Exercise 8

An exothermic homogeneous first-order liquid-phase chemical reaction was studied in a straight, circular mono-channel microreactor.

The reaction could be run quasi-isothermally using 80% w/w of solvent.

Data

Flowrate $\dot{Q} = 1.5 \cdot 10^{-7} m^3 s^{-1}$

Molecular weight of reactant A $MW = 0.21\ kg\ mol^{-1}$

Kinetics

$r = kc_A (mol \cdot m^{-3} \cdot s^{-1})$ $\qquad k = 50\ s^{-1}$

Reactor dimensions

Diameter $D = 2 \cdot 10^{-4}\ m$

Length $L = 0.1\ m$

Fluid properties (assume independent of concentration)

Density $\rho = 900\ kg\ m^{-3}$

Viscosity $\mu = 1.2 \cdot 10^{-3} Pa \cdot s$

Heat capacity $c_p = 2200\ J\ kg^{-1}\ K^{-1}$

Heat conductivity $\lambda = 0.2\ W\ m^{-1}\ K^{-1}$

Nusselt number $Nu = 3.66$ (valid in laminar regime)

Questions

Design a reactor capable of processing (same conversion) quasi-isothermally the same molar flowrate of the reactant using only 40% w/w of solvent in the feed.

1. Propose a mono-channel design
2. Propose a multichannel design to maintain the pressure drop equal or smaller than in the first study. Pressure drop for circular channel in laminar regime $\Delta p = L \frac{32\, \mu\, u_m}{D^2}$

Answers

First order reaction → $X = 1 - \exp(-\frac{\tau}{t_{hom}})$; $t_{hom} = \frac{1}{kc_0^{n-1}} = \frac{1}{k} \neq f(c_0) \rightarrow \boldsymbol{\tau = constant}$

Solvent mass fraction decreases from 80% to 40% → increase in $c_{A,0}$ by a factor of 3

→ Volumetric flowrate $\dot{Q}$ will decrease by a factor of 3 ($\dot{n}_{A,0} = \dot{Q} \cdot c_0 = constant$)

→ Reactor volume will decrease by a factor of 3 since $\tau = \frac{V}{\dot{Q}} = constant$

Characteristic time for heat transfer $t_{heat} = \frac{\rho\, c_p}{\lambda} \frac{R^2}{Nu}$ must decrease by a factor of 3 since the same amount of heat is released in a 3 times smaller volume → $D_2 = \frac{D_1}{\sqrt{3}}$ and $L_2 D_2^2 = \frac{1}{3} L_1 D_1^2 \rightarrow L_1 = L_2$

Pressure drop $\Delta p = L \frac{32\, \mu\, u_m}{D^2}$ will increase by a factor of $\frac{L_2}{L_1}\left(\frac{D_1}{D_2}\right)^2 = 3$

$(u_m \propto \frac{Q}{D^2}$ is constant since $\frac{Q_1}{Q_2} = \left(\frac{D_2}{D_1}\right)^2 = 3)$

Second design proposed: use two channels with same diameter as case above but with length divided by two (thus keeping the same total volume) → velocity divided by two in each channel and length divided by two→ pressure drop divided by four, i.e., ¾ only of initial value during the study.

n	1	
k_hom	5.00E+01	s-1
MW	0.2	kg/mol
ro	900	kg/m^3
Nu	3.66	
cp	2200	J kg-1 K-1
lambda	0.2	W m-1 K-1
mu	1.20E-03	Pa*s

		R1	R2	R3
F	m^3/s	1.50E-07	5.00E-08	5.00E-08
Solvent mass frac	kg/kg	80%	40%	40%
Reactant mass frac	kg/kg	20%	60%	60%
C0	mol/m^3	900	2700	2700
Mol flow rate reactant	mol/s	1.35E-04	1.35E-04	1.35E-04
Lc	m	1.00E-01	1.00E-01	5.00E-02
Dc	m	2.00E-04	1.15E-04	1.15E-04
Ac	m^2	6.28E-05	3.63E-05	1.81E-05
Sc	m^2	3.14E-08	1.05E-08	1.05E-08
Nc	-	1	1	2
Vc	m^3	3.14E-09	1.05E-09	5.24E-10
Vreac	m^3	3.14E-09	1.05E-09	1.05E-09
dh	m	2.00E-04	1.15E-04	1.15E-04
Ac/Vc	m-1	2.0E+04	3.5E+04	3.5E+04
u	m/s	4.8E+00	4.8E+00	2.4E+00
h=U	W m-2 K-1	3660	6339	6339
t_hom	s	0.02	0.02	0.02
t_heat	s	0.11	0.04	0.04
Tau	s	0.021	0.021	0.021
Da	-	1.05	1.05	1.05
NTU	-	0.77	2.32	2.32
X		65%	65%	65%
UA		2.3E-01	2.3E-01	2.3E-01
Re		716	413	207
Dp	bar	4.58	13.75	3.44