Example 12: Fixed bed reactors for liquids (dynamic)

A Simple Reaction System

An example modified from one by Parulekar (2007) which was modified from one by Folger (1999)

A --> B	reaction 0
B --> C	reaction 1

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

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

dynamic fluid energy balance

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

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

where

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

dynamic mass balance (1D)

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

B.C. $\omega(0, 0) := \omega_0$ ω_0 could be a function of time but it is not in this example

where θp_{ave} = radial average of particle temperatures

Data from Example 8 are included in the collapsed area below.

Dynamic forcing functions

cubic transition function

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

feed temperature

$$temp := \frac{T_f + 50\Delta°C}{T_0}$$

$$Tin := \begin{pmatrix} temp \\ temp - \frac{10\Delta°C}{T_0} \end{pmatrix}$$ feed temperature

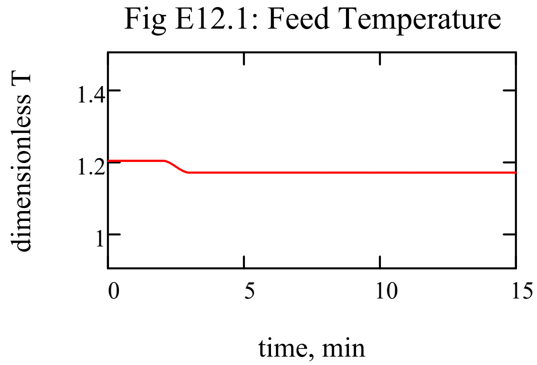
wall temperature not used for this adiabatic case

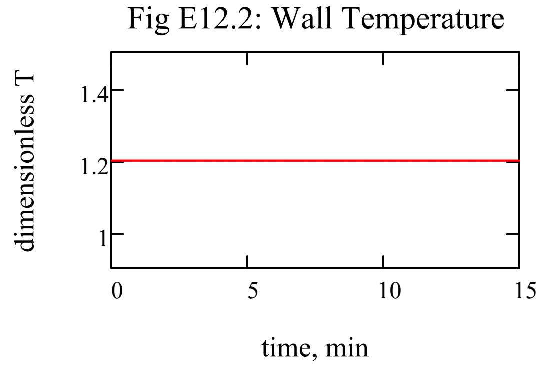
$$Twall := temp$$

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

$$Tf(t) := SR(t, 2\cdot min, Tin_0, 3\cdot min, Tin_1)$$

$$Tw(t) := SR(t, 10\cdot min, Tj_0, 15\cdot min, Tj_1)$$





Correlations for heat and mass transfer parameters, liquid systems

$$\rho_f := \rho f(\omega_0, \theta_0, 1)$$

density is constant for liquids so a new variable without arguments is used in this model

$$Rey_p := \frac{G \cdot d_p}{\mu(T_0)}$$ Reynolds number $Rey_p = 125$

$$Pr := \frac{Cp(\omega_0, \theta_0) \cdot \mu(T_0)}{k_f}$$ Prandtl number $Pr = 15.509$

$$v := \frac{G}{\rho_f}$$ velocity $v = 0.05\frac{m}{s}$

$$Sc := \frac{\mu(T_0)}{\rho_f \cdot D_f}$$ Schmidt number $Sc = 1 \times 10^3$

$$Gr := g \cdot B \cdot d_p^{\,3} \cdot 2 \cdot K \cdot \left(\frac{\rho_f}{\mu(T_0)}\right)^2$$ Grashof number $Gr = 61.292$

Ergun equation parameters

MacDonald et al (1979)

$\alpha_P := 180$ $\beta_P := if(smooth = \text{"yes"}, 1.8, 4.0)$ $f_k := \beta_P + \alpha_P \cdot \frac{(1-\varepsilon)}{Rey_p}$

The parameter correlations below may be used for long, industrial reactors. Assume that "long" means 5 ft or longer.

wall heat transfer coefficients

Li and Finlayson (1977)

This correlation was developed with gases, but no correlation for liquids has been found. The pilot plant should therefore be used to determine a better estimate for h_w. The forms below may be used as a framework, with the data used to update the leading coefficient and the power of Rey_p.

