PRACTICAL SESSION 3

EXERCISE 1

balance equations for a PFR with heat exchange

$$\begin{cases} \dfrac{d\dot{F}_j}{dV} = R_j \\[2ex] \dot{F}_{tot}\,\tilde{C}_{p,tot}\,\dfrac{dT}{dV} = U(T_e - T)\,\dfrac{p_w}{A} + \dot{Q}_R \end{cases}$$

$+$

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

Hp: $T_e = \text{const}$

$A = \text{const}$ (cross section area) $\Longrightarrow dV = A\,dz$

$$\begin{cases} \dfrac{d\dot{F}_j}{dz} = A R_j \\[2ex] \dot{F}_{tot}\,\tilde{C}_{p,tot}\,\dfrac{dT}{dz} = U(T_e - T)\cdot\dfrac{p_w}{A}\cdot A + \dot{Q}_R A \end{cases}$$

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

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

$\dot{Q}_R = \text{heat release} = -\widetilde{\Delta H}_R \cdot r$

Implementation in MATLAB

$X_{out} = 99.57\%$

$T_{out} = 366.72\,°C$

$T_{max} = 411.6\,°C$ @ $109.8\,m$

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

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

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

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

Implemented in MATLAB

$X_{out} = 99.39\%$

$T_{out} = 406.93\ °C$

$T_{max} = 406.93\ °C$ @ $z = 150$ m

EXERCISE 3

balance equations for a PFR with heat exchange

COUNTER-CURRENT CONFIGURATION

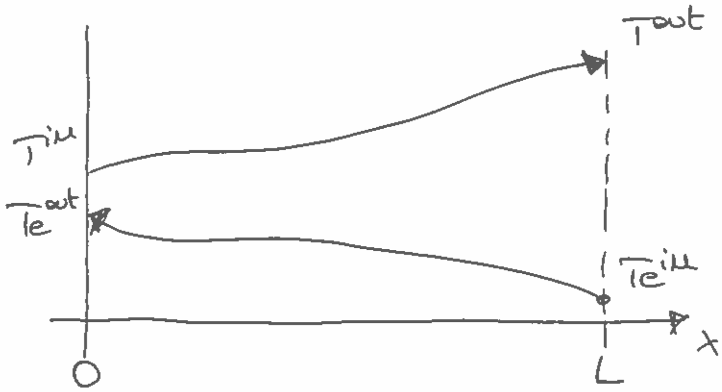
$$\begin{cases} \dfrac{d\dot{F}_j}{dV} = R_j \\[2mm] \dot{F}_{tot}\tilde{C}p_{tot}\dfrac{dT}{dV} = U(T_e - T)\dfrac{pw}{A} + \dot{Q}_R \\[2mm] \dot{F}_e\tilde{C}p_e\dfrac{dT_e}{dV} = U(T_e - T)\dfrac{pw}{A} \end{cases}$$

$\oplus$ initial/boundary conditions

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

$$\begin{cases} \dfrac{d\dot{F}_j}{dz} = R_j A \\[2mm] \dfrac{dT}{dz} = \dfrac{A}{\dot{F}_{tot}\tilde{C}p_{tot}}\left[U(T_e - T)\dfrac{pw}{A} + \dot{Q}_R\right] \\[2mm] \dfrac{dT_e}{dz} = \dfrac{A}{\dot{F}_e\tilde{C}p_e} U(T_e - T)\dfrac{pw}{A} \end{cases} \oplus \begin{cases} \dot{F}_j(x=0) = \dot{F}_j^{in} \\ T(x=0) = T^{in} \\ T_e(x=L) = T_e^{in} \end{cases}$$

BVP



SHOOTING METHOD
BVP → IVP

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

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

underrelaxation factor (for stability reasons)   calculated   target

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

Implementation in MATLAB

$X_{out} = 99.9\%$
$T_{out} = 409\,°C$

$T_{max} = 439\,°C$ @ 99.96

EXERCISE 4

Inclusion of pressure drop equation

$$
\begin{cases}
\dfrac{dF_j}{dz} = A R_j \\[2mm]
\dfrac{dT}{dz} = \dfrac{A}{F_{tot} \hat{C}p_{tot}} \left[U(T_e - T) \dfrac{p_w}{A} + \dot{Q}_R \right] \\[2mm]
\dfrac{dT_e}{dz} = \dfrac{A}{F_e \hat{C}p_e} \left[U(T_e - T) \dfrac{p_w}{A} + \dot{Q}_R \right] \\[2mm]
\dfrac{dp}{dz} = -\rho v \dfrac{dv}{dz} + \rho g_z - \tau_{wall} \dfrac{p_w}{A}
\end{cases}
$$

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

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

$\rho g_z = 0$ 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 $\dfrac{dv}{dt}$?
not necessarily

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

$$= -\frac{F_{tot}}{A} \frac{1}{C_{tot}^2} \frac{dC_{tot}}{dz} = -\frac{F_{tot}}{A C_{tot}^2} \frac{d}{dt}\left(\frac{P}{RT} \right) =$$

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

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

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

pressure drop 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

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

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

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

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