CHG 4304 Advanced Materials in Chemical Engineering

University of Ottawa

Assignment #2 Solution

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2. 1)
Given:
The gadolinium bar dimensions are 3.2 x 4.8 mm and a length of 25 cm.
The heating zone travels at a speed of 2.5 cm/h for 20 times from left to right over the bar.
The length of the heating zone is 4 cm.
Composition of impurities initially in bar and at various distances from the left side of the bar after 20 passes of the heated zone is given in the table below:

Element	Initial concentration in bar (ppm)	Conc. 1 cm from the left side of the bar (ppm)	Conc. 1/4 from the left side of the bar (ppm)	Conc. middle of the bar (ppm)	Conc. 3/4 from the left side of the bar (ppm)
C	320	210	288	341	419
Fe	10	1	0.3	2.5	68
W	5	1	1.5	2	8
Al	4	0.2	0.6	1	6
Si	2	0.2	0.25	0.5	2
Ti	2	0.1	0.1	0.9	7
Zr	9	12	10	9	60
Cu	2	0.4	0.3	0.3	10

a) Find the value of k_{eff} for each impurity after 20 passes.
b) Use the Hume Rothery rules for solid solutions to explain the differences in the values of k_{eff} observed amongst the 8 impurities? Discuss why you can or cannot use these rules. Support your answer numerically.

Solution:

1- To determine the effective partition coefficient (k_{eff}) for each impurity, equation (8.20) has to be applied.

$$\frac{x_s}{x_0^L} = 1-(1-k_{eff})\exp\left(-\frac{k_{eff}}{L_{zone}}y\right)$$

$$0 = 1-(1-k_{eff})\exp\left(-\frac{k_{eff}}{L_{zone}}y\right)-\frac{x_s}{x_0^L}$$

Note: Equation (8.20) can be used only when the concentration at specific position is equal or less than the initial concentration. This means that Eq. (8.20) cannot be applied for the concentration at ¾ of the length.
By inserting the compositions in excel file and using Solver, k_{eff} can be found by reducing the sum of the squares.

Element	**Initial concentration**	**Concentration at 1cm**	**Concentration at ¼ of the length**	**Concentration at the middle**	**Concentration at ¾ of the length**	$X_{at\ 1cm} / X_{initial}$	$X_{at\ 1/4} / X_{initial}$	$X_{at\ mid} / X_{initial}$	k_{eff}	X_s/X_0 (eq.8.20) at 1cm	X_s/X_0 (eq.8.20) at ¼ of the length	X_s/X_0 (eq.8.20) at the middle	$[(X_{at\ 1cm} / X_{initial}) - (X_s/X_0\ (eq.8.20)\ at\ 1cm)]^2$	$[(X_{at\ 1/4} / X_{initial}) - (X_s/X_0\ (eq.8.20)\ at\ 1/4\ of\ the\ length)]^2$	$[(X_{at\ mid} / X_{initial}) - (X_s/X_0\ (eq.8.20)\ at\ the\ middle)]^2$	**Sum of the three squares for each element**
C	320	210	288	341	419	0.656	0.9	1.065	**0.652**	0.704	0.874	0.954	0.0023	0.0006	0.0123	0.015
Fe	10	1	0.3	2.5	68	0.1	0.03	0.25	**0.052**	0.065	0.127	0.196	0.0012	0.0095	0.0028	0.013
W	5	1	1.5	2	8	0.2	0.3	0.4	**0.131**	0.159	0.293	0.424	0.0016	4.7E-5	0.0006	0.002
Al	4	0.2	0.6	1	6	0.05	0.15	0.25	**0.064**	0.079	0.154	0.235	0.0008	2E-5	0.0002	0.001
Si	2	0.2	0.25	0.5	2	0.1	0.125	0.25	**0.06**	0.073	0.144	0.220	0.0006	0.0003	0.0008	0.001
Ti	2	0.1	0.1	0.9	7	0.05	0.05	0.45	**0.089**	0.109	0.207	0.311	0.0035	0.0249	0.0193	0.047
Zr	9	12	10	9	60	1.333	1.11	1	**1.487**	1.335	1.047	10..4	6.2E-6	0.004	2.2E-5	0.004
Cu	2	0.4	0.3	0.3	10	0.2	0.15	0.15	**0.056**	0.0693	0.135	0.208	0.017	0.0002	0.0033	0.020

