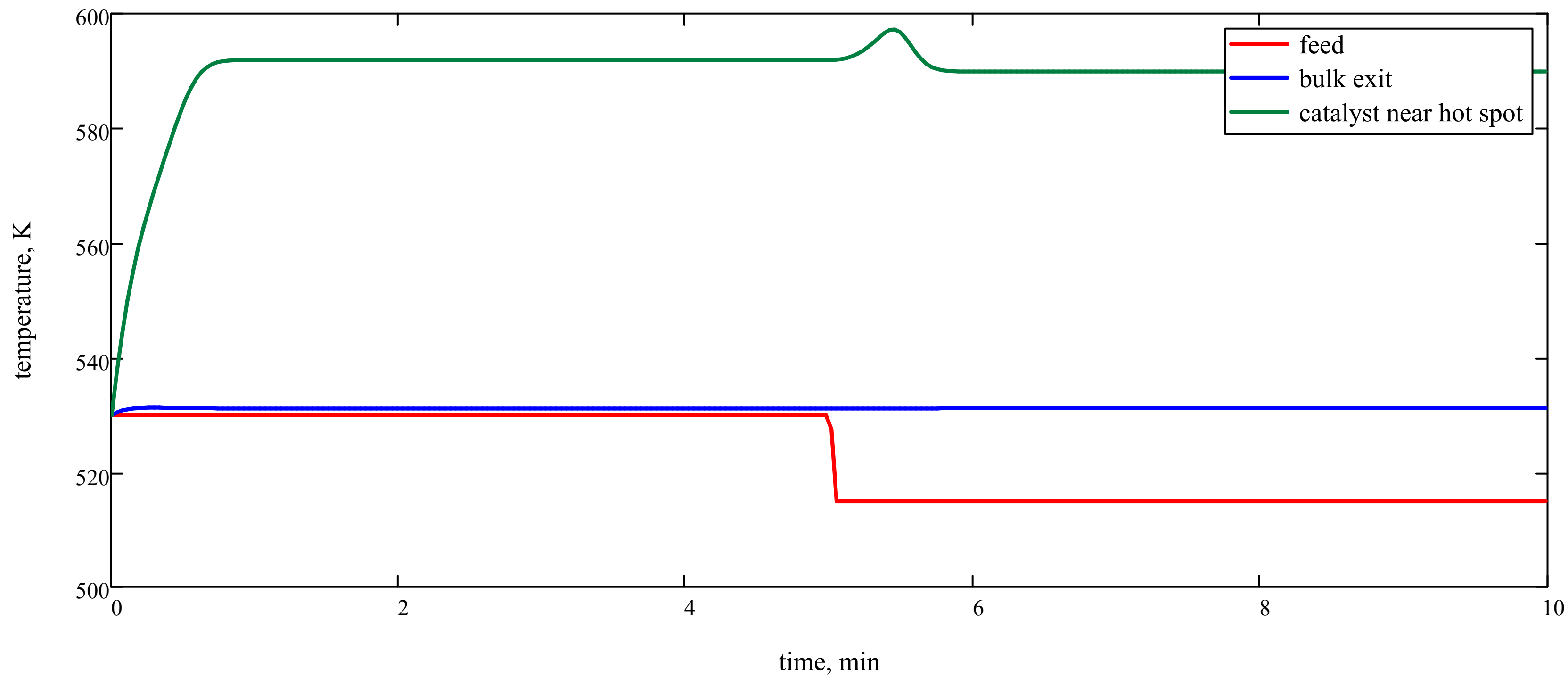
Radial average velocity

$$v_{ave_{j,k}} := 2 \cdot kx^2 \cdot \left[\sum_{i=1}^{NR} \frac{[vel(i, j, k) \cdot i + vel(i-1, j, k) \cdot (i-1)]}{2}\right]$$

Mixing cup (bulk) gas temperature

$$T_{b_{j,k}} := \frac{2 \cdot kx^2 \cdot \sum_{i=1}^{NR} \frac{(\Theta f_k)_{i,j} \cdot vel(i,j,k) \cdot i + (\Theta f_k)_{i-1,j} \cdot vel(i-1,j,k) \cdot (i-1)}{2}}{v_{ave_{j,k}}}$$

Fig E11.3: Dynamic Temperatures



The "wrong way" behavior shown by the rise in the green curve for the hot spot is very minor for this example. The heat transfer at the wall moderates much of the dynamics imposed at the inlet.

axial profiles near the halfway point in time

Fig E11.4: Averge Wt Fraction of "comp"

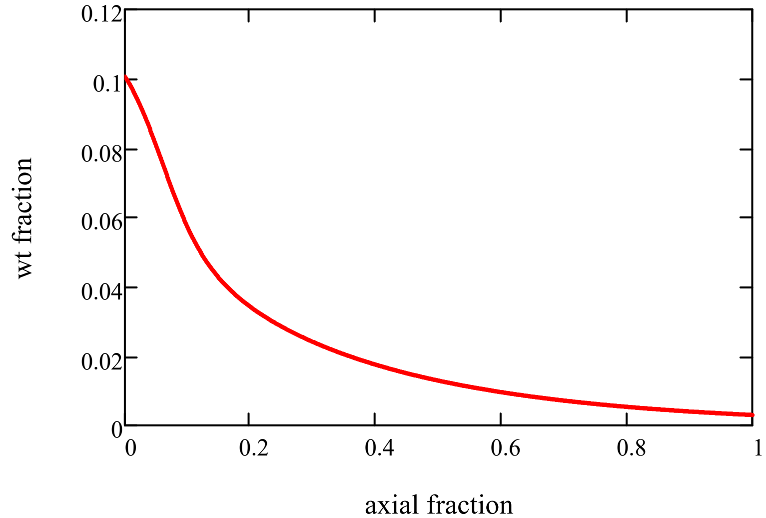
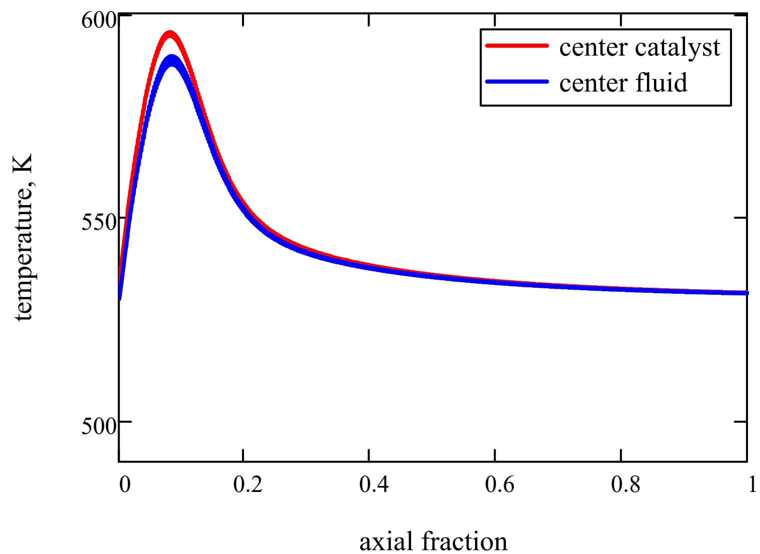


Fig E11.5: Temperatures



The peak centerline catalyst temperature before the change in feed temperature is 595 K. This result is 15 K higher than the peak temperature calculated in Example 7 with the steady state model using the collocation method. Comparisons with a simple system also resulted in lower peak temperatures with the collocation method.

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