Chemical Reaction Engineering

Practical Session 6

14 December 2018

Non-ideal reactors

1. ***Compartment model (2 parameters)***

The following irreversible reaction occurs in liquid phase in a non-ideal mixed reactor: $A \rightarrow Products$. The reaction is second order, i.e. $r = kC_A^2$, with a kinetic constant equal to $k = 2\ \frac{m^3}{kmol\ min}$. The total reactor volume is $V = 0.7\ l$ and the total volumetric flow rate is $Q = 0.7\ l/min$. The inlet mixture is pure A at concentration $C_A^{in} = 10\ \frac{kmol}{m^3}$.

In order to evaluate deviations from ideality, a step experiment was performed ($C_0 = 1\frac{kmol}{m^3}$), and the tracer concentration at the outlet was measured, according to what reported in the table below.

1. Estimate the fraction of dead volume and the fraction of by passing volumetric flow rate on the basis of experimental data, by adopting a two-parameter compartment model.
2. Estimate the outlet concentration and conversion according to the compartment model.
3. Compare the performances of the real reactor with the performances of the corresponding ideal CSTR.

$\boldsymbol{t\ (min)}$	0	0.5	1	1.5	2	2.5	3	3.5	4	5
$\boldsymbol{C_{out}\left(\frac{kmol}{m^3}\right)}$	0.04214	0.43449	0.66865	0.81223	0.881173	0.93673	0.962299	0.978663	0.982717	0.995

2. ***Segregated model (0 parameters)***

Repeat the previous exercise describing the non-ideal behavior through the perfectly segregated model.

3. ***Maximum Mixedness Model (0 parameters)***

Repeat the previous exercise describing the non-ideal behavior through the Maximum Mixedness Model.

4. ***Non-ideal tubular reactor (1 parameter)***

The following second-order reaction $A \rightarrow Products$ is carried out in a tubular reactor. The kinetic constant is $k = 0.1\ \frac{m^3}{kmol\ s}$ and the reaction occurs in liquid phase. The reactor is $L = 30\ m$ long and has a diameter of $D = 4\ cm$. The inlet mixture is pure A at concentration $C_A^{in} = 10\ \frac{kmol}{m^3}$ and its velocity is $v = 8.1\ m/s$. The Residence Time Distribution function was experimentally measured and reported in the table below (closed/closed boundary conditions can be assumed).

1. Estimate the Peclet number and the effective dispersion coefficient according to the Dispersion Model.
2. Estimate the number of equivalent CSTR according to the Tanks in Series model and the corresponding outlet concentration and conversion of A. Make a comparison with the ideal plug flow reactor.

time (s)	E (1/s)
0	0
0.1	0
0.2	0
0.3	0
0.4	0
0.5	0
1	0
2	0
2.2	0.010641
2.4	0.042563
2.6	0.085126
2.8	0.12769
3	0.255379
3.2	0.681011
3.4	0.851264
3.6	0.851264
3.8	0.766137
4	0.427055
4.2	0.284704
4.4	0.170253
4.6	0.12769
4.8	0.085126
5	0.042563
6	0.021282
7	0
8	0