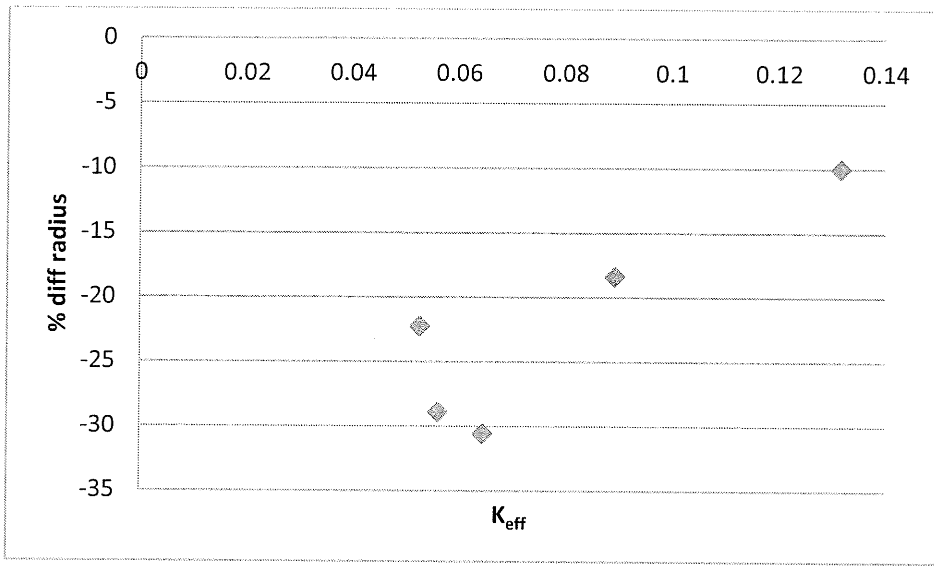
2- The Hume Rothery rules for solid solution can be used to explain the differences in the k_{eff}.
3- The conditions favoring substitutional solid solution are:
   - Diff % in radius < 15%
   - Proximity in periodic table (i.e. similar electronegativities)
   - Valency, All else being equal, a metal will have a greater tendency to dissolve a metal of higher valency than one of lower valency.

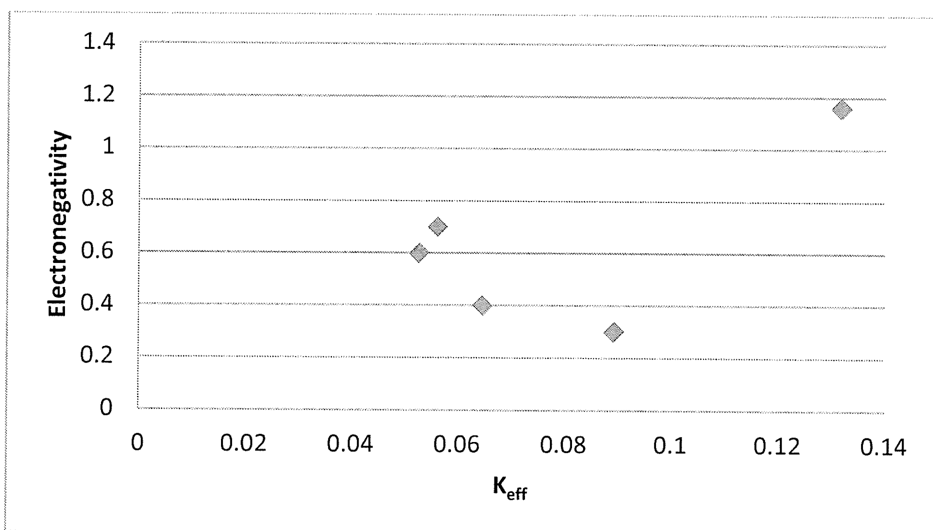
The physical properties of the impurities are in the table below:

Element	**Atom radius (R) nm**	**% diff radius** $\left(\frac{R - R_{Gad}}{R_{Gad}}\right) * 100$	**Electronegativity (E)**	**E-E$_{Gad}$**	**Structure**	**Ox**	k_{eff}
Gadolinium	0.18		1.2		HCP	3	
C	0.077	-57.2	2.55	1.35		4	**0.652**
Fe	0.14	-22.2	1.8	0.6	BCC	3	**0.052**
W	0.162	-10	2.36		BCC	6	**0.131**
Al	0.125	-30.5	1.6	1.16	FCC	3	**0.064**
Si	0.11	-38.88	1.8	0.6		4	**0.06**
Ti	0.147	-18.3	1.5	0.3	HCP	4	**0.089**
Zr	0.16	-11.1	1.33	0.13	HCP	4	**1.487**
Cu	0.128	-28.8	1.9	0.7	FCC	4	**0.056**

From the calculation in the above tables:

- The element **Fe, Al**, **Si**, **Ti**, **Cu**, are less soluble as the % diff radius > 15%, and the k_{eff} values are very low.
- **W** is more soluble than the above as % diff radius < 15%.
- **Zr** is the most soluble as k_{eff} is the highest, % diff radius < 15%, its electronegativity is very close to Gadolinium and it has the same structure (HCP) as Gadolinium.





