

## 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 %  $^{54}\text{Fe}$  ( $A = 53.940$  u), 91.66 %  $^{56}\text{Fe}$  ( $A = 55.935$  u), 2.19 %  $^{57}\text{Fe}$  ( $A = 56.935$  u), and 0.33 %  $^{58}\text{Fe}$  ( $A = 57.993$  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

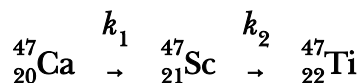
- A) table of  $C$  values
- B) table of  $t$  values
- C) determine the index  $i$
- D) create four separate plot  $C$ ,  $\ln C$ ,  $1/C$ ,  $1/C^2$  against  $t$  (no calculations necessary!)
- E) the linear plot identifies the reaction order
- F) calculate  $k$

**#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  $^{47}\text{Ca}$  and  $^{47}\text{Sc}$  are 4.7 d and 3.4 d, respectively.



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  $\text{Bconc}(t)$  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  $\text{Brate}(t)$