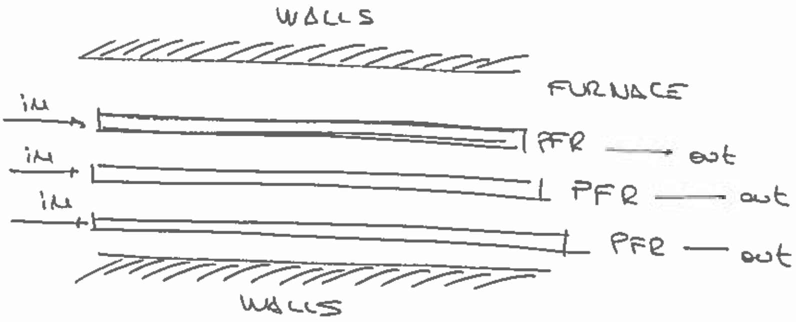
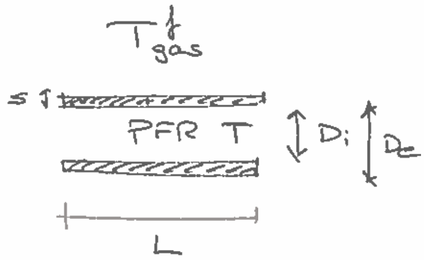
PRACTICAL SESSION 4

EXERCISE 1





$$\begin{cases} C_3H_8 \rightarrow C_2H_4 + CH_4 \\ C_3H_8 \rightarrow C_3H_6 + H_2 \end{cases}$$

endothermic reactions !
heat must be supplied from the external environment
↓
FURNACES

High temperatures → high thickness of tubes $s = 1\ cm$
because of high resistences of tubes.

2 parallel reactions
change of moles
non isothermal conditions
heat exchange with constant T external environment

$\rho \neq$ const

GOVERNING EQUATIONS

$$\begin{cases} \dfrac{d\dot{F}_i}{dz} = R_i A \\ \dot{m}_{TOT} \hat{C}_p \dfrac{dT}{dz} = A\left(\dot{Q}_R + U_i\left(T_{gas}^{f} - T\right)\dfrac{4}{D_i}\right) \end{cases}$$

$$A = \frac{\pi D_i^2}{4}$$

$$\dot{m}_{TOT} \hat{C}_p = \dot{F}_{tot} \tilde{C}_p$$

$$\dot{Q}_R = \text{heat release} = -\sum_{j=1}^{2} \widetilde{\Delta H}_j^R r_j = -\sum_{j=1}^{NS} \tilde{H}_j R_j$$

negative because the reactions are endothermic

HEAT EXCHANGE

$$\frac{1}{UA} = \frac{1}{h_i A_i} + \frac{1}{h_e A_e} + \frac{s}{K_{wall} A_{ln}}$$

$$\begin{cases} A_i = \pi D_i L \\ A_e = \pi D_e L \\ A_{ln} = \dfrac{A_e - A_i}{\ln \frac{A_e}{A_i}} = \dfrac{\pi L (D_e - D_i)}{\ln \frac{D_e}{D_i}} \end{cases}$$

$$\frac{1}{U_i A_i} = \frac{1}{h_i A_i} + \frac{1}{h_e A_e} + \frac{s}{K_w} \frac{1}{A_{ln}} =$$

$$\Rightarrow \quad \frac{1}{U_i} = \frac{1}{h_i} + \frac{D_i}{h_e D_e} + \frac{s}{K_w} \frac{D_i}{\frac{D_e - D_i}{\ln \frac{D_e}{D_i}}}$$

$$\frac{1}{U_i} = \frac{1}{h_i} + \frac{1}{h_e} \frac{D_i}{D_e} + \frac{s}{K_w} \frac{D_i}{D_e - D_i} \ln \frac{D_e}{D_i}$$

$$\frac{1}{U_e} = \frac{1}{h_i} \frac{D_e}{D_i} + \frac{1}{h_e} + \frac{s}{K_w} \frac{D_e}{D_e - D_i} \ln \frac{D_e}{D_i}$$

$$U_i D_i = U_e D_e \longrightarrow U_i = U_e \frac{D_e}{D_i}$$

O.D. EQUATIONS

6 equations for species

1 equation for T

$$\begin{cases} \dfrac{d\dot{F}_i}{dz} = R_i A \\ \\ \dfrac{dT}{dz} = \dfrac{A \left[\dot{Q}_R + U_i (T_{gas}^f - T) \, 4/D_i \right]}{\dot{m}_{TOT} \, \hat{C}_p} \end{cases}$$

