10c Computational Study of System Dynamics (Mathcad)

These five problems are similar to those found in a textbook. Instead of giving keystrokes, only the “flow” of solving the problem is given.

**#1** Naturally occurring atomic iron consists of 5.82 % $^{54}$Fe ($A = 53.940$ u), 91.66 % $^{56}$Fe ($A = 55.935$ u), 2.19 % $^{57}$Fe ($A = 56.935$ u), and 0.33 % $^{58}$Fe ($A = 57.993$ u). Determine the value of the average atomic mass of Fe (the value that appears in the periodic table).

A) table of $w$ values  
B) table of $A$ values  
C) determine the index $i$  
D) average is found by summing up over $i$ the product of $w_i A_i$

**#2** Calculate the number of moles of $(C_2H_5)_2$ that will occupy 62.9 L at 175 °C and 0.750 bar assuming van der Waals behavior

\[
\left( P + \frac{an^2}{V^2} \right) (V - nb) = nRT
\]

where $a = 19.00$ L$^2$ bar mol$^{-2}$, $b = 0.1214$ L mol$^{-1}$, and $R = 0.08314$ L bar K$^{-1}$ mol$^{-1}$.

A) define vol(n) as above equation with $nRT$ moved to the right side  
B) use seed guess as $n = 1$ or value from ideal gas law  
C) use root function to solve for $n$ with limits between 0 and 100

**#3** A quick graphical method for determining the order of reaction $n$ and rate constant $k$ is to make a series of plots of functions of concentration $C$ against time $t$ according to the following table

<table>
<thead>
<tr>
<th>$n$</th>
<th>y axis</th>
<th>x axis</th>
<th>slope ($m$)</th>
<th>intercept ($b$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>$C$</td>
<td>$t$</td>
<td>$-k_0$</td>
<td>$C_0$</td>
</tr>
<tr>
<td>1</td>
<td>$\ln C$</td>
<td>$t$</td>
<td>$-k_1$</td>
<td>$\ln C_0$</td>
</tr>
<tr>
<td>2</td>
<td>$C^{-1}$</td>
<td>$t$</td>
<td>$k_2$</td>
<td>$C_0^{-1}$</td>
</tr>
<tr>
<td>3</td>
<td>$C^2$</td>
<td>$t$</td>
<td>$2k_3$</td>
<td>$C_0^{-2}$</td>
</tr>
</tbody>
</table>

Determine the reaction order and rate constant for the decomposition of nitrogen trioxide

<table>
<thead>
<tr>
<th>$t$/s</th>
<th>0</th>
<th>184</th>
<th>526</th>
<th>867</th>
<th>1877</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C$/M</td>
<td>2.33</td>
<td>2.08</td>
<td>1.67</td>
<td>1.36</td>
<td>0.72</td>
</tr>
</tbody>
</table>
A) table of C values
B) table of t values
C) determine the index i
D) create four separate plot C, ln C, 1/C, 1/C^2 against t (no calculations necessary!)
E) the linear plot identifies the reaction order
F) calculate k

#4 The Arrhenius equation implies that a plot of ln k against 1/T is linear with a slope \( m = -E_a/R \) where \( T \) is the absolute temperature, \( k \) is the rate constant, \( E_a \) is the activation energy, and \( R = 8.314 \text{ J K}^{-1} \text{ mol}^{-1} \). Calculate the activation energy for the decomposition of acetaldehyde

<table>
<thead>
<tr>
<th>( T/(^\circ\text{C}) )</th>
<th>430</th>
<th>460</th>
<th>486</th>
<th>518</th>
<th>538</th>
<th>563</th>
<th>592</th>
</tr>
</thead>
<tbody>
<tr>
<td>( k )</td>
<td>0.0110</td>
<td>0.0352</td>
<td>0.105</td>
<td>0.343</td>
<td>0.79</td>
<td>2.14</td>
<td>4.95</td>
</tr>
</tbody>
</table>

A) table of \( T \) values
B) table of \( k \) values
C) determine the index i
D) define lnk, and display (if desired)
E) define invT, as 1/(T + 273) and display (if desired)
F) find the slope and the intercept using Mathcad functions
G) define the least squares line for plotting (see Mathcad Chat #8)
H) plot lnk and the least squares line
I) calculate \( E_a \) from the slope

#5 The half lives for the nuclear decay of \(^{47}\text{Ca}\) and \(^{47}\text{Sc}\) are 4.7 d and 3.4 d, respectively.

\[
\begin{align*}
^{20}\text{Ca} & \quad ^{47}\text{Ca} & \quad ^{47}\text{Sc} & \quad ^{47}\text{Ti} \\
& \quad k_1 & \quad k_2 & \quad \text{decay}
\end{align*}
\]

Starting with one mole of \(^{47}\text{Ca}\), prepare a plot of the amount of each nuclide as a function of time up to 25 d using the differential rate laws. The integrated rate law for \(^{47}\text{Sc}\) is given in the \(jCE\) paper by Andraos. Find the time at which the amount of \(^{47}\text{Sc}\) is a maximum.

A) this looks like Mathcad Chat #11!
B) find the two rate constants by \( k = (\ln 2)/t_{1/2} \)
C) because \( t \) was used in an earlier exercise, it might be best to reset the value 0 to 100
D) define Bconc(t) in terms of the equation from Andraos
E) define Brate(t) as the derivative with respect to \( t \) of Bconc(t)
F) find the time for the maximum of B by find the root of Brate(t)