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

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 $R = 8.314\ \mathrm{J\ K^{-1}\ mol^{-1}}$. Calculate the activation energy for the decomposition of acetaldehyde

T/(°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 lnk_i and display (if desired)
E) define invT_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 lnk 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.

$$^{47}_{20}\mathrm{Ca} \xrightarrow{k_1} {}^{47}_{21}\mathrm{Sc} \xrightarrow{k_2} {}^{47}_{22}\mathrm{Ti}$$

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 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)