$\oplus$

initial conditions

$$\begin{cases} \dot{F}_i (z=0) = \dot{F}_i^{in} \\ T(z=0) = T_{in} \end{cases}$$

FORMATION RATES OF SPECIES

$$\begin{cases} R_{C_3H_8} = -r_1 - r_2 \\ R_{C_2H_4} = +r_1 \\ R_{CH_4} = +r_1 \\ R_{C_3H_6} = +r_2 \\ R_{H_2} = +r_2 \\ R_{H_2O} = 0 \end{cases}$$

$$\begin{cases} r_1 = K_1 \cdot C_{C_3H_8} \\ r_2 = K_2 \, C_{C_3H_8} \end{cases}$$

REACTION RATES

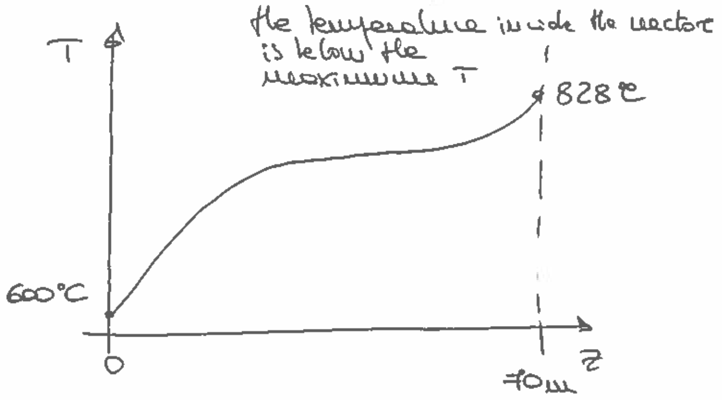
INTERNAL HEAT EXCHANGE COEFFICIENT

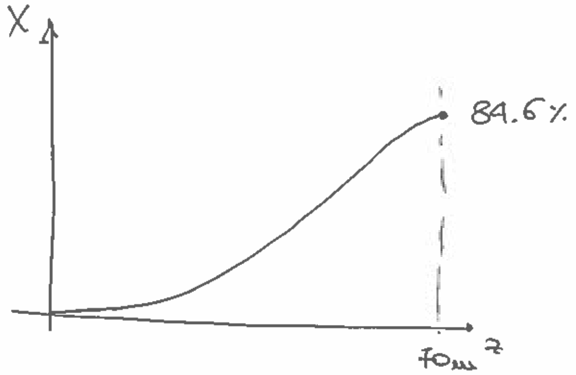
$$h_i = \frac{Nu_i \cdot \lambda_{mix}}{D_i}$$

$$Nu_i = 0.023\, Re^{0.80} \cdot Pr^{1/3}$$

DITTUS-BOELTER CORRELATION

$$Re = \frac{\rho v D_i}{\mu_{mix}} \qquad Pr = \frac{\nu}{\alpha} = \frac{\mu_{mix}}{\hat{C}p\, \lambda_{mix}}$$

