

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 $(\text{C}_2\text{H}_5)_2$ 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 $a = 19.00 \text{ L}^2 \text{ bar mol}^{-2}$, $b = 0.1214 \text{ L mol}^{-1}$, and $R = 0.08314 \text{ L bar K}^{-1} \text{ mol}^{-1}$.

- 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

n	y axis	x axis	slope (m)	intercept (b)
0	C	t	$-k_0$	C_0
1	$\ln C$	t	$-k_1$	$\ln C_0$
2	C^{-1}	t	k_2	C_0^{-1}
3	C^{-2}	t	$2k_3$	C_0^{-2}

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

$t/(s)$	0	184	526	867	1877
$C/(M)$	2.33	2.08	1.67	1.36	0.72

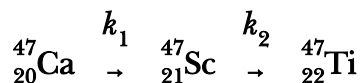
- A) table of C values
- B) table of t values
- C) determine the index i
- D) create four separate plot C , $\ln C$, $1/C$, $1/C^2$ against t (no calculations necessary!)
- E) the linear plot identifies the reaction order
- F) calculate k

#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

$T/(\text{°C})$	430	460	486	518	538	563	592
k	0.0110	0.0352	0.105	0.343	0.79	2.14	4.95

- A) table of T values
- B) table of k values
- C) determine the index i
- D) define $\ln k_i$ and display (if desired)
- E) define $\text{inv}T_i$ 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 $\ln k$ and the least squares line
- I) calculate E_a from the slope

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



Starting with one mole of ^{47}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}Sc is given in the *JCE* paper by Andraos. Find the time at which the amount of ^{47}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 $\text{Bconc}(t)$ in terms of the equation from Andraos
- E) define $\text{Brate}(t)$ as the derivative with respect to t of $\text{Bconc}(t)$
- F) find the time for the maximum of B by find the root of $\text{Brate}(t)$