9. REVERSIBLE, EXOTHERMIC, GAS PHASE REACTION IN A CATALYTIC REACTOR

9.1 Numerical Methods

Simultaneous ordinary differential equations with known initial conditions.

9.2 Concepts Utilized

Design of a gas phase catalytic reactor with pressure drop for a first order reversible gas phase reaction.

9.3 Course Useage

Reaction Engineering

9.4 Problem Statement

The elementary gas phase reaction $2A \rightleftharpoons C$ is carried out in a packed bed reactor. There is a heat exchanger surrounding the reactor, and there is a pressure drop along the length of the reactor.
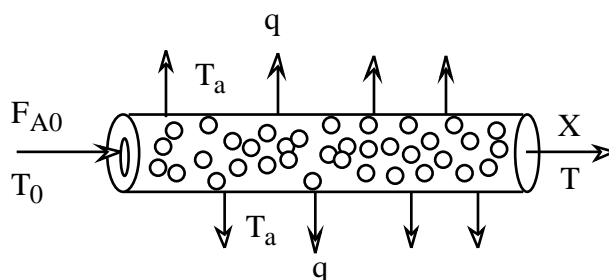

Figure 3 Packed Bed Catalytic Reactor

The various parameters values for this reactor design problem are summarized in Table (3).

Table 3 Parameter Values for Problem 9.

C_{PA} = 40.0 J/g-mol·K	R = 8.314 J/g-mol·K
C_{PC} = 80.0 J/g-mol·K	F_{A0} = 5.0 g-mol/min
ΔH_R = - 40,000 J/g-mol	Ua = 0.8 J/kg·min·K
E_A = 41,800 J/g-mol·K	T_a = 500 K
k = 0.5 dm^6/kg·min·mol @ 450 K	α = 0.015 kg^{-1}
K_C = 25,000 dm^3/g-mol @ 450 K	P_0 = 10 atm
C_{A0} = 0.271 g-mol/dm^3	y_{A0} = 1.0 (Pure A feed)
T_0 = 450 K	

(a)   Plot the conversion (X), reduced pressure (y) and temperature (T $\times 10^{-3}$) along the reactor from $W = 0$ kg up to $W = 20$ kg.

(b)   Around 16 kg of catalyst you will observe a "knee" in the conversion profile. Explain why this knee occurs and what parameters affect the knee.

(c)   Plot the concentration profiles for reactant A and product C from $W = 0$ kg up to $W = 20$ kg.

Addition Information

The notation used here and the following equations and relationships for this particular problem are adapted from the textbook by Fogler.[2] The problem is to be worked assuming plug flow with no radial gradients of concentrations and temperature at any location within the catalyst bed. The reactor design will use the conversion of A designated by X and the temperature T which are both functions of location within the catalyst bed specified by the catalyst weight W.

The general reactor design expression for a catalytic reaction in terms of conversion is a mole balance on reactant A given by

$$F_{A0}\frac{dX}{dW} = -r'_A \tag{30}$$

The simple catalytic reaction rate expression for this reversible reaction is

$$-r'_A = k\left[C_A^2 - \frac{C_C}{K_C}\right] \tag{31}$$

where the rate constant is based on reactant A and follows the Arrhenius expression

$$k = k(@\ T=450°K)\exp\frac{E_A}{R}\left[\frac{1}{450} - \frac{1}{T}\right] \tag{32}$$

and the equilibrium constant variation with temperature can be determined from van't Hoff's equation with $\Delta \tilde{C}_P = 0$

$$K_C = K_C(@\ T=450°K)\exp\frac{\Delta H_R}{R}\left[\frac{1}{450} - \frac{1}{T}\right] \tag{33}$$

The stoichiometry for $2A \rightleftharpoons C$ and the stoichiometric table for a gas allow the concentrations to be expressed as a function of conversion and temperature while allowing for volumetric changes due to decrease in moles during the reaction. Therefore

$$C_A = C_{A0}\left(\frac{1-X}{1+\varepsilon X}\right)\frac{P}{P_0}\frac{T_0}{T} = C_{A0}\left(\frac{1-X}{1-0.5X}\right)y\frac{T_0}{T} \tag{34}$$

and

$$y = \frac{P}{P_0}$$

$$C_C = \left(\frac{0.5\,C_{A0}X}{1-0.5X}\right)y\frac{T_0}{T} \tag{35}$$

The pressure drop can be expressed as a differential equation (see Fogler[2] for details)

$$\frac{d\left(\frac{P}{P_0}\right)}{dW} = \frac{-\alpha(1+\varepsilon X)}{2}\frac{P_0}{P}\frac{T}{T_0} \tag{36}$$

or

$$\frac{dy}{dW} = \frac{-\alpha(1-0.5X)}{2y}\frac{T}{T_0} \tag{37}$$

The general energy balance may be written at

$$\frac{dT}{dW} = \frac{U_a(T_a - T) + r'_A(\Delta H_R)}{F_{A0}\left(\sum \theta_i C_{Pi} + X\Delta\tilde{C}_P\right)} \tag{38}$$

which for only reactant A in the reactor feed simplifies to

$$\frac{dT}{dW} = \frac{U_a(T_a - T) + r'_A(\Delta H_R)}{F_{A0}(C_{PA})} \tag{39}$$