case values: $Rey_p = 125$ $\frac{d_p}{D_t} = 0.122$

$$h_{w\_cyl} := .18 \cdot Rey_p^{0.93} \cdot Pr^{\frac{1}{3}} \cdot \frac{k_f}{d_p}$$ for $20 \le Rey_p \le 800$ and $.03 \le \frac{d_p}{D_t} < .3$

$$h_{w\_sph} := .19 \cdot Rey_p^{0.79} \cdot Pr^{\frac{1}{3}} \cdot \frac{k_f}{d_p}$$ for $20 \le Rey_p \le 7600$ and $.05 \le \frac{d_p}{D_t} < .2$

$$h_w := if\left(shape = \text{"cylinder"}, h_{w\_cyl}, h_{w\_sph}\right)$$

catalyst effective radial conductivity

$$k_{es} := (1-\varepsilon) \cdot k_s$$

conductivity of catalyst phase

effective radial thermal dispersion coefficient of fluid in heterogeneous model

The correlation by Yagi and Kunii (1960) as shown in Himmelblau and Bischoff (1968) is used below. The catalyst phase contribution to the stagnant term has been excluded for this heterogeneous model.

$$a := 0.2 - .7 \cdot \frac{d_p}{D_t}$$

Fig A.6 in Himmelblau and Bischoff, cylinders curve

$$k_{ef} := k_f \cdot \varepsilon \cdot \left(1 + a \cdot Pr \cdot Rey_p\right)$$

Biot number for wall heat transfer

$$Bi_w := \frac{h_w \cdot Ri}{k_{ef} + k_{es}}$$

$$Bi := if\left(adiabatic, 0, Bi_w\right)$$

no heat transfer at wall if adiabatic

effective radial mass diffusivity

The function below was derived from curves for liquids in Fig A.4 in Himmelblau and Bischoff (1968).

$$D_e := \frac{v \cdot d_p}{\varepsilon} \cdot \left[10^{\left(-0.2 \cdot log\left(\frac{Rey_p}{\varepsilon}\right) - 1.1\right)} \right]$$

for $.01 \le \frac{Rey_p}{} \le 20$

but D_e and the range for $\frac{Rey_p}{\varepsilon}$ may not be critical

particle to fluid heat transfer coefficient

Baptista et al (1997) liquids

$$Nu_s := 2 + 0.025 \cdot Pr^{\frac{1}{3}} \cdot Gr^{\frac{1}{2}}$$

static liquid Nusselt number

$$h_s := \frac{k_f}{d_p} \cdot \left(Nu_s + .20 \cdot Pr^{.38} \cdot Rey_p^{.67}\right)$$

for $\left(Rey_p \le 800\right)$ $69 \le Pr \le 1810$

$2.8 \le Gr \le 4840$

particle to fluid mass transfer coefficient

<u>for gases and liquids</u> Wakao and Kaguei correlation for h and the Colburn analogy

$$k_{sg} := \frac{D_f}{d_p} \cdot \left(2 + 1.1 \cdot Sc^{\frac{1}{3}} \cdot Rey_p^{.6}\right)$$

$$k_{sg} = 8.053 \times 10^{-5} \frac{m}{s}$$

Parameter groups used in the model equations

fluid radial energy dispersion

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

$$\alpha_{Hf} = 2.706$$

particle radial energy dispersion

$$\alpha_{Hp} := \frac{k_{es} \cdot \rho_f \cdot L}{G \cdot \rho_c \cdot Cp_c \cdot Ri^2}$$

$$\alpha_{Hp} = 2.144$$

fluid to particle heat transfer

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

$$\alpha_{FP} = 21.075$$

particle to fluid heat transfer

$$\alpha_{PF} := \frac{h_s \cdot L \cdot \rho_f \cdot a_p}{G \cdot \rho_c \cdot Cp_c}$$

$$\alpha_{PF} = 215.603$$

particle to fluid mass transfer

$$\alpha_{MFP} := \frac{k_{sg} \cdot L \cdot a_p \cdot \rho_f}{G}$$

$$\alpha_{MFP} = 3.896$$

Numerical difference functions

Formulas have been divided into sub functions to fit to page.

