Problem 3:

Adiabatic batch reactor. Consider the liquid phase reaction \( A \rightarrow B \) conducted in a batch reactor of volume 2 m\(^3\). The rate constant is given by \( k = 10^5 e^{-\frac{4000}{T}} \) s\(^{-1}\). The reactor is charged with pure A of 4000 moles at a temperature of 300 K. Determine the time it takes to obtain 50% conversion if (a) it is conducted isothermally and (b) it is conducted adiabatically.

Data: \( -\Delta H = 20000 \) J/mol A reacted. \( C_{p-A} = C_{p-B} = 100 \) J/mol/K.

(a) Isothermal case:

For a first order reaction at constant volume and temperature, we know that \( C_A = C_{A0} e^{-kt} \). Initial concentration is 2000 mol/m\(^3\). Final concentration is 1000 mol/m\(^3\). \( k = 2.6012 \times 10^{-4} \) s\(^{-1}\).

Therefore, \( t = -\frac{1}{k} \ln \left( \frac{C_A}{C_{A0}} \right) = 3363 \) s = 56 min

(b) Adiabatic case:

Mass balance: \( \frac{dN_A}{dt} = (r_A) V \)

\( N_{A0} \frac{dx}{dt} = (-r_A) V = kC_{A0} (1-x) V = kN_{A0} (1-x) \)

\( \frac{dx}{dt} = k (1-x) \).

Energy balance: Energy released = energy needed to increase the temperature

\[ (-\Delta H) (-r_A) V = \frac{d}{dt} \left( \sum_i N_i C_{p-i} T \right) \]

In this particular case,

\[ (-\Delta H) (-r_A) V = N_{A0} C_{p-A} \frac{dT}{dt} \]

\[ (-\Delta H) N_{A0} \frac{dx}{dt} = N_{A0} C_{p-A} \frac{dT}{dx} \]

\[ \frac{dT}{dx} = \frac{(-\Delta H)}{C_{p-A}} \]

Therefore, create a table for different values of \( x \) and get values of \( T \), and then values of \( k \), and then evaluate the following expression.
\[ dt = \frac{dx}{k(1-x)} \]

<table>
<thead>
<tr>
<th>( x )</th>
<th>( T(\text{K}) )</th>
<th>( k(\text{s}^{-1}) )</th>
<th>( 1/(k \times (1-x)) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>300</td>
<td>2e-4</td>
<td>4852</td>
</tr>
<tr>
<td>0.1</td>
<td>320</td>
<td>7.2e-4</td>
<td>1544</td>
</tr>
<tr>
<td>0.2</td>
<td>340</td>
<td>0.0022</td>
<td>577</td>
</tr>
<tr>
<td>0.3</td>
<td>360</td>
<td>0.0058</td>
<td>247</td>
</tr>
<tr>
<td>0.4</td>
<td>380</td>
<td>0.0139</td>
<td>120</td>
</tr>
<tr>
<td>0.5</td>
<td>400</td>
<td>0.0306</td>
<td>65.4</td>
</tr>
</tbody>
</table>

Trapezoidal integration shows that 50% conversion comes in approximately 494 seconds.

Precise integration is to be done using the expression for \( T \) in \( k \) and then using numerical integration.

If \( \Delta H \) and \( C_{p-A} \) are functions of temperatures, to find the conversion and temperature for a given time, integrate \( \frac{dx}{dt} \) and \( \frac{dT}{dt} \) together.

i.e.
\[
\frac{dx}{dt} = \frac{(-r_A)V}{N_{A_0}}
\]
\[
\frac{dT}{dt} = \left( -\Delta H \right) \frac{(-r_A)V}{\sum_i N_i C_{p-i}}
\]

To find the time it takes to get a conversion, integrate \( \frac{dt}{dx} \) and \( \frac{dT}{dx} \) together.

i.e.
\[
\frac{dt}{dx} = \frac{N_{A_0}}{(-r_A)V}
\]
\[
\frac{dT}{dx} = \left( -\Delta H \right) \frac{N_{A_0}}{\sum_i N_i C_{p-i}}
\]