PRACTICAL SESSION 3

EXERCISE 1

balance equations for a PFR with heat exchange

$$\begin{cases} \dfrac{dF_j}{dV} = R_j \\ F_{tot}\,\tilde{c}_{p\,tot}\,\dfrac{dT}{dV} = U(T_e - T)\,\dfrac{p_w}{A} + Q_R \end{cases}$$

$\oplus$

initial conditions

$$\begin{cases} F_j(V=0) = F_j^{in} \\ T(V=0) = T^{in} \end{cases}$$

Hp: $T_e = const$

$A = const$ (cross section area) $\Rightarrow dV = A\,dz$

$$\begin{cases} \dfrac{dF_j}{dz} = A R_j \\ F_{tot}\,\tilde{c}_{p\,tot}\,\dfrac{dT}{dz} = U(T_e - T)\cdot\dfrac{p_w}{A}\cdot A + Q_R A \end{cases}$$

$$\frac{p_w}{A} = \frac{\text{perimeter}}{\text{cross section area}} = \frac{4}{D}$$

A = cross section area $= \dfrac{\pi D^2}{4}$

Q_R = heat release $= -\Delta H_R \cdot r$

Implementation in MATLAB

$X_{out} = 99.5\%$

$T_{out} = 356.72\,°C$

$T_{max} = 911.6\,°C$ @ $109.8\,m$

Analysis with constraints

$U_{min} = 75.96\ \dfrac{kcal}{m^2 h K}$

$X = 99.6\%$

EXERCISE 2

balance equations for a PFR with heat exchange

CO-CURRENT CONFIGURATION

$$\begin{cases} \dfrac{d\dot{F}_j}{dV} = R_j \\ \dot{F}_{tot}\,\bar{C}_{p\,tot}\,\dfrac{dT}{dV} = U(T_e - T)\dfrac{p_w}{A} + \dot{Q}_R \\ \dot{F}_e\,\tilde{C}_{pe}\,\dfrac{dT_e}{dV_e} = -U(T_e - T)\dfrac{p_w}{A} \end{cases}$$

⊕ initial conditions

$$\begin{cases} \dot{F}_j(V=0) = \dot{F}_j^{in} \\ T(V=0) = T^{in} \\ T_e(V=0) = T_e^{in} \end{cases}$$

$$\begin{cases} \dfrac{d\dot{F}_j}{dz} = R_j A \\ \dfrac{dT}{dz} = \dfrac{A}{\dot{F}_{tot}\,\tilde{C}_{p\,tot}}\left[U(T_e - T)\dfrac{p_w}{A} + \dot{Q}_R\right] \\ \dfrac{dT_e}{dz} = -\dfrac{A_e}{\dot{F}_e\,\tilde{C}_{pe}}\left[U(T_e - T)\dfrac{p_w}{A}\right] \end{cases}$$

Implemented in MATLAB

$X_{out} = 99.39\,\%$

$T_{out} = 406.93\,°C$

$T_{max} = 406.93\,°C$ @ $z = 150$ mm

EXERCISE 3

balance equations for a PFR with heat exchange

COUNTER-CURRENT CONFIGURATION

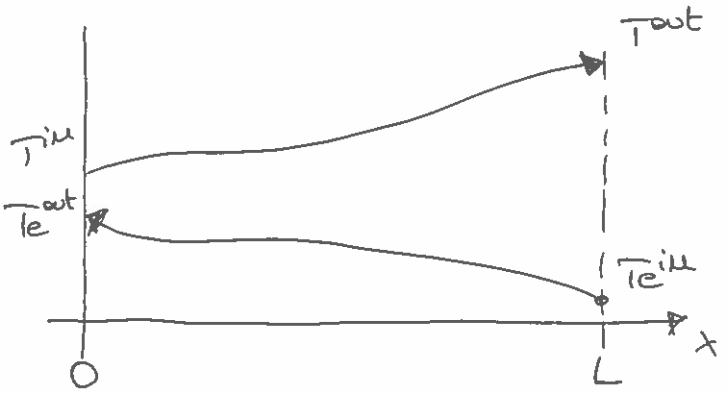
$$\begin{cases} \dfrac{dF_j}{dV} = R_j \\ \dot{F}_{tot}\,\tilde{c}_{p_{tot}}\,\dfrac{dT}{dV} = U(T_e - T)\dfrac{p_w}{A} + \dot{Q}_e \\ \dot{F}_e\,\tilde{c}_{p_e}\,\dfrac{dT_e}{dV_e} = U(T_e - T)\dfrac{p_w}{A} \end{cases}$$