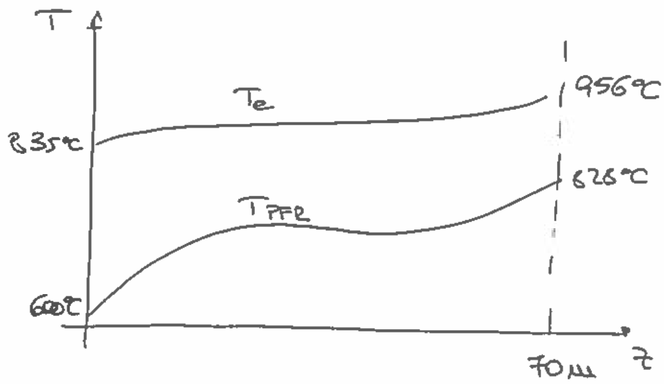




Estimation of temperature of external surface of PFR (which has to be < Tmax)

$$U_i \cdot \pi D_i L \left(T_{gas}^{f} - T\right) = h_e \cdot \pi D_e L \cdot \left(T_g^{f} - T_e\right)$$

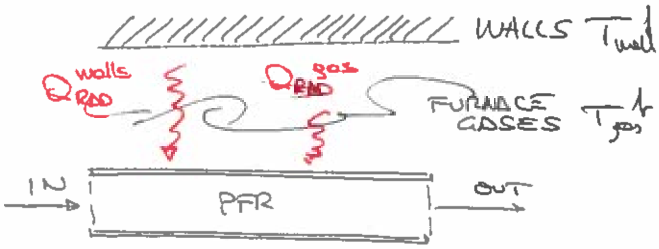
$$T_e(z) = T_{gas}^{f} - \frac{U_i D_i}{h_e D_e}\left(T_{gas}^{f} - T(z)\right)$$



The external wall temperature is below the maximum!

✓

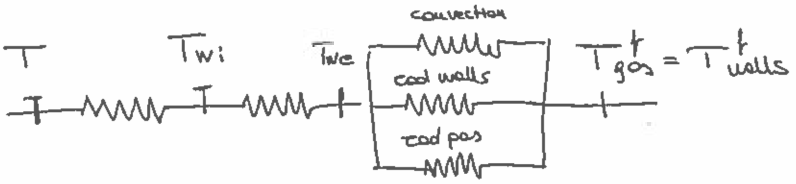
EXERCISE 2 / EXERCISE 3



two additional contributions have to be accounted for

– radiation from the ~~surface~~ walls of the furnace

– radiation from the gas in the furnace



$$\begin{cases} Q^{rad}_{wall} = F\sigma\varepsilon\left(T_f^{wall\,4} - T_e^4\right)\cdot A_e \\ Q^{rad}_{gas} = \beta\left(T_f^{gas\,4} - T_e^4\right)\cdot A_e \end{cases}$$

continuity of fluxes

$$Q_{conv} + Q^{gas}_{rad} + Q^{walls}_{rad} = Q_{int/wall}$$

$$h_e A_e\left(T^f_{gas} - T_e\right) + F\sigma\varepsilon\left(T^{f\,4}_{wall} - T_{we}^4\right)A_e + \beta A_e\left(T^{f\,4}_{gas} - T_{we}^4\right) =$$

$$= A_e \cdot U_e'\left(T_{we} - T\right)$$

$$\Rightarrow \boxed{h_e\left(T^f_{gas} - T_{we}\right) + F\sigma\varepsilon\left(T^{f\,4}_{wall} - T_{we}^4\right) + \beta\left(T^{f\,4}_{gas} - T_{we}^4\right) = U_e'\left(T_{we} - T\right)}$$

! non linear equation in T_{we}

$$\frac{1}{U_e' A_e} = \frac{1}{h_i A_i} + \frac{s}{\lambda_{wall} A_{ln}}$$

$$\frac{1}{U_e'} = \frac{1}{h_i}\frac{D_e}{D_i} + \frac{s}{\lambda_{wall}}\cdot\frac{D_e}{D_e - D_i}\cdot\ln\frac{D_e}{D_i}$$

ENERGY BALANCE EQUATION

$$\dot{m}_{tot}\hat{C}_p\frac{dT}{dz} = A\left[\dot{Q}_R + U_e'\cdot\frac{4}{D_e}\left(T_{we} - T\right)\right]$$

! be careful

$U_e' D_e = U_i' D_i$

$$= A\left[\dot{Q}_R + U_i'\frac{4}{D_i}\left(T_{we} - T\right)\right]$$

EQUATIONS:

ODE + NLS

$\Downarrow$

DAE: DIFFERENTIAL-ALGEBRAIC EQUATIONS

EXERCISE 2

we solve the NL algebraic equations inside the ODE system

EXERCISE 3

we solve the whole system of equations (ODE+NL) as a DAE

$$
\begin{cases}
\dfrac{dF_i}{dz} = R_i A \\[2ex]
\dfrac{dT}{dz} = \dfrac{A\left[\dot{Q}_R + U_i'(T_{we} - T)\, 4/D_i\right]}{\dot{m}_{tot}\, \hat{C}_p} \\[2ex]
h_e\left(T'_{gas} - T_{we}\right) + F\sigma\varepsilon\left(T'^4_{wall} - T^4_{we}\right) + \beta\left(T'^4_{gas} - T^4_{we}\right) - U_e'\left(T_{we} - T\right) = 0
\end{cases}
$$

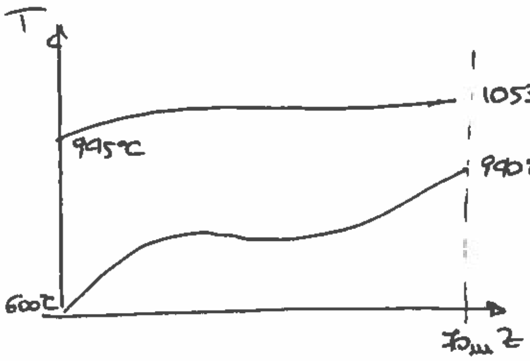
+ initial conditions for ODEs

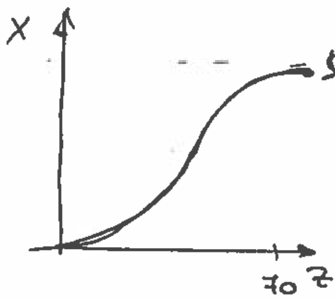
$$
\begin{cases}
F_i(z=0) = F_i^{in} \\
T(z=0) = T^{in}
\end{cases}
$$

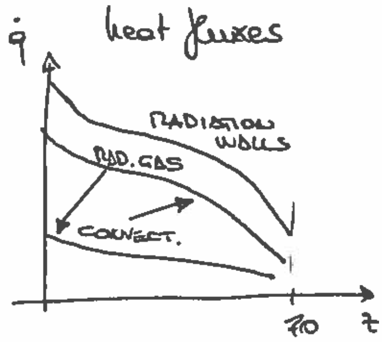
+ guess solution for algebraic variable T_{we}

$$T_{we}(z=0) = T_{we}^{\text{first guess}}$$

! the max temperature constraint is not satisfied







EXERCISE 4

The equation of pressure is added

$$\frac{dp}{dz} = -\rho v \frac{dv}{dz} + \rho g_z - \tau_{wall} \frac{p_w}{A}$$

$$\tau_{wall} = \frac{1}{2}\rho v^2 f$$

$$\frac{p_w}{A} = \frac{4}{D_i}$$

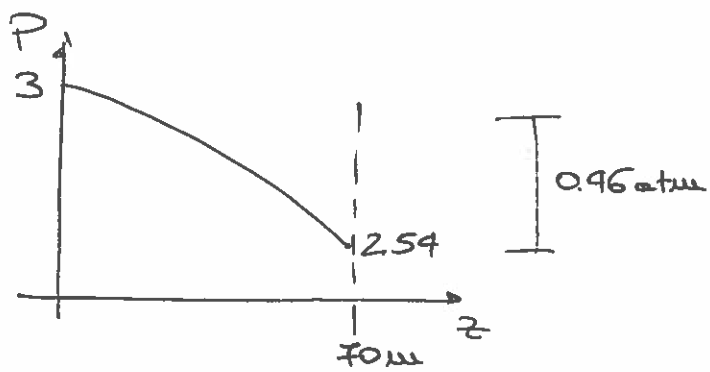
$$\Rightarrow \frac{dp}{dz} = -\rho v \frac{dv}{dz} + \rho g_z - \frac{1}{2}\rho v^2 f \cdot \frac{4}{D_i}$$