Inlet particle energy

implicit interphase term, approximate. reaction term

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

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

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

fluid energy balance

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

mass balance

$$Eyn\_1(\omega,\theta f,p,\theta p,y,n,h,kx,ky,A,NR) := h \cdot \left(\frac{L}{G} \cdot Mw_n \cdot Rxn\left(\omega_y, Ave(\theta p,y,kx,NR), p_y, Ave(A,y,kx,NR)\right)_n\right)$$

$$Eyn(\omega,\theta f,p,\theta p,y,n,h,kx,ky,A,NR) := \left(\omega_y\right)_n - h\cdot\frac{\left[\left(\omega_y\right)_n - \left(\omega_{y-1}\right)_n\right]}{ky} \ldots$$
$$+ Eyn\_1(\omega,\theta f,p,\theta p,y,n,h,kx,ky,A,NR)$$

steady state pressure equation, pressure does not vary radially

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

particle energy balance

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

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

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

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

centerline

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

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

wall

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

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

Formulas for implicit steps

interior

fluid energy balance

$$Ixyf\_0(\theta f,\omega 2,\theta f2,p,\theta p2,x,y,h,kx,ky,A) := h \cdot \alpha_{Hf} \cdot \left(\frac{\theta f2_{x+1,y}}{kx^2} + \frac{\theta f2_{x-1,y}}{kx^2} - \frac{\theta f2_{x-1,y}}{kx^2 \cdot x}\right)$$

$$Ixyf\_1(\theta f,\omega 2,\theta f2,p,\theta p2,x,y,h,kx,ky,A) := h \cdot \alpha_{FP} \cdot \theta p2_{x,y} + \frac{h}{ky} \cdot \theta f2_{x,y-1}$$

$$Ixyf\_N(\theta f,\omega 2,\theta f2,p,\theta p2,x,y,h,kx,ky,A) := \theta f_{x,y} + Ixyf\_0(\theta f,\omega 2,\theta f2,p,\theta p2,x,y,h,kx,ky,A) \ldots$$
$$+ Ixyf\_1(\theta f,\omega 2,\theta f2,p,\theta p2,x,y,h,kx,ky,A)$$

$$Ixyf\_D(\theta f, \omega 2, \theta f2, p, \theta p2, x, y, h, kx, ky, A) := 1 + h \cdot \alpha_{FP} + \frac{h}{ky} \; ... \\ + h \cdot \alpha_{Hf}\left(\frac{2}{kx^2} - \frac{1}{kx^2 \cdot x}\right)$$

$$Ixyf(\theta f, \omega 2, \theta f2, p, \theta p2, x, y, h, kx, ky, A) := \frac{Ixyf\_N(\theta f, \omega 2, \theta f2, p, \theta p2, x, y, h, kx, ky, A)}{Ixyf\_D(\theta f, \omega 2, \theta f2, p, \theta p2, x, y, h, kx, ky, A)}$$

particle energy balance

$$Ixypt\_0(\theta p, \omega 2, \theta f2, p, \theta p2, x, y, h, kx, ky, A) := h \cdot \alpha_{Hp} \cdot \left(\frac{\theta p2_{x+1,y}}{kx^2} + \frac{\theta p2_{x-1,y}}{kx^2} - \frac{\theta p2_{x-1,y}}{kx^2 \cdot x}\right)$$

$$Ixypt\_1(\theta p, \omega 2, \theta f2, p, \theta p2, x, y, h, kx, ky, A) := h \cdot \alpha_{PF} \cdot \theta f2_{x,y}$$

$$Ixypt\_2(\theta p, \omega 2, \theta f2, p, \theta p2, x, y, h, kx, ky, A) := \frac{h \cdot L \cdot \rho_f \cdot Qr\left(\omega 2_y, \frac{\theta p2_{x+1,y} + \theta p2_{x-1,y}}{2}, p_y, \frac{A_{x+1,y} + A_{x-1,y}}{2}\right)}{G \cdot \rho_c \cdot Cp_c \cdot T_0}$$