⊕ initial/boundary conditions

$$\begin{cases} \dot{F}_j(V=0) = \dot{F}_j^{in} \\ T(V=0) = T^{in} \\ T_e(V=V_{TOT}) = T_e^{in} \end{cases}$$

$$\begin{cases} \dfrac{dF_j}{dz} = R_j A \\ \dfrac{dT}{dz} = \dfrac{A}{\dot{F}_{tot}\,\tilde{c}_{p_{tot}}}\left[U(T_e - T)\dfrac{p_w}{A} + \dot{Q}_R\right] \\ \dfrac{dT_e}{dz} = \dfrac{A_e}{\dot{F}_e\,\tilde{c}_{p_e}}\,U(T_e - T)\dfrac{p_w}{A} \end{cases} \quad \oplus \quad \begin{cases} \dot{F}_j(x=0) = \dot{F}_j^{in} \\ T(x=0) = T^{in} \\ T_e(x=L) = T_e^{in} \end{cases}$$

BVP



SHOOTING METHOD
BVP → IVP

$$\begin{cases} \dot{F}_j(x=0) = \dot{F}_j^{in} \\ T(x=0) = T^{in} \\ T_e(x=0) = T_{e,guess}^{out} \end{cases}$$

$$T_{e,guess}^{out\,(k+1)} = T_{e,guess}^{out\,(k)} - \alpha\left(T_{e,calc}^{in} - T_e^{in}\right)$$

α: under-relaxation factor (for stability reasons)
$T_{e,calc}^{in}$: calculated
T_e^{in}: target

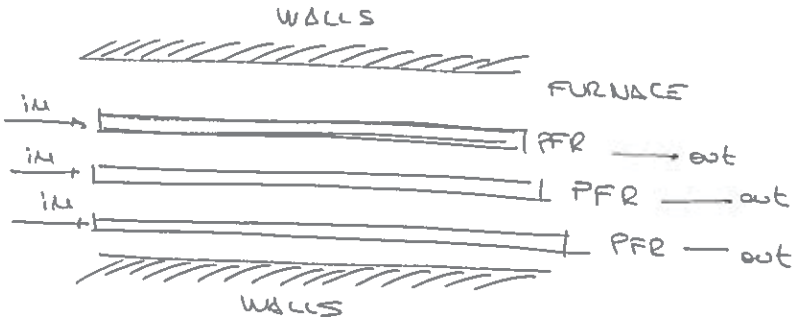
Stop criterium: if $\left(T_{e,calc}^{in} - T_e^{in}\right) < \varepsilon$

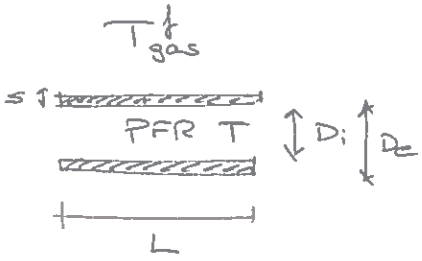
Implementation in MATLAB

$X_{out} = 99.9\%$ $\quad T_{out} = 405\,°C$ $\quad T_{max} = 439\,°C$ @ 99.96 kg

PRACTICAL SESSION 3

EXERCISE 4





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

endothermic reactions !

heat must be supplied from the external environment

↓

FURNACES

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

2 parallel reactions
change of moles
non isothermal conditions
heat exchange with constant T external environment $\Big\{ \rho \neq const$

GOVERNING EQUATIONS

$$\begin{cases} \dfrac{dF_i}{dz} = R_i A \qquad A = \dfrac{\pi D_i^2}{4} \\ \dot{m}_{TOT}\, \hat{C}_p \dfrac{dT}{dt} = A\left(Q_R + U_i (T_{gas} - T) \dfrac{4}{D_i} \right) \end{cases}$$

