**Problem 2**

**Given**

\[ A \rightarrow R + S; \quad -r_A = kC_A; \quad \text{Inlet temperature, } T_0; \quad \text{Rate constant at a given temperature; } \]

The activation energy \( E_A \); Reaction enthalpy, \( \Delta H_{298} \); Liquid phase density, \( \rho \); Liquid phase specific heat capacity, \( c_p \); \( C_{A0} \); Reactor volume, \( V \); Inlet volumetric flow, \( \nu \);

**Calculate**

Conversions, reactor temperatures and heat duties for several different modes of operation.

**Solution**

Theory: HSF Chapter 8. Compare the algorithm on page 399.

**Stoichiometric table:**

<table>
<thead>
<tr>
<th>In</th>
<th>Prod</th>
<th>Out</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>( F_{A0} )</td>
<td>( -F_{A0}x_A )</td>
</tr>
<tr>
<td>R</td>
<td>0</td>
<td>( F_{A0}x_A )</td>
</tr>
<tr>
<td>S</td>
<td>0</td>
<td>( F_{A0}x_A )</td>
</tr>
<tr>
<td>I</td>
<td>( F_{I0} )</td>
<td>( F_{I0} )</td>
</tr>
</tbody>
</table>

**Concentrations:**

Since this is a liquid phase system with a constant density the volumetric flow may be assumed constant \( \nu = \nu_0 \):

\[ C_A = \frac{F_A}{\nu} = \frac{F_{A0}}{\nu_0} (1 - x_A) = C_{A0} (1 - x_A) \]

**Mole balance:**

\[ V = F_{A0} x_A = \nu C_{A0} \frac{x_A}{k(T)C_{A0} (1 - x_A)} = \frac{\nu}{k(T)} \frac{x_A}{1 - x_A} \]

This gives

\[ x_A = \frac{k(T)}{1 + k(T) \nu} \frac{V}{\nu} = \frac{k(T) \nu}{1 + k(T) \nu} \]

(1)

where

\[ k(T) = k(298) \exp \left[ -\frac{E_A}{R} \left( \frac{1}{T} - \frac{1}{298} \right) \right] \]
Energy balance:

Applying equation 8-22 from HSF gives

\[
\dot{Q} - \int_{T_0}^{T} \left( F_{A0} c_{pl} + F_{I0} c_{pl} \right) \delta H \, dT - \Delta H_{298} F_{A0} x_A = 0
\]

Since the second term is the enthalpy change as the result of changing the temperature of the flow from \( T \) to \( T_0 \) we may also write this as follows assuming that the specific heat capacity, the reaction enthalpy and the volumetric flow are constant

\[
\dot{Q} - \rho v c_p (T - T_0) - \Delta H_{298} v C_{A0} x_A = 0
\]  

(2)

a) Isothermal reactor:

Calculate the conversion from Equation 1 for the reactor temperature 298K. The heat duty, \( \dot{Q} \), is calculated from Equation 2. The conversion becomes 0.09 and 26 kW must be removed from the reactor (negative \( \dot{Q} \)).

b. Adiabatic reactor with inlet temperature 298K:

First set \( \dot{Q} \) equal to zero in the energy balance and solve for \( x_A \). We obtain

\[
x_A = \frac{\rho v c_p}{C_{A0} (\Delta H_{298})} (T - T_0)
\]  

(3)

Plot Equation 3 and Equation 1 on the same graph with \( x_A \) as functions of \( T \). The result can be read from the intersection of the two curves. The diagrams below give the conversion 0.17 and the temperature 311 K.

c) Adiabatic reactor with the reactor temperature 363 K:

Calculate the conversion for the reactor temperature 363 K from Equation 1. This gives \( x_A = 0.67 \). The inlet temperature, \( T_0 \), required is calculated from Equation 2 with \( \dot{Q} = 0 \). This gives the inlet temperature 312 K.

d) Non-adiabatic reactor with the reactor temperature 363 K and inlet temperature 298 K:

The conversion is the same as in case c). The heat duty is calculated from Equation 2. The rate of heat which must be added becomes \( \dot{Q} = 51.3 \) kW.
Problem 3

a)

\[ D_{\text{max}} = \mu_{\text{max}} \left( 1 - K_s \frac{1}{K_s + S_0} \right) = 0.5 \text{ hr}^{-1} \left( 1 - \frac{2}{\sqrt{2} + 50} \right) = 0.402 \text{ hr}^{-1} \]

b)

Get the concentration of substrate coming out of first tank.

\[ S_1 = \frac{D \cdot K_s}{\mu_{\text{max}} - D} = \frac{(0.402)(2)}{0.5 - 0.402} = 8.2 \text{ g/L} \]

Get biomass concentration coming out of first tank and into second tank.

\[ X_1 = Y \left( S_0 - \frac{D \cdot K_s}{\mu_{\text{max}} - D} \right) = 1 \left( 50 - \frac{(0.402)(2)}{0.5 - 0.402} \right) = 41.8 \text{ g/L} \]

For subsequent tanks, use:

\[ D(S_1 - S_2) - \frac{\mu_{\text{max}} S_2 X_2}{Y(S_2 + K_s)} = 0 \]

Use yield coefficient \( Y \) to substitute for \( X_2 \): \( X_2 = Y(S_1 - S_2) \).

\[ D(S_1 - S_2) - \frac{\mu_{\text{max}} S_2 (X_1 + Y(S_1 - S_2))}{Y(S_2 + K_s)} = 0 \]

Use goal seek in Excel to find:

\[ S_2 = 0.293 \text{ g/L} \]

Therefore, 2 tanks suffice.