$$Ixypt\_N(\theta p, \omega 2, \theta f2, p, \theta p2, x, y, h, kx, ky, A) := \theta p_{x,y} + Ixypt\_0(\theta p, \omega 2, \theta f2, p, \theta p2, x, y, h, kx, ky, A) \; ... \\ + Ixypt\_1(\theta p, \omega 2, \theta f2, p, \theta p2, x, y, h, kx, ky, A) \; ... \\ + Ixypt\_2(\theta p, \omega 2, \theta f2, p, \theta p2, x, y, h, kx, ky, A)$$

$$Ixypt\_D(\theta p, \omega 2, \theta f2, p, \theta p2, x, y, h, kx, ky, A) := 1 + h \cdot \alpha_{PF} + h \cdot \alpha_{Hp}\left(\frac{2}{kx^2} - \frac{1}{kx^2 \cdot x}\right)$$

$$Ixypt(\theta p, \omega 2, \theta f2, p, \theta p2, x, y, h, kx, ky, A) := \frac{Ixypt\_N(\theta p, \omega 2, \theta f2, p, \theta p2, x, y, h, kx, ky, A)}{Ixypt\_D(\theta p, \omega 2, \theta f2, p, \theta p2, x, y, h, kx, ky, A)}$$

centerline

$I0yf\,(\theta f2, y, kx, ky) := \theta f2_{1,y}$ fluid energy boundary condition

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

wall

$IRyf\,(\theta f2, NR, y, kx, ky, Tw) := \dfrac{\theta f2_{NR-1,y} + kx \cdot Bi \cdot Tw}{1 + kx \cdot Bi}$ fluid energy boundary condition

$IRypt(\theta p2, NR, y, h, kx, Tw) := Tw$ particle energy B.C. (option 1), not used for this example

$IRypt(\theta p2, NR, y, h, kx, Tw) := \dfrac{\theta p2_{NR-1,y} + kx \cdot Bi \cdot Tw}{1 + kx \cdot Bi}$ particle energy B.C. (option 2)

$Dyn\_1(Cf, Tf, IT, IM, Tw, A, NR, NY, v, tf) :=$

"Dynamics of a 2D Reactor for Liquids"

$brk \leftarrow 0$

"Tmax is the maximum dimensionless temperature allowed, used to exit with partial results"

$Tmax \leftarrow 5$

"NR and NY must be even integers"

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

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

$h \leftarrow min\left[\varepsilon \cdot ky, ky \cdot \frac{\left(\rho_c \cdot Cp_c + \varepsilon \cdot \rho_f \cdot Cp(Cf, Tf(0))\right)}{\rho_f \cdot Cp(Cf, Tf(0))}\right]$

"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"

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

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

"pressure profile"

$p_0 \leftarrow 1$

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

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

```
ω2 ← ω
θf2 ← θf
θp2 ← θp
"initialize the output matrices"
Ω_0 ← ω
Θf_0 ← θf
Θp_0 ← θp
"r is the time step number "
r ← 0
tv_0 ← 0
t ← 0
k ← 0
while t ≤ tf
    "Solve  for one time step"
    for n ∈ 0 .. NC − 1
        (ω2_0)_n ← Cf_n
        for y ∈ 1 .. NY
            (ω2_y)_n ← Eyn(ω, θf, p, θp, y, n, h, kx, ky, A, NR)
    for x ∈ 0, 1 .. NR
        θf2_{x,0} ← Tf(t · L/v)
    "Use simi-implicit step at inlet for particle temperature"
    for x ∈ 0 .. NR
        θp2_{x,0} ← Ix0pt(ω2, θf2, p, x, kx, ky, A)
    ""
    ""
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```
"βh is the even-odd indicator for the time step"
βh ← if(trunc(r/2) · 2 = r, 1, 0)
if βh = 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 ∈ 1, 3 .. NY − 1
        for x ∈ 1, 3 .. NR − 1
            θf2[x,y] ← Exyf(ω, θf, p, θp, x, y, h, kx, ky, A)
            θp2[x,y] ← Exypt(ω, θf, p, θp, x, y, h, kx, ky, A)
    for y ∈ 2, 4 .. NY
        θf2[0,y] ← E0yf(ω, θf, p, θp, y, h, kx, ky, A)
        θp2[0,y] ← E0ypt(ω, θf, p, θp, y, h, kx, ky, A)
        "page break"
        "page break"
        for x ∈ 2, 4 .. NR − 2
            θf2[x,y] ← Exyf(ω, θf, p, θp, x, y, h, kx, ky, A)
            θp2[x,y] ← Exypt(ω, θf, p, θp, x, y, h, kx, ky, A)
        θf2[NR,y] ← ERyf(ω, θf, p, θp, NR, y, h, kx, ky, A)
        θp2[NR,y] ← ERypt(ω, θf, p, θp, NR, y, h, kx, ky, A)
    "implicit step: (odd y + even x) and (even y + odd x)"
    for y ∈ 1, 3 .. NY − 1
        θf2[0,y] ← I0yf(θf2, y, kx, ky)
        θp2[0,y] ← I0ypt(θp2, y, kx, ky)
        for x ∈ 2, 4 .. NR − 2
            θf2[x,y] ← Ixyf(θf, ω2, θf2, p, θp2, x, y, h, kx, ky, A)
```

