CP303 – Simulation Set #2 (July-October 2013)

Simulation of Non-isothermal Batch Reactors

[Choose one of the problems given in this set and solve it entirely.
Consultation sessions with the course instructors are available on request.]

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(1) An endothermic third-order reaction $3A \longrightarrow 2B + C$ is carried out in a batch reactor. The reaction mixture is heated up till 400^{o}C. During the heating up period, 10% of A is converted.

Additional Data:

Initial number of moles $N_{A0} = 10.2$ kmol;
Volume of the reactor $V = 1$ m^3 = constant;
Total mass $m_T = 950$ kg;
Mean specific heat $c_{pm} = 0.59$ kcal/kg.K;
Heat of reaction $\Delta H = 25{,}000$ kcal/kmol of A reacted;
Reaction rate constant k in m^6/kmol^2.s is given by

$$\ln(k) = -\frac{10,000}{RT} + 5 \quad \text{where} \quad R = 1.9858 \text{ kcal/kmol.K.}$$

(i) Starting from the mass balance for A over the batch reactor, show that the differential equation describing the rate of change of conversion of A is given by the following:

$$\frac{dx_A}{dt} = k\, C_{A0}^2\, (1 - x_A)^3 \quad \text{where } C_{A0} = N_{A0}/V$$

(ii) Starting from the energy balance for A over the batch reactor, show that the differential equation describing the rate of change of temperature under adiabatic condition is given by the following:

$$\frac{dT}{dt} = -\frac{\Delta H\, V\, C_{A0}}{m_T\, C_{pm}} \frac{dx_A}{dt}$$

(iii) Solve the differential equation of part (i) for isothermal operating condition and the differential equations of parts (i) and (ii) for adiabatic operating condition using MATLAB™ and plot the following:

(a) conversion of A as function of t for isothermal and adiabatic operations

(b) temperature as function of t for isothermal and adiabatic operations

(c) conversion of A as function of temperature for isothermal and adiabatic operations

(d) rate of reaction as function of t for isothermal and adiabatic operations

(iv) Discuss why conversion of A stabilizes about 0.7 for adiabatic operation whereas it surpasses 0.95 for isothermal operation.

(2) The elementary, liquid-phase reversible reaction $A \rightleftharpoons R$ has the rate coefficient parameters A_f = 7 sec^{-1}, E_f = 10,000 kcal/kmol, A_b = 5000 sec^{-1} and E_b = 20,000 kcal/kmol, where the subscripts f and b refer to forward and backward reactions, respectively. The reaction is to be carried out in a batch reactor with a maximum allowed temperature of T_{max} = 800 K. Initially, only A is present in the reactor, and the expected final conversion of A (x_{Af}) is set at 0.8.

(i) Show that the equilibrium conversion of A is given by

$$x_{A,eqm} = k_f/(k_f + k_b)$$

and plot the $x_{A,eqm}$ versus temperature T profile.

Also, determine the temperature above which it is not possible to reach x_{Af} = 0.8.

(ii) Starting from the mass balance for A over the batch reactor, show that the differential equation describing the rate of change of conversion of A is given by the following:

$$\frac{dx_A}{dt} = k_f\,(1 - x_A) - k_b\,x_A$$

where k_f and k_b are the forward and backward specific reaction rates, respectively.

(iii) For the isothermal operation of the reactor, show that the time taken to reach x_{Af} is given by

$$t_f = -\frac{1}{k_f + k_b}\,\ln\left[1 - \frac{x_{Af}}{x_{A,eqm}}\right]$$

and plot the t_f (in min) versus T profile for x_{Af} = 0.8 in the range of T = 300 to 800 K.

Also, determine the isothermal operating temperature that minimizes the processing time as well as the corresponding minimum processing time.

(iv) For the nonisothermal operation of the reactor, the optimum temperature profile is given by $\partial(-r_A)/\partial T$ = 0, where $(-r_A)$ is the rate of reation of A. Hence, show that the optimum temperature profile is related to x_A by

$$T_{opt} = \frac{E_f - E_b}{R\,\ln\left[(A_f E_f / A_b E_b)\,(1 - x_A)/x_A\right]}$$

and plot the optimum temperature profile as function of x_A.

(v) Solve the differential equation of part (ii) using the optimum temperature profile with the help of MATLAB™ and plot the processing time (in hour) as function of x_A. Determine the processing time for x_{Af} = 0.8.

(vi) Would you recommend the isothermal operation to reach x_{Af} = 0.8 or the non-isothermal operation with optimum temperature profile for the same task?

Explain your answer.