

PRACTICAL SESSION 3

EXERCISE 1

balance equations
for a PFR with
heat exchange

$$\frac{d\dot{F}_j}{dV} = R_j$$

$$\dot{F}_{tot} \tilde{C}_{p,tot} \frac{dT}{dV} = U(T_e - T) \frac{P_w}{A} + Q_R$$

⊕

initial conditions

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

Hyp: $T_e = \text{const}$

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

$$\frac{d\dot{F}_j}{dz} = A R_j$$

$$\dot{F}_{tot} \tilde{C}_{p,tot} \frac{dT}{dz} = U(T_e - T) \cdot \frac{P_w}{A} \cdot A + Q_R A$$

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

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

$$\dot{Q}_R = \text{heat release} = - \Delta \hat{H}_R \cdot \dot{\nu}$$

Implementation in MATLAB

$$X_{at} = 99.5\%$$

$$T_{out} = 356.72^\circ\text{C}$$

$$T_{max} = 411.6^\circ\text{C} @ 109.8 \text{ m}$$

Analysis with
constraints

$$U_{min} = 75.96 \frac{\text{W}}{\text{m}^2\text{K}}$$

$$X = 99.6\%$$

EXERCISE 2

balance equations
for a PFR with
heat exchange

CO-CURRENT
CONFIGURATION

$$\left\{ \begin{aligned} \frac{d\dot{F}_j}{dV} &= R_j \\ \dot{F}_{tot} \bar{C}_{p,tot} \frac{dT}{dV} &= U(T_e - T) \frac{p_w}{A} + \dot{Q}_R \\ \dot{F}_e \tilde{C}_{pe} \frac{dT_e}{dV} &= -U(T_e - T) \frac{p_w}{A} \end{aligned} \right.$$

⊕ initial
conditions

$$\left\{ \begin{aligned} \dot{F}_j(V=0) &= \dot{F}_j^{in} \\ T(V=0) &= T^{in} \\ T_e(V=0) &= T_e^{in} \end{aligned} \right.$$

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

Implemented in MATLAB

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

$$T_{out} = 406.93^\circ\text{C}$$

$$T_{max} = 406.93^\circ\text{C} @ z = 150 \text{ mm}$$

EXERCISE 3

balance equations for
a PFR with heat
exchange

COUNTER-CURRENT
CONFIGURATION

$$\frac{dF_j}{dV} = R_j$$

$$\dot{F}_{tot} \tilde{C}_{p,tot} \frac{dT}{dV} = U(T_e - T) \frac{p_w}{A} + \dot{Q}_R$$

$$\dot{F}_e \tilde{C}_{p,e} \frac{dT_e}{dV} = U(T_e - T) \frac{p_w}{A}$$

⊕ initial/boundary conditions

$$\left\{ \begin{array}{l} \dot{F}_j(V=0) = \dot{F}_j^{in} \\ T(V=0) = T^{in} \\ T_e(V=V_{TOT}) = T_e^{in} \end{array} \right.$$

$$\frac{dF_j}{dz} = R_j A$$

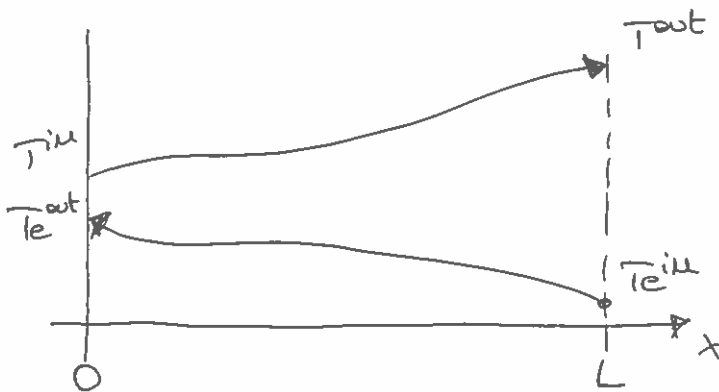
$$\frac{dT}{dz} = \frac{A}{\dot{F}_{tot} \tilde{C}_{p,tot}} \left[U(T_e - T) \frac{p_w}{A} + \dot{Q}_R \right]$$

$$\frac{dT_e}{dz} = \frac{A}{\dot{F}_e \tilde{C}_{p,e}} U(T_e - T) \frac{p_w}{A}$$

⊕

$$\left\{ \begin{array}{l} \dot{F}_j(x=0) = \dot{F}_j^{in} \\ T(x=0) = T^{in} \\ T_e(x=L) = T_e^{in} \end{array} \right.$$

BVP



SHOOTING METHOD

BVP → IVP

$$\left\{ \begin{array}{l} \dot{F}_j(x=0) = \dot{F}_j^{in} \\ T(x=0) = T^{in} \\ T_e(x=0) = T_{e,guess}^{out} \end{array} \right.$$

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

under relaxation factor / for stability reasons calculated target

Stop criterion: if $(T_{e,calc}^{in} - T_e^{in}) < \epsilon$

Implementation
in MATLAB

$T_{out} = 90^\circ\text{C}$
 $T_{out} = 90^\circ\text{C}$

$T_{max} = 93^\circ\text{C}$ @ 99.96%

EXERCISE 4

Inclusion of pressure drop equation

$$\left\{ \begin{array}{l} \frac{d\dot{F}_i}{dt} = \dot{A}R_i \\ \frac{dT}{dt} = \frac{A}{\dot{F}_{tot}\bar{C}_{tot}} \left[U(T_e - T) \frac{p_w}{A} + \dot{Q}_R \right] \\ \frac{dT_e}{dt} = \frac{A}{\dot{F}_e \bar{C}_e} \left[U(T_e - T) \frac{p_w}{A} + \dot{Q}_R \right] \\ \frac{dp}{dt} = -\rho v \frac{dv}{dt} + \rho g_z - \tau_{wall} \frac{p_w}{A} \end{array} \right.$$

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

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

$\rho g_z = 0$ 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

$$\frac{dp}{dt} = -\frac{pv^2}{T} \frac{dT}{dt} + \frac{pv^2}{P} \frac{dP}{dt} - \frac{2}{D} pv^2 f$$

$$\frac{dp}{dt} = \frac{-\frac{pv^2}{T} \frac{dT}{dt} - \frac{2}{D} pv^2 f}{1 - \frac{pv^2}{P}}$$

final system of equations

$$\left\{ \begin{array}{l} \frac{dF_j}{dt} = \dot{L}_j A \\ \frac{dT}{dt} = \frac{\dot{A}}{\dot{F}_{tot} \dot{C}_{tot}} [U(T_e - T) \frac{P_w}{A} + \dot{Q}_2] \\ \frac{dT_e}{dt} = \frac{\dot{A}}{\dot{F}_e \dot{C}_{Fe}} [U(T_e - T) \frac{P_w}{A}] \\ \frac{dp}{dt} = \frac{-\frac{pv^2}{T} \frac{dT}{dt} - \frac{2}{D} pv^2 f}{1 - \frac{pv^2}{P}} \end{array} \right.$$

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

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

Implementation in MATLAB

$$P_{at} = 2.98 \text{ atm}$$

Analytical (approximate) formula

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

$$\tilde{P}_{at} \approx 2.57 \text{ atm}$$