$$\theta p2_{x,y} \leftarrow Ixypt(\theta p, \omega 2, \theta f2, p, \theta p2, x, y, h, kx, ky, A)$$

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$$\theta f2_{NR,y} \leftarrow IRyf\left(\theta f2, NR, y, h, kx, Tw\left(t \cdot \frac{L}{v}\right)\right)$$

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

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

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

$$\theta f2_{x,y} \leftarrow Ixyf(\theta f, \omega 2, \theta f2, p, \theta p2, x, y, h, kx, ky, A)$$

$$\theta p2_{x,y} \leftarrow Ixypt(\theta p, \omega 2, \theta f2, p, \theta p2, x, y, h, kx, ky, A)$$

$if\ \ \beta h = 0$

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

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

$$\theta f2_{0,y} \leftarrow E0yf(\omega, \theta f, p, \theta p, y, h, kx, ky, A)$$

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

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

$$\theta f2_{x,y} \leftarrow Exyf(\omega, \theta f, p, \theta p, x, y, h, kx, ky, A)$$

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

$$\theta f2_{NR,y} \leftarrow ERyf(\omega, \theta f, p, \theta p, NR, y, h, kx, ky, A)$$

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

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

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

$$\theta f2_{x,y} \leftarrow Exyf(\omega, \theta f, p, \theta p, x, y, h, kx, ky, A)$$

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

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

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

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

$\theta f2_{x,y} \leftarrow Ixyf(\theta f, \omega 2, \theta f2, p, \theta p2, x, y, h, kx, ky, A)$

$\theta p2_{x,y} \leftarrow Ixypt(\theta p, \omega 2, \theta f2, p, \theta p2, x, y, h, kx, ky, A)$

"page break"

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

$\theta f2_{0,y} \leftarrow I0yf(\theta f2, y, kx, ky)$

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

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

$\theta f2_{x,y} \leftarrow Ixyf(\theta f, \omega 2, \theta f2, p, \theta p2, x, y, h, kx, ky, A)$

$\theta p2_{x,y} \leftarrow Ixypt(\theta p, \omega 2, \theta f2, p, \theta p2, x, y, h, kx, ky, A)$

$$\theta f2_{NR,y} \leftarrow IRyf\left(\theta f2, NR, y, h, kx, Tw\left(t \cdot \frac{L}{v}\right)\right)$$

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

"the new values now become the old values for the next time step"

$\omega \leftarrow \omega 2$

$\theta f \leftarrow \theta f2$

$\theta p \leftarrow \theta p2$

$t \leftarrow t + h$

"page break"

"save to output at the sample time"

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

$k \leftarrow k + 1$

$\Omega_k \leftarrow \omega$

$$\Theta f_k \leftarrow \theta f$$
$$\Theta p_k \leftarrow \theta p$$
$$tv_k \leftarrow t$$
"check for extreme temperatures and exit if any found"
$$for\ \ y \in 1..NY$$
$$brk \leftarrow 1\ \ if\ \ \theta f_{0,y} > Tmax$$
$$break\ \ if\ \ brk = 1$$
$$r \leftarrow r + 1$$
$$(\Omega\ \ \Theta f\ \ p\ \ \Theta p\ \ h\ \ tv\ \ brk)$$