Assignment # 2

2.2 Solution :

$$1 \text{ Barrer} = 3.348 * 10^{-19} \frac{\text{kmol.m}}{m^2.s.pa} = 7.5 * 10^{-14} \frac{cm^3 \text{ STP} . cm}{cm^2. s. pa}$$

a)

$$J = P_M * \frac{\Delta P}{\Delta x}$$

$$J = 550 * 3.348 * 10^{-19} \frac{\cancel{\text{kmol}}, \cancel{m}}{m^2 s, \cancel{pa}} * \frac{(880-101) * 10^3 \cancel{pa}}{45 * 10^{-6} \cancel{m}} * \frac{1000 \text{ mol}}{\cancel{\text{kmol}}}$$

$$J = 31876.68 * 10^{-7} \frac{\text{mol}}{m^2.s} = 3.1876 * 10^{-7} \frac{\text{mol}}{cm^2.s}$$

b)

$$\text{flowrate} = J * A = 31876.68 * 10^{-7} \frac{\text{mol}}{m^2.s} * 10 m^2 * \frac{3600 s'}{hr}$$

$$= 114.75 \frac{\text{mol}}{hr}$$

c)

$$P_M = P_{M_0} \exp\left(-\frac{Q_p}{RT}\right)$$

$$Q_p = -\left(\ln \frac{P_M}{P_{M_0}}\right) * RT$$

$$Q_p = -\left(\ln \frac{550 * 7.5 * 10^{-14} \frac{cm^3 STP\ cm}{cm^2, s.\ pa}}{1.2 * 10^{-8} \frac{cm^3\ STP\ cm}{cm^2 . s . pa}}\right) * 8.314 \frac{J}{mol.k} * 325 K$$

$$= -\ln(0.00343) * 8.314 * 325$$

$$Q_p = 15.328 \text{ kJ/mol}.$$

$$P_{M_{500k}} = P_{M_0} \exp\left(\frac{-Q_P}{RT}\right)$$

$$P_{M_{500k}} = 1.2 * 10^{-8} \frac{cm^3\ STP\ cm}{cm^2 \cdot s \cdot Pa} \exp\left(\frac{-15328\ J/mol}{8.314\ \frac{J}{mol\cdot K} * 500k}\right)$$

$$P_{M_{500k}} = 3 * 10^{-10} \frac{cm^3\ STP\ cm}{cm^2 \cdot s \cdot Pa} = 1.339 * 10^{-15} \frac{kmol \cdot m}{m^2 \cdot s \cdot Pa}$$

$$J_{500k} = P_{M_{500k}} * \frac{\Delta P}{\Delta x}$$

$$= 1.339 * 10^{-15} \frac{kmol \cdot m}{m^2 \cdot s \cdot Pa} * \frac{(880-101) * 10^3\ Pa}{45 * 10^{-6}\ m}$$

$$J_{500k} = 23.179 * 10^{-6} \frac{kmol}{m^2 \cdot s} = 2.3179 * 10^{-2} \frac{mol}{m^2 \cdot s}$$

$$\text{flowrate}_{(500k)} = 2.3179 * 10^{-2} \frac{mol}{m^2 \cdot s} * 10\ m^2$$

$$= 0.23179 \frac{mol}{s} * \frac{3600\ s}{hr}$$

$$\text{Flowrate}_{500k} = 834.444 \frac{mol}{hr.} = 0.834 \frac{kmol}{hr.}$$

Assignment # 2

2.3 Solution:

a) The maximum load ~~that~~ can be applied without plastic deformation (F_y)

$$F_y = \sigma_y A_o \quad \text{------} \quad eq\ (7.1)$$

$$F_y = 290 * 10^6 \frac{N}{m^2} * 600 * 10^{-6} m^2$$

$$\boxed{F_y = 174000\ N}$$

b) The maximum length to which the sample may be deformed without plastic deformation is determined from eq 7.2 and 7.5

$$\varepsilon = \frac{L_i - L_o}{L_o} = \frac{L_i}{L_o} - 1 \Rightarrow$$

$$L_i = L_o(\varepsilon + 1)$$

and $$\varepsilon = \frac{\sigma}{E} \quad \text{------} \quad (7.5)$$

$$L_i = L_o\left(\frac{\sigma}{E} + 1\right)$$

$$L_i = 140\left(\frac{290\ Mpa}{115 * 10^3\ Mpa} + 1\right)$$

$$L_i = 140.353\ mm$$