usually negligible

it depends on the PFR direction with respect to $\vec{g}$
if horizontal, is 0

$$\frac{dp}{dz} = -\frac{1}{2}\rho v^2 f \cdot \frac{4}{D_i}$$

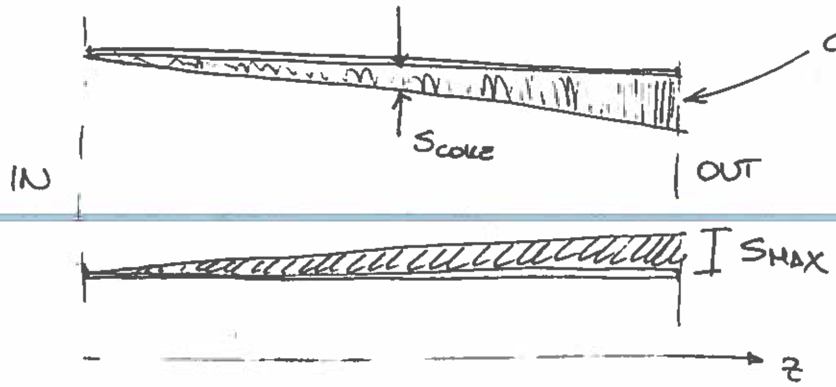
$$f = \frac{0.079}{Re^{1/4}}$$ BLASIUS FORMULA



no significant changes on the reactor performances

EXERCISE 5

Formation of coke along the reactor

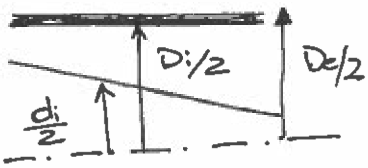


$$S_{COKE} = \frac{z}{L} \cdot S_{MAX}$$

Effects
1. reduction of residence time because of higher velocities in the reactor
2. increase of wall resistances

REVISION OF THERMAL RESISTANCES

$$d_i \overset{\text{def}}{=} D_i - 2 s_{coke}$$



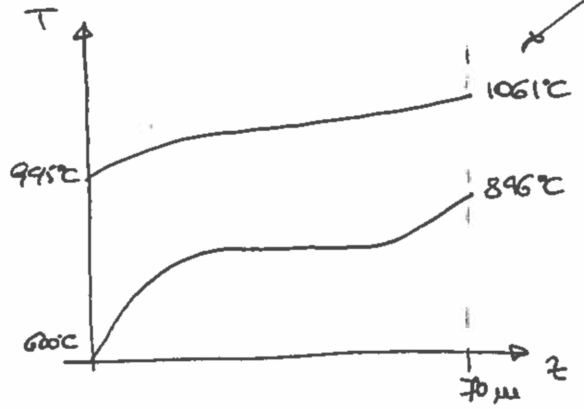
$$\frac{1}{U_e'} = \frac{1}{h_i}\frac{D_e}{d_i} + \frac{s}{\lambda_{wall}} \cdot \frac{D_e}{D_e - D_i} \ln\frac{D_e}{D_i} +$$

$$+ \frac{s_{coke}}{\lambda_{coke}} \cdot \frac{D_i}{D_i - d_i} + \ln\frac{D_i}{d_i}$$

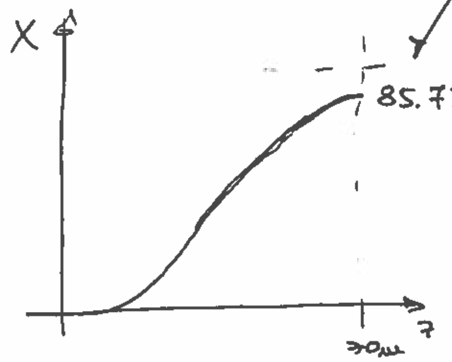
$$\tilde{A}_i = \frac{\pi}{4} d_i^2$$ $\Longrightarrow$ this is the new cross section area to be accounted for in the mass and energy balance equations

