Quiz Question:

The following reaction is to be carried out in the liquid phase

\[ \text{NaOH} + \text{CH}_3\text{COOC}_2\text{H}_5 \longrightarrow \text{CH}_3\text{COO}^-\text{Na}^+ + \text{C}_2\text{H}_5\text{OH} \]

The initial concentrations are 0.2 M in NaOH and 0.25 M in CH\textsubscript{3}COOC\textsubscript{2}H\textsubscript{5} with k=5.2 \times 10^{-5} \text{ m}^3/\text{mol s} at 20 °C with E = 42,810 J/mol. Design a set of operating conditions to produce 200 mol/day of ethanol in a semibatch reactor and not operate above 35° C and below a concentration of NaOH of 0.02 M. The semibatch reactor you have available is 1.5 m in diameter and 2.5 m tall.

Differential Equations

Explicit Equations
Writing the Semi-batch Reactor Equations in Terms of Conversion

Startup of CSTRs  MUST USE CONCENTRATION
Semi-batch reactors  Three variables can be used to formulate and solve: Concentration, $C_j$, number of moles, $N_j$, and conversion, $X$.

So far we have talked about writing the semibatch equations in terms of concentration.
For this discussion we will consider a reversible reaction

\[ A + B \rightleftharpoons C + D \]

B is being fed to the vat containing only A initially. The reaction is first order with respect to A and B.

What should we do first?

**Stoichiometric Tables:** *Used to express concentration as a function of conversion.*
\[ \text{A} + \text{B} \leftrightarrow \text{C} + \text{D} \]

<table>
<thead>
<tr>
<th>Species</th>
<th>Initially (mol)</th>
<th>Change (mol)</th>
<th>Remaining (mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>( N_{A0} )</td>
<td>(-N_{A0}X )</td>
<td>( N_A = )</td>
</tr>
<tr>
<td>B</td>
<td>( N_{B0} )</td>
<td></td>
<td>( N_B = )</td>
</tr>
<tr>
<td>C</td>
<td>( N_{C0} )</td>
<td></td>
<td>( N_C = )</td>
</tr>
<tr>
<td>D</td>
<td>( N_{D0} )</td>
<td></td>
<td>( N_D = )</td>
</tr>
</tbody>
</table>
Let's describe the number of moles of A remaining at any time $t$.

<table>
<thead>
<tr>
<th>Number of moles of A in the vat at time $t$</th>
<th>Number of moles of A in the vat initially</th>
<th>Number of moles of A reacted up to time $t$</th>
</tr>
</thead>
</table>

$$N_A = N_{A0} - N_{A0}X$$
How do we describe for species B?

\[
N_B = N_{Bi} + \int_0^t F_{B0} \, dt - N_{A0} X
\]
Species A is the limiting reactant

STEP 1 of Algorithm: **Write the mole balance** in terms of conversion

\[
[\text{Rate in}] - [\text{Rate out}] + [\text{Rate of Gen}] = [\text{Rate of Acc}]
\]

\[
0 - 0 + r_A V(t) = \frac{dN_A}{dt}
\]

\[
N_A = N_{A0}(1 - X) \quad \quad dN_A = -N_{A0}dX
\]

Differentiate with respect to time:

\[
-r_A V(t) = N_{A0} \frac{dX}{dt}
\]
STEP 2: Rate Law

A + B ←→ C + D

Recall reversible

STEP 3: Stoichiometry

\[ C_A = \frac{N_A}{V} = \frac{N_{A0}(1 - X)}{V_0 + v_0 t} \]

Semibatch reactor volume as function of time
STEP 4: Combine

\[-r_A V(t) = N_{A_0} \frac{dX}{dt}\]

\[-r_{A,NET} = k \left( C_A C_B - \frac{C_C C_D}{K_C} \right)\]

\[C_A = \frac{N_{A_0} (1 - X)}{V_0 + v_0 t}\]

\[C_B = \frac{N_{Bi} + F_{B_0} t - N_{A_0} X}{V_0 + v_0 t}\]

\[C_C = \frac{N_{A_0} X}{V_0 + v_0 t}\]

\[C_D = \frac{N_{A_0} X}{V_0 + v_0 t}\]
FOR YOU TO DO -

Equilibrium Conversion pg. 225
Reactive Distillation: CD module – go thru (fair game for a quiz)

Last HOMEWORK FOR CH. 4 – DUE DATE 3/16/07

Last Quiz Question:
Polymath Soln – Worth 5 pts

Worth 10 pts each
P4-23 - Last Lecture example (Finish-Polymath)
P4-32 – On CD parts a and b