Exercise 22

Determine the maximum internal diameter in a cylindrical microchannel allowing stable operation for a fast first-order exothermic reaction. Stability criteria: $\Delta T'_{max} = 1.2$

Estimate the hot spot temperature.

(Calculate de conversion and temperature profile in the reactor - requires numerical integration)

Assumptions

- The main heat transfer resistance is on reaction channel side
- The laminar temperature profile is established

Data

Cooling temperature $T_c = 50°C$

Inlet temperature $T_0 = 50°C$

Rate constant at cooling temperature $k_{50°C} = 0.2\ s^{-1}$

Activation energy $E = 80\ kJ\ mol^{-1}$

Reaction enthalpy $\Delta H_r = -150\ kJ\ mol^{-1}$

Inlet concentration $c_{1,0} = 0.7\ kmol\ m^{-3}$

Space time : $\tau = 15\ s$

Reaction mixture properties:

$\rho(kg\ m^{-3})$	867
$c_p(J\ kg^{-1}K^{-1})$	1720
$\lambda\ (W\ K^{-1}\ m^{-1})$	0.141
$\mu\ (Pa \cdot s)$	$5.8\ 10^{-4}$

Solution

$$\Delta T_{ad} = \frac{-\Delta H_r\ c_{10}}{\rho\ c_p}$$

$$\gamma = \frac{E}{RT_c}$$

$$S' = \Delta T_{ad} \frac{E}{RT_c^2}$$

$$N'_{min} = 2.72\ S' - B\sqrt{S'} \quad \text{with} \quad B = 3.37\ \text{(n=1)}$$

$$N' = \frac{Ua}{\rho c_p} \frac{1}{k(T_c) c_{1,0}^{n-1}} = \frac{Ua}{\rho c_p} \frac{1}{k(T_c)} \quad \rightarrow \quad Ua = h_r a = N' \rho\ c_p\ k(T_c)$$

$$Nu_\infty = 3.66\ (cylindrical\ channel)$$

$$Ua = h_r a = h_r \frac{A}{V} = \frac{Nu_\infty \cdot \lambda_f}{d_t}\frac{4}{d_t} \rightarrow d_t = 2\sqrt{\frac{Nu_\infty \, \lambda_f}{h_r a}}$$

$$\Delta T'_{max} = \frac{T_{max} - T_c}{T_c}\gamma \rightarrow T_{max} = T_c + \Delta T'_{max}\frac{T_c}{\gamma}$$

B	3.37	
Dtad	70.41	K
gamma	29.8	
S'	6.49	
N'min	9.08	
Ua=hra	2.71E+06	W/m^3 K
Nu inf	3.66	
d	8.73E-04	m
DT'max	1.2	
Tmax	336	K
Dtmax	13.0	K

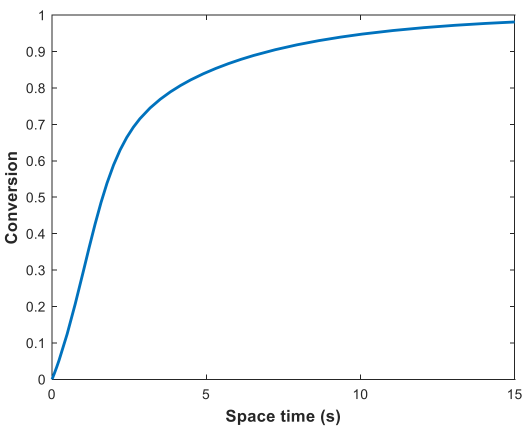
Simulation in PFR with $\tau = 15\ s$:

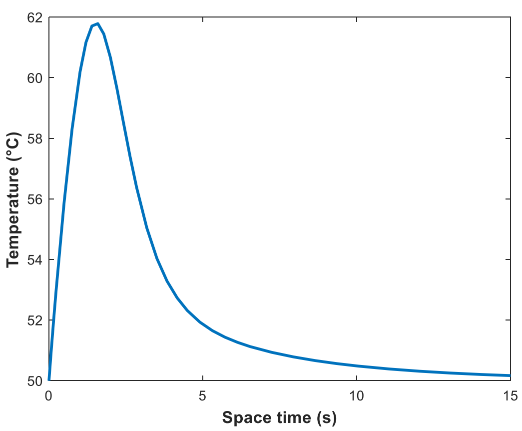
System of 2 following coupled ODEs to be solved numerically (e.g., using Matlab)

$$\frac{dT}{d\tau} = \frac{Ua(T_c - T) + k_0 \exp[-E/(RT)]\, c\, (-\Delta H_r)}{\rho c_p}$$

$$\frac{dc}{d\tau} = -k_0 \exp\left[-\frac{E}{RT}\right] c$$

Where $k_0 = \frac{k_{323K}}{\exp[-E/(R \cdot 323)]}$





Hot-spot (numerical simulation): 62°C

Hot-spot (estimation): 63°C

➔good agreement!

Conversion after 15s: 98%