Homework 6 Due April 27

1. Problem 9.8. Add (K) Plot the major ions on the trilinear diagram with three x symbols.

2. The following analyses of water are from the perched aquifer beneath the Pantex Plant.

Constituent	Measurement
Calcium	34.6 mg/L
Magnesium	33.4 mg/L
Sodium	26.5 mg/L
Potassium	5.7 mg/L
Bicarbonate	298 mg/L
Sulfate	26.0 mg/L
Chloride	24.0 mg/L
Temperature	15°C
pH	7.28

[a] Calculate the ionic strength of the water.
[b] Plot the major ions on the trilinear diagram with three circle (o) symbols.
[c] Find the P_{CO2} in bar for this water in the aquifer. Consider only the carbonate equilibrium, and use the activities.
[d] When the water is brought to the surface, it comes in contact with the atmosphere. The CO_2 degasses and the P_{CO2} in the water drops to $10^{-3.5}$ bar, with the other dissolved concentrations (except pH) and temperature are unchanged. Find the pH of the water after it was brought to the surface. Consider only the carbonate equilibrium and use the activities.

4. Problem 10.1.

5. Problem 10.5.

6. Problem 10.7.

Cations

Anions
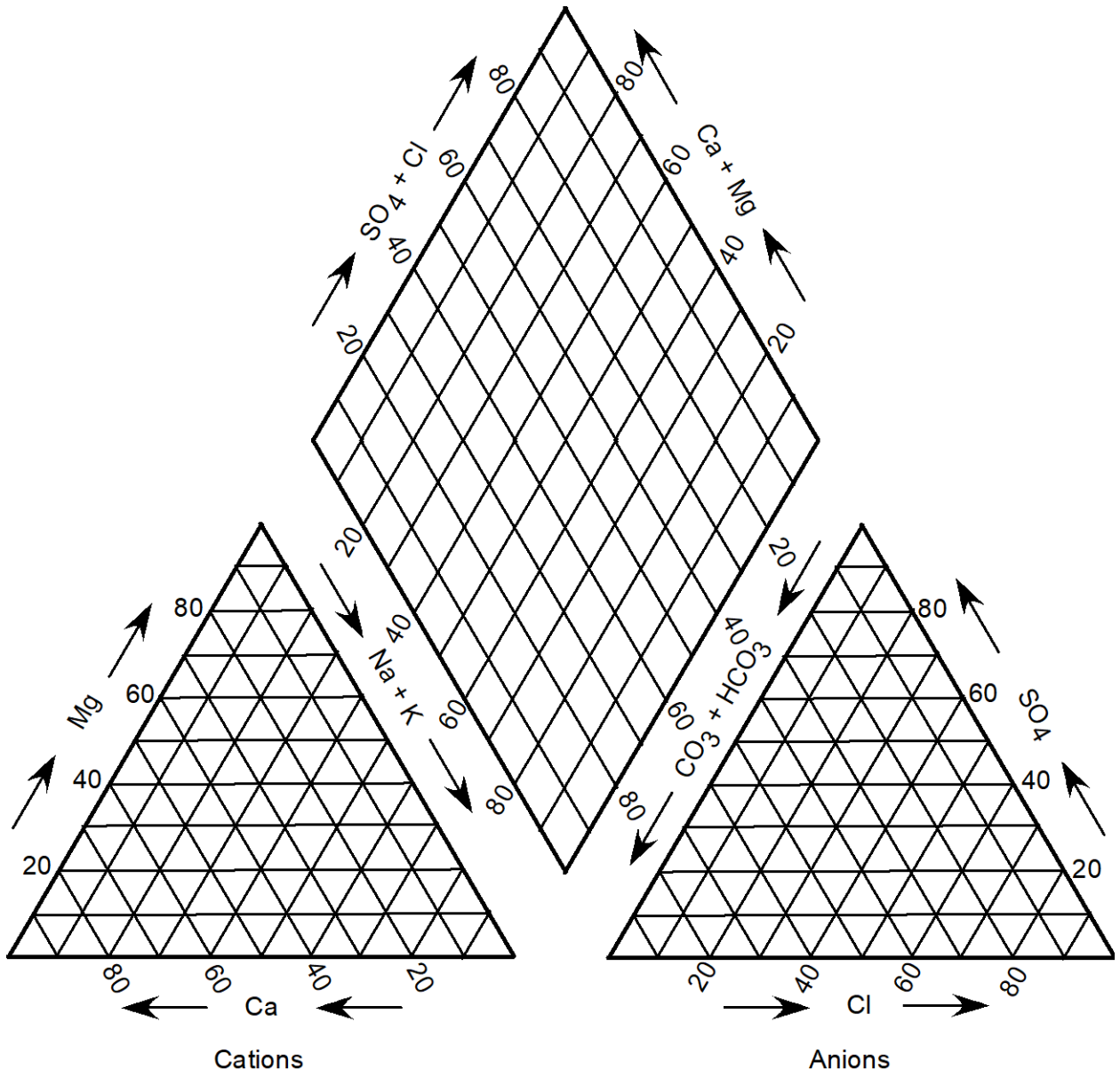
9d/ Given: K_{sp} for $CaSO_4 = 10^{-4.5}$

