Problem 1 (10 pts)

Consider a chemical reaction where species $A$ decomposes to form $B$ and $C$,

$$ A \xrightarrow{k} B + C $$

As you will learn in your kinetics class, there are a few possible ways that this reaction may proceed. From these, we obtain the following equations for the concentration of $A$, $c_A$ as a function of time:

$$ c_A = c_A^0 \exp (-kt) \quad \text{First order reaction} \quad (1) $$

$$ c_A = \frac{c_A^0}{1 + ktc_A^0} \quad \text{Second order reaction} \quad (2) $$

If we take the natural log of (1) then we find

$$ \ln c_A = \ln c_A^0 - kt. $$

Therefore, if we plot $\ln c_A$ as a function of $t$ then we should obtain a straight line if the reaction is first order. Similarly, if we rearrange (2) we find

$$ \frac{1}{c_A} = \frac{1}{c_A^0} + kt. $$

Therefore, if we plot $\frac{1}{c_A}$ as a function of $t$ then we should obtain a straight line if the reaction is second order.

From the data shown in Table 1, make plots of $\frac{1}{c_A}$ versus $t$ and $\ln c_A$ versus $t$, and plot these on the same figure. Use them to conclude whether the reaction is first or second order. Be sure to label your plot axes.

You may use either MATLAB or Excel to solve this problem. In either case, you must clearly indicate whether the reaction is first or second order.

<table>
<thead>
<tr>
<th>$t$ (s)</th>
<th>0</th>
<th>0.43</th>
<th>0.86</th>
<th>1.29</th>
<th>1.71</th>
<th>2.14</th>
<th>2.57</th>
<th>3.00</th>
</tr>
</thead>
<tbody>
<tr>
<td>$c_A$ (mol/cm$^3$)</td>
<td>0.96</td>
<td>0.64</td>
<td>0.40</td>
<td>0.27</td>
<td>0.18</td>
<td>0.12</td>
<td>0.07</td>
<td>0.049</td>
</tr>
</tbody>
</table>

Table 1: The concentration of species $A$ as a function of time.
**Problem 2 (10 pts)**

The ideal gas law can be written as

\[ \rho = \frac{pW}{RT} \]

where \( \rho \) is the density of the gas, \( W \) is its molecular weight, \( R = 0.0820574587 \ \text{L} \cdot \text{atm} / \text{mol} \cdot \text{K} \) is the gas constant, and \( T \) is the temperature.

Plot the density of Hydrogen (H\(_2\)), Nitrogen (N\(_2\)), Argon (Ar), and Chlorine (Cl\(_2\)) as functions of temperature at pressures of 1, 5, and 10 atm. Your plot should look like Figure 1. You must use loops to accomplish this. An algorithm might look like:

1. Define a vector of molecular weights
2. Define a vector of species names
3. Define the temperature points
4. for each species
   - calculate the density at all temperatures for \( p=1 \text{ atm} \).
   - calculate the density at all temperatures for \( p=5 \text{ atm} \).
   - calculate the density at all temperatures for \( p=10 \text{ atm} \).
5. select the appropriate sub-plot
6. plot the density vs. temperature for each pressure
7. create axis labels and legend
8. end

![Figure 1: Your plot for Problem 2 should look like this.](image-url)
Problem 3 (10 pts)

The heat capacity of a material indicates how much heat (thermal energy) the material must absorb to change its temperature. It is often fit to a polynomial form such as

\[ C_p = a + bT + cT^2 + dT^3, \]  \hspace{1cm} (3)

\[ C_p = a + bT + cT^{-2}. \]  \hspace{1cm} (4)

Table 2 shows the coefficients for several chemical compounds, along with the equation that should be used to calculate \( C_p \). For example, to determine \( C_p \) for steam we use (3):

\[ C_p = (33.46) + (6.88 \times 10^{-3}) T + (7.604 \times 10^{-6}) T^2 + (-3.593 \times 10^{-9}) T^3, \]

and the units for temperature would be °C. The units of \( C_p \) would be \( \frac{J}{mol \cdot °C} \). Similarly, for CaCO\(_3\), we use (4):

\[ C_p = (82.34) + (4.975 \times 10^{-2})T - (1.287 \times 10^6)T^{-2}, \]

and the units for temperature would be K and the units for \( C_p \) would be \( \frac{J}{mol \cdot K} \).

<table>
<thead>
<tr>
<th>Compound</th>
<th>Eqn.</th>
<th>T Unit</th>
<th>( a )</th>
<th>( b )</th>
<th>( c )</th>
<th>( d )</th>
<th>T Range (units of T)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hydrogen (H(_2))</td>
<td>(3)</td>
<td>Celsius</td>
<td>28.84</td>
<td>7.65 \times 10^{-5}</td>
<td>3.288 \times 10^{-6}</td>
<td>-8.698 \times 10^{-10}</td>
<td>0-1500</td>
</tr>
<tr>
<td>Calcium Carbonate (CaCO(_3))</td>
<td>(4)</td>
<td>Kelvin</td>
<td>82.34</td>
<td>4.975 \times 10^{-2}</td>
<td>-1.287 \times 10^{-6}</td>
<td>-</td>
<td>273-1033</td>
</tr>
<tr>
<td>Steam (H(_2)O)</td>
<td>(3)</td>
<td>Celsius</td>
<td>33.46</td>
<td>6.88 \times 10^{-3}</td>
<td>7.604 \times 10^{-6}</td>
<td>-3.593 \times 10^{-9}</td>
<td>0-1500</td>
</tr>
<tr>
<td>Copper (Cu)</td>
<td>(3)</td>
<td>Kelvin</td>
<td>22.76</td>
<td>6.117 \times 10^{-3}</td>
<td>0</td>
<td>0</td>
<td>273-1357</td>
</tr>
<tr>
<td>Propane (C(_3)H(_8))</td>
<td>(3)</td>
<td>Celsius</td>
<td>68.032</td>
<td>0.2259</td>
<td>-1.311 \times 10^{-4}</td>
<td>3.171 \times 10^{-8}</td>
<td>0-1200</td>
</tr>
</tbody>
</table>

Table 2: Heat capacity data for several compounds. Units for \( C_p \) are \( \frac{J}{mol \cdot K} \) or \( \frac{J}{mol \cdot °C} \), depending on the unit of temperature indicated in the table. Data are from Elementary Principles of Chemical Processes, Felder & Rousseau, 2\(^{nd}\) edition, (1986).

Write a MATLAB script to have the user select the compound and then plot \( C_p \) as a function of \( T \) over the valid temperature range for that compound. Be sure to label the axes appropriately.

You may want to start with the file posted on the class web site.