$nr := 8$ last radial position for tubular reactor, must be even number

$NR := if(adiabatic, 4, nr)$ use the minimum NR (4) for adiabatic reactor $NR = 4$

$n := 0..NC - 1$

$NZ := 400$ last axial position, must be even number
NZ may need to be increased if results are unstable or error occurs

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

initial conditions

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

$IM := \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$ initial mass fractions $\sum IM = 1$

radial range index

$i := 0 .. NR$

axial range index

$j := 0 .. NZ$

$A_{i,j} := .01$

activity profile

$t_{ss} := \frac{L}{v} = 0.667 \cdot min$

time to steady state

$tend := 8 \cdot min$

simulation end time

$\tau_f := tend \cdot \frac{v}{L}$

dimensionless end time

$time1 := time(0)$ monitor computation time (requires CTRL F9 or "Calculate worksheet" to reset the timers)

$$(\Omega \;\; \Theta f \;\; p \;\; \Theta p \;\; h \;\; tv \;\; break) := Dyn\_l\left(\omega_0, Tf, IT, IM, Tw, A, NR, NZ, v, \tau_f\right)$$

$time2 := time(0)$

$calc\_time := time2 - time1$

$calc\_time = 346.97$ seconds

$h = 1.24 \times 10^{-3}$ dimensionless time step used

$break = 0$ 0 = completed simulation, 1 = interrupted by high temperature

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

$NT = 101$

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

$r_i := \frac{i}{NR}$

$z_j := \frac{j}{NZ}$

$t_k := tv_k \cdot \frac{L}{v}$

$p_{NZ} = 0.931$ outlet pressure as fraction of inlet pressure

Radial average catalyst temperature

$$T_{c_{j,k}} := 2 \cdot kx^2 \cdot \left[\sum_{i=1}^{NR} \frac{\left[(\Theta p_k)_{i,j} \cdot i + (\Theta p_k)_{i-1,j} \cdot (i-1) \right]}{2} \right]$$

Mixing cup (bulk) liquid temperature

$$T_{b_{j,k}} := 2 \cdot kx^2 \cdot \left[\sum_{i=1}^{NR} \frac{(\Theta f_k)_{i,j} \cdot i + (\Theta f_k)_{i-1,j} \cdot (i-1)}{2} \right]$$

Fig E12.3: Temperature at Inlet and Outlet

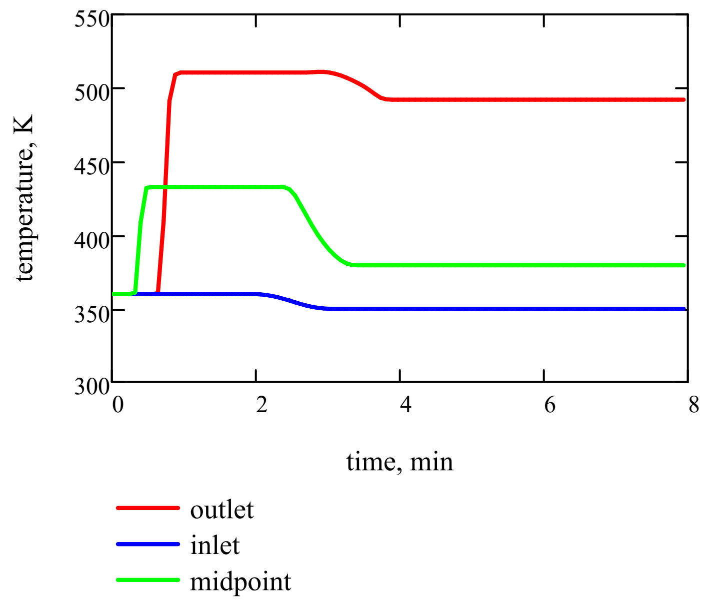
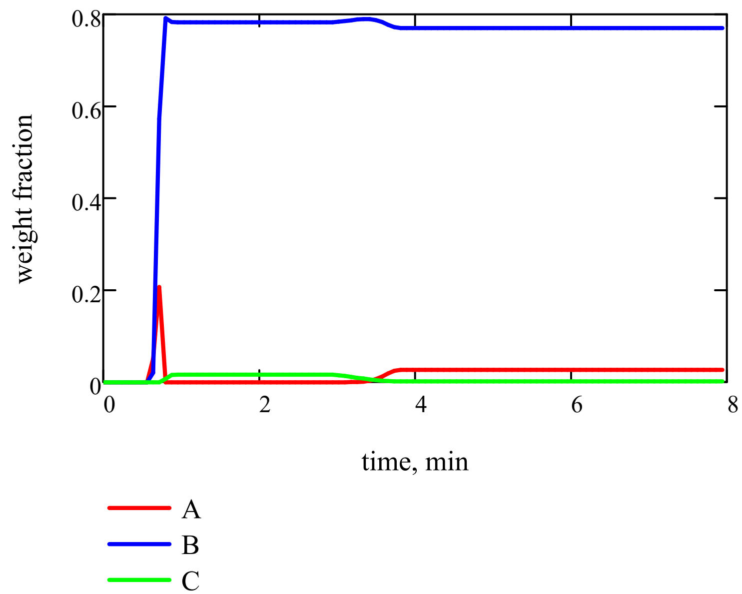