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

Q_R = heat whose $= -\sum_{1}^{2}{}_j \tilde{\Delta H}^R_j \tau_j =$

$= -\sum_{1}^{NS}{}_j \tilde{H}_j R_j$

↓ negative because the reactions are endothermic

HEAT EXCHANGE

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

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

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

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

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

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

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

O.D. EQUATIONS

6 equations for species
1 equation for T

$$\begin{cases} \dfrac{dF_i}{dz} = R_i A \\ \dfrac{dT}{dz} = \dfrac{A \left[Q_R + U_i (T_{gas}^t - T) \pi D_i \right]}{\dot{m}_{TOT} \hat{C}_p} \end{cases}$$

$\oplus$

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

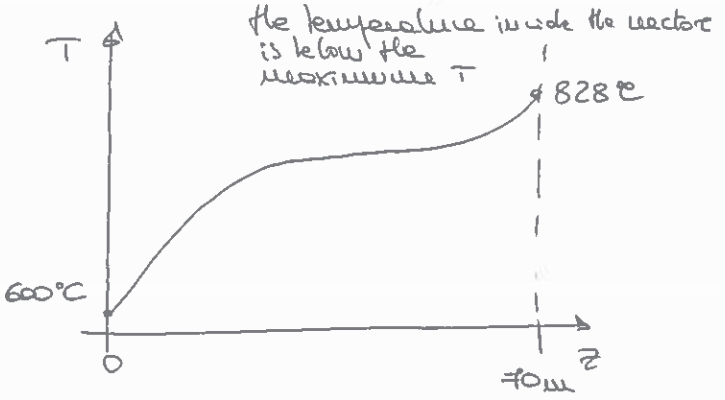
INTERNAL HEAT EXCHANGE COEFFICIENT

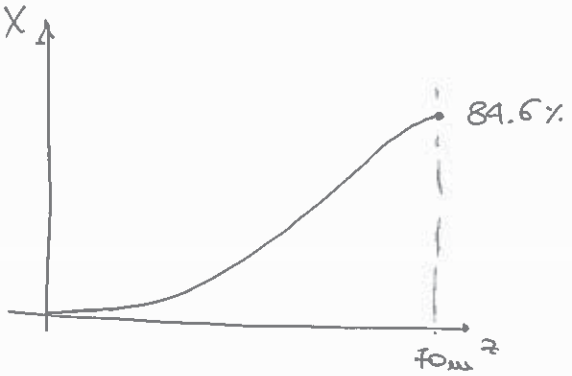
$$h_i = \frac{Nu_i \cdot \lambda_{mix}}{D_i}$$

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

DITTUS-BOELTER CORRELATION

$$Re = \frac{\rho v D_i}{\mu_{mix}} \qquad Pr = \frac{\nu}{\alpha} = \frac{\mu_{mix}}{\hat{c}_p \lambda_{mix}}$$

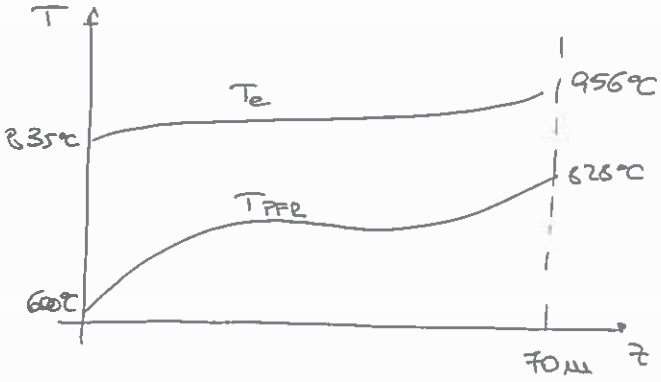




Estimation of temperature of external surface of PFR (which has to be < T_{max})

$$U_i \cdot \pi D_i L \left(T_{gas}^{1} - T\right) = h_e \cdot \pi D_e L \cdot \left(T_g^{1} - T_e\right)$$

$$T_e(z) = T_{gas}^{1} - \frac{U_i D_i}{h_e D_e}\left(T_{gas}^{1} - T(z)\right)$$