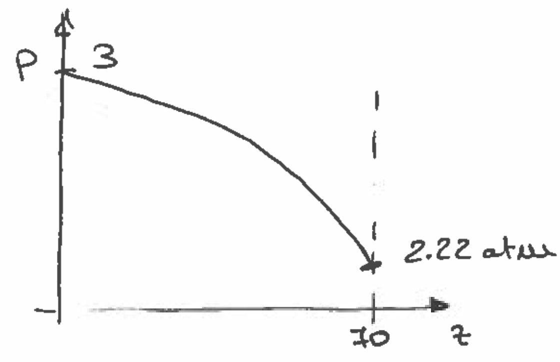
$$\begin{cases} \dfrac{dF_i}{dz} = R_i \tilde{A} \\[2ex] \dfrac{dT}{dz} = \dfrac{\tilde{A}\left[\dot{Q}_R + U_i'(T_{we} - T)\, 4/D_i\right]}{\dot{m}_{tot}\, \hat{c}_p} \\[2ex] h_e\left(T_{gas}^f - T_{we}\right) + \sigma\varepsilon\left(T_{wall}^{f\,4} - T_{we}^4\right) + \beta\left(T_{gas}^{f\,4} - T_{we}^4\right) - U_e'\left(T_{we} - T\right) = 0 \end{cases}$$

! at maximum

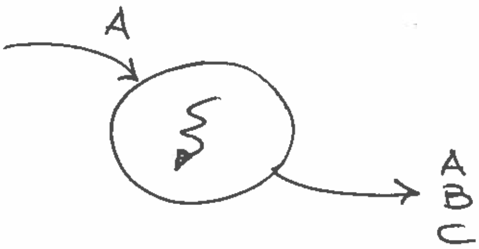


sharp reduction in conversion !!





EXERCISE 7



$$\begin{cases} A \rightarrow B \\ A \rightarrow C \end{cases}$$

reactions in parallel
isothermal conditions
constant density
steady-state conditions

$$\begin{cases} \dfrac{C_{A\,in} - C_A}{\tau} = K_1 C_A + K_2 C_A \\[2ex] \dfrac{C_{B\,in} - C_B}{\tau} = -K_1 C_A \\[2ex] \dfrac{C_{C\,in} - C_C}{\tau} = -K_2 C_A \end{cases}$$

$$\begin{cases} R_A = -K_1 C_A - K_2 C_A \\ R_B = K_1 C_A \\ R_C = K_2 C_A \end{cases}$$

$$K_{tot} \overset{\text{def}}{=} K_1 + K_2$$

$$C_{A\,in} - C_A = (K_1 + K_2) C_A \tau \qquad C_{A\,in} - C_A = K_{tot} \tau C_A$$

$$C_A = \frac{C_{A\,in}}{1 + K_{tot}\tau}$$

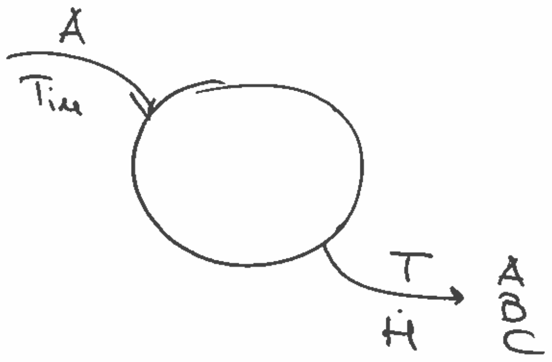
$$\frac{C_{B\,in} - C_B}{\tau} = -K_1 C_A \qquad C_{B\,in} - C_B = -K_1 C_A \tau$$

$$C_B = C_{B\,in} + K_1 C_A \tau = C_{B\,in} + \frac{K_1 \tau C_{A\,in}}{1 + K_{tot}\tau}$$

$$\begin{cases} C_A = \dfrac{C_{A\,in}}{1 + K_{tot}\tau} \\[2ex] C_B = C_{B\,in} + \dfrac{K_1 \tau C_{A\,in}}{1 + K_{tot}\tau} \\[2ex] C_C = C_{C\,in} + \dfrac{K_2 \tau C_{A\,in}}{1 + K_{tot}\tau} \end{cases}$$