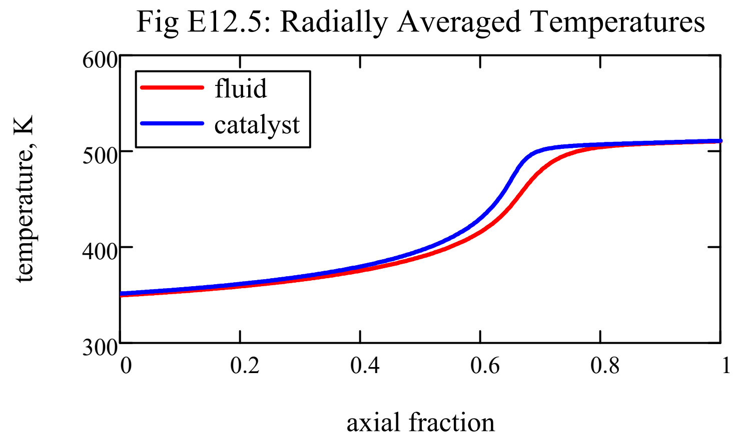
Fig E12.4: Bulk Exit Composition of A and B

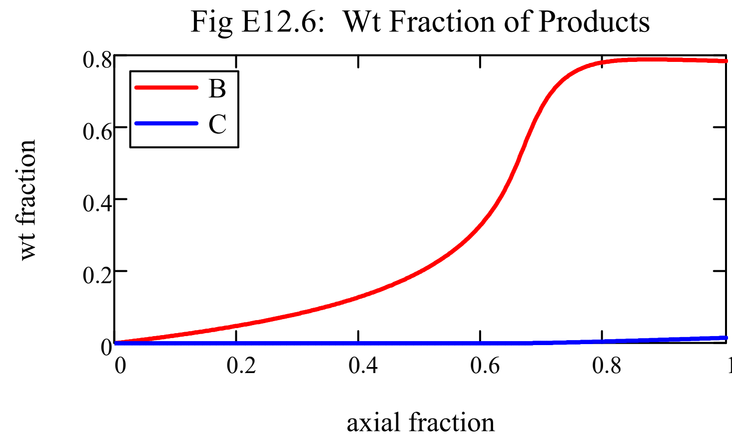


$t_{plot} := 3.1 \cdot min$ The time chosen for the plots below.

$$kk := trunc\left(\frac{t_{plot}}{t_{NT}} \cdot NT\right) = 39$$

axial profiles at $t_{kk} = 3.017 \cdot min$ ***with*** $Tin_0 \cdot T_0 = 360\,K$ ***initial feed temperature***





Summary

- This case included 20% inerts by weight. Without the inerts, the temperatures near the exit became excessive.
- The "wrong way" temperature response is not evident with this system.
- The fixed bed was effective in selectively producing the intermediate product, "B".
- The hopscotch method was effective for an adiabatic

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Exercise:

- Explore the performance of a non-adiabatic tubular reactor with a constant wall temperature.