Chemical Reaction Engineering

Practical Session 1

13 November 2020

Plug-Flow and Batch Reactors

1. Reactions in series in a Plug-Flow Reactor

Build up the numerical model of a plug flow reactor, with an internal diameter of 8 cm and a length of 100 m. The following reactions occur within the PFR:

$$A \xrightarrow{k_1} B \xrightarrow{k_2} C$$

The reactor works at a temperature of 750 $°C$, a pressure of 3 bar and is fed by a molar flow of A ($MW = 25\ kg/kmol$) equal to 20 $kmol/h$.

Considering both the reactions as first-order:

$$\begin{cases} r_1 = k_1 C_A \\ r_2 = k_2 C_B \end{cases} \qquad \begin{cases} k_1 = A_1 e^{-\frac{E_1}{RT}} & A_1 = 1.2 \cdot 10^8\ s^{-1} & E_1 = 37000\ cal/mol \\ k_2 = A_2 e^{-\frac{E_2}{RT}} & A_2 = 4 \cdot 10^8\ s^{-1} & E_2 = 39000\ cal/mol \end{cases}$$

evaluate the concentration profiles of the different compounds throughout the reactor. Do this in two ways:

i. Analytical resolution of the differential system.
ii. Numerical resolution of the differential system through one of the ODE solvers available in MATLAB®.

Compare the obtained yield Y_C in both the approaches: $Y_C = \frac{C_C}{C_A^0}$

2. Parallel reactions in a Batch reactor

The species B is produced from species A ($MW = 35$ kg/kmol), according to the following kinetic mechanism, through which a secondary product C is formed, too:

$$A \xrightarrow{k_1} B \quad r_1 = k_1 C_A \quad k_1 = A_1 e^{-\frac{E_1}{RT}} \qquad A_1 = 8 \cdot 10^4\ h^{-1} \qquad E_1 = 8000\ cal/mol$$

$$A \xrightarrow{k_2} C \quad r_1 = k_2 C_A \quad k_2 = A_2 e^{-\frac{E_2}{RT}} \qquad A_2 = 1 \cdot 10^5\ h^{-1} \qquad E_2 = 10000\ cal/mol$$

The reaction is carried in liquid phase ($\rho = 800 \frac{kg}{m^3}$) at a temperature of 100 $°C$.

Considering a conversion of A equal to 98%, evaluate the daily productivity of B, knowing that the reactor volume is $V = 1\ m^3$ and the overall downtime for reactor loading, unloading and cleaning is $t_D = 1\ h$.

Knowing that the operating costs C_F for single cycle vary according the cost function reported below (as function of downtime and residence time), evaluate the optimal conversion of A, and the corresponding daily productivity of B. The revenue obtained from product selling are equal to $15\ \$/kg$.

$$C_F(\tau) = C_1 t_D + C_2 \tau + C_3 \qquad \begin{cases} C_1 = 100\ \$/h \\ C_2 = 25\ \$/h \\ C_3 = 8000\ \$ \end{cases}$$

Continuously Stirred Tank Reactors (CSTR)

3. *Parallel reactions in a CSTR*

The species B is produced through an irreversible, first-order reaction $A \rightarrow B$ in liquid phase in a CSTR reactor. At the same time, a second unwanted reaction of degradation of A giving C occurs: $A \rightarrow C$. Determine the required volume to obtain 95% of A conversion, and the corresponding concentrations of B and C (volumetric inlet flow $Q = 4\ l/min$). Considering that the inlet flow contains $2\ mol/l$ of A, evaluate yield and selectivity of B in such conditions. What is the required time to maximize the yield of B? And the selectivity?

$$\begin{cases} r_1 = k_1 C_A \\ r_2 = k_2 C_A \end{cases} \qquad \begin{cases} k_1 = 0.5\ min^{-1} \\ k_2 = 0.1\ min^{-1} \end{cases}$$

The yield and selectivity of B with respect to A are defined respectively as:

$$Y_B = \frac{C_B}{C_A^0} \qquad \sigma_B = \frac{C_B}{C_A^0 - C_A}$$

Suggested exercises

4. Optimization of batch operations

Starting from species A, the species B must be produced in an isothermal batch reactor:

$$A \overset{k_1}{\rightarrow} B \overset{k_2}{\rightarrow} C$$

The kinetic constants k_1 and k_1 are respectively:

$$\begin{cases} k_1 = A_1 e^{-\frac{E_1}{RT}} & A_1 = 1.5 \cdot 10^4\ h^{-1} & E_1 = 9000\ cal/mol \\ k_2 = A_2 e^{-\frac{E_2}{RT}} & A_2 = 6 \cdot 10^6\ h^{-1} & E_2 = 19000\ cal/mol \end{cases}$$

The reactor works at a temperature of $500\ K$ with a liquid mixture. Its volume is $0.5\ m^3$, and at the beginning of each cycle $20\ kmol$ of A are introduced.

Knowing that the total time required for reactor loading, unloading, and cleaning is $1\ h$:

i. Evaluate the reaction time to maximize the yield of B.
ii. Define the optimal conditions to maximize the daily production of B. In detail, evaluate:
   - cycle length (sum of reaction and downtimes)

- conversion of A per cycle
- number of cycles per day
- daily production of B

5. Isothermal Plug Flow Reactor: QSSA

Repeat the first exercise (#1) considering the new set of kinetic parameters:

$$\begin{cases} r_1 = k_1 C_A \\ r_2 = k_2 C_B \end{cases} \qquad \begin{cases} k_1 = A_1 e^{-\frac{E_1}{RT}} & A_1 = 2 \cdot 10^8\ s^{-1} & E_1 = 40000\ cal/mol \\ k_2 = A_2 e^{-\frac{E_2}{RT}} & A_2 = 4 \cdot 10^8\ s^{-1} & E_2 = 26000\ cal/mol \end{cases}$$

In particular, evaluate the species concentration profiles in three ways:

i. Analytical solution of the differential system.
ii. Numerical resolution of the differential system through one of the ODE solvers available in MATLAB®.
iii. Numerical resolution of the differential system through the hypothesis of pseudo steady-state of B.

Compare the yield of C obtained with the three methods, and evaluate the distance between the analytical and the numerical resolution in terms of maximum error on C_B.