ANALYTICAL SOLUTION

EXERCISE 8



Same exercise 7 but
ADIABATIC CONDITIONS

↓

ENERGY EQUATION

$$\underbrace{\dot{H}_{in}}_{\text{inlet}} = \underbrace{\dot{H}_{out}}_{\text{outlet}}$$

$$\begin{cases} \dot{H}_{in} = \dot{F}_{in}\,\tilde{H}_{in} \\ \dot{H}_{out} = \dot{F}_{out}\,\tilde{H}_{out} \end{cases}$$

$\dot{F}_{in} = \dot{F}_{out}$ (constant density, liquid)

ENERGY EQUATION $\tilde{H}_{in} = \tilde{H}_{out}$

$$\begin{cases} \tilde{H}_{in} = \sum_i \dfrac{C_i^{in}}{C_{TOT}}\,\tilde{H}_i(T_{in}) \\ \tilde{H}_{out} = \sum_i \dfrac{C_i}{C_{TOT}}\,\tilde{H}_i(T) \end{cases}$$

$$\tilde{H}_i(T) = \tilde{H}_i(T_0) + \tilde{c}_{p_i}(T-T_0) = \tilde{H}_i^0 + \tilde{c}_{p_i}(T-T_0)$$

system of NL equations

4 unknowns
4 equations

C_A, C_B, C_C, T

$$\begin{cases} C_{A_{in}} - C_A + R_A\tau = 0 \\ C_{B_{in}} - C_B + R_B\tau = 0 \\ C_{C_{in}} - C_C + R_C\tau = 0 \\ \tilde{H}_{in} - \tilde{H}_{out} = 0 \end{cases}$$

+ FIRST GUESS SOLUTION

↑

very important

EXERCISE 9

Same exercise 8, but solution with FALSE TRANSIENT method

NLS

$$\begin{cases} 0 = \dfrac{C_A^{in} - C_A}{\tau} + R_A \\ 0 = \dfrac{C_B^{in} - C_B}{\tau} + R_B \\ 0 = \dfrac{C_C^{in} - C_C}{\tau} + R_C \\ 0 = \dot{H}_{in} - \dot{H}_{out} \end{cases}$$

transformation in ODEs

ODEs

$$\begin{cases} \dfrac{dC_A}{dt} = \dfrac{C_A^{in} - C_A}{\tau} + R_A \\ \dfrac{dC_B}{dt} = \dfrac{C_B^{in} - C_B}{\tau} + R_B \\ \dfrac{dC_C}{dt} = \dfrac{C_C^{in} - C_C}{\tau} + R_C \\ \dfrac{dH}{dt} = \dot{H}_{in} - \dot{H}_{out} \end{cases}$$

+ initial conditions

$$\frac{dH}{dt} = \frac{d}{dt}(N\tilde{H}) = N\frac{d\tilde{H}}{dt} = N\tilde{C}_p\frac{dT}{dt}$$

$$\frac{dT}{dt} = \frac{\dot{H}_{in} - \dot{H}_{out}}{N\tilde{C}_p} = \frac{\dot{F}(\tilde{H}_{in} - \tilde{H}_{out})}{N\tilde{C}_p} =$$

$$= \frac{1}{\tilde{C}_p}\frac{\tilde{H}_{in} - \tilde{H}_{out}}{\tau}$$

FINAL SYSTEM OF ODES

$$\begin{cases} \dfrac{dC_i}{dt} = \dfrac{C_i^{in} - C_i}{\tau} + R_i \\ \dfrac{dT}{dt} = \dfrac{1}{\tilde{C}_p}\dfrac{\tilde{H}_{in} - \tilde{H}_{out}}{\tau} \end{cases}$$