The external wall temperature is below the maximum! ✓

EXERCISE 5

Derivation of pressure loop equation

$$\begin{cases} \dfrac{d\dot{F}_j}{dt} = \dot{A}\dot{R}_j \\ \dfrac{dT}{dt} = \dfrac{A}{\dot{F}_{tot}\bar{C}_{tot}}\left[U(T_e - T)\dfrac{p_w}{A} + \dot{Q}_R\right] \\ \dfrac{dT_e}{dt} = \dfrac{A_e}{\dot{F}_e \bar{C}_{pe}}\left[U(T_e - T)\dfrac{p_w}{A} + \dot{Q}_R\right] \\ \dfrac{dp}{dt} = -\rho v \dfrac{dv}{dz} + \rho g_z - \tau_{wall}\dfrac{p_w}{A} \end{cases}$$

$$\frac{p_w}{A} = \frac{4}{D} \qquad \tau_{wall} = \frac{1}{2}\rho v^2 f \qquad f = \frac{0.079}{Re^{1/4}}$$

pressure loop equation: $\dfrac{dp}{dz} = -\rho v \dfrac{dv}{dt} + \rho g_z - \dfrac{1}{2}\rho v^2 f \cdot \dfrac{4}{D}$

$\rho g_z = 0$ if reactor is horizontal

$$\frac{dp}{dt} = -\rho v \frac{dv}{dt} - \frac{1}{2}\rho v^2 f \cdot \frac{4}{D}$$

↑ do we need an additional equation for $\frac{dv}{dt}$? not necessarily

$$\frac{dv}{dt} = \frac{d}{dt}\left(\frac{\dot{F}_{tot}}{C_{tot} A}\right) = \frac{\dot{F}_{tot}}{A}\frac{d}{dt}\left(\frac{1}{C_{tot}}\right)$$

$$= -\frac{\dot{F}_{tot}}{A}\frac{1}{C_{tot}^2}\frac{dC_{tot}}{dt} = -\frac{\dot{F}_{tot}}{A C_{tot}^2}\frac{d}{dt}\left(\frac{p}{RT}\right) =$$

$$= -\frac{V}{C_{tot}}\frac{d}{dt}\left(\frac{p}{RT}\right) = -\frac{V}{C_{tot}}\left[\frac{p}{RT}\cdot T\frac{d}{dt}\left(\frac{1}{T}\right) + \frac{p}{RT}\cdot\frac{1}{p}\frac{dp}{dt}\right] =$$

$$= -v\left(-\frac{1}{T}\frac{dT}{dt} + \frac{1}{p}\frac{dp}{dt}\right)$$

$$\rho v \frac{dv}{dt} = \frac{\rho v^2}{T}\frac{dT}{dt} - \frac{\rho v^2}{p}\frac{dp}{dt}$$

pressure loop equation

$$\frac{dp}{dt} = -\frac{\rho v^2}{T}\frac{dT}{dt} + \frac{\rho v^2}{p}\frac{dp}{dt} - \frac{2}{D}\rho v^2 f$$

$$\frac{dp}{dt} = \frac{-\frac{\rho v^2}{T}\frac{dT}{dt} - \frac{2}{D}\rho v^2 f}{1 - \frac{\rho v^2}{p}}$$

final system of equations

$$\begin{cases} \frac{dF_j}{dt} = k_j A \\ \frac{dT}{dt} = \frac{A}{F_{tot} C_{tot}} \left[U(T_e - T)\frac{\rho w}{A} + \dot{Q}_e \right] \\ \frac{dT_e}{dt} = \frac{A}{F_e C_{pe}} \left[U(T_e - T)\frac{\rho w}{A} \right] \\ \frac{dp}{dt} = \frac{-\frac{\rho v^2}{T}\frac{dT}{dt} - \frac{2}{D}\rho v^2 f}{1 - \frac{\rho v^2}{p}} \end{cases}$$

usually the $\rho v \frac{dv}{dt}$ term is negligible

if we neglect it, we have: $\frac{dp}{dt} = -\frac{2}{D}\rho v^2 f$

Implementation in MATLAB

$P_{out} = 2.98$ atm

Analytical (approximate) formula

$$\tilde{P} = P_0 \sqrt{1 - \alpha_p A x}$$

$$\tilde{P}_{out} \simeq 2.57 \text{ atm}$$