Find: Solubility of Ca^{2+} at equilibrium w/ $CaSO_4$.

Ignore other molecules

$$CaSO_4 \rightleftharpoons Ca^{2+} + SO_4^{2-}$$

$$K_{sp} = [Ca^{2+}][SO_4^{2-}] = 10^{-4.5}$$

\# moles $Ca^{2+} = $ \# moles SO_4^{2-}

$$K_{sp} = [Ca^{2+}]^2 = 10^{-4.5}$$

$$\boxed{\begin{array}{l} [Ca^{2+}] = 10^{-2.25} \text{ mol/L} \\ \\ [Ca^{2+}] = 5.6 \times 10^{-3} \text{ moles/L} \end{array}}$$

Problem 9.8
Given: Tabulated groundwater analyses with major ions, pH = 7.8, TDS = 542 mg/L
Find: See statements in each section below

You can follow the format recommended on page 382. $\boxed{10}$[a] $\boxed{10}$[c] $\boxed{5}$[d] $\boxed{10}$[e]

$\underline{80\ total}$

Ion	Formula Weight (g)	Charge z_i	Ionic Radius a_i	Conc. (mg/L)	m_i (mol/L)	Activity Coef. γ_i	Chemical Activity α_i	Conc. (meq/L)
Cations								
Calcium	40	2	6	83.27	2.08E-03	0.673	1.40E-03	4.16
Magnesium	24.3	2	8	24.32	1.00E-03	0.887	6.88E-04	2.00
Sodium	23	1	4	18.33	7.97E-04	0.901	7.18E-04	0.80
Potassium	39.1	1	3	2.34	5.98E-05	0.898	5.37E-05	0.06
Total				128.26				7.02
Anions								
Sulfate	96	-2	4	23.45	2.44E-04	0.658	1.61E-04	0.49
Bicarbonate	61	-1	4	366.78	6.01E-03	0.901	5.42E-03	6.01
Chloride	35.5	-1	3	12.5	3.52E-04	0.898	3.16E-04	0.35
Total				402.73				6.85

[b] Ionic Strength

$$I = \frac{1}{2}\sum m_i z_i^2$$ I =   1.03E-02 $\boxed{5}$

[c] Activity Coefficient   Assume T = 25 C unless told otherwise

$$-\log \gamma_i = \frac{A z_i^2 \sqrt{I}}{1 + a_i B \sqrt{I}}$$ A =   0.5085
                                                             B =   0.3281

[d] Activity $\boxed{\alpha_i = \gamma_i m_i}$

[e] Convert to meq/L

$$\boxed{\#\frac{meq}{L} = \#\frac{mg}{L}\frac{meq}{\#mg}}$$

[f] Cation-anion balance

$$Error = 100\left|\frac{\sum_{cations} m_i z_i - \sum_{anions} m_i z_i}{\sum_{cations} m_i z_i + \sum_{anions} m_i z_i}\right|$$ Error =   1.21   % OK $\boxed{5}$

[g] K_{iap} of CaSO$_4$

$$\boxed{K_{iap} = \alpha_{Ca^{2+}} \cdot \alpha_{SO_4^{2-}}}$$ K_{iap} =   2.25E-07 $\boxed{5}$

[h] Compare K_{iap} to K_{sp} K_{sp} =   3.16E-05 > K_{iap} so undersaturated with respect to anhydrite $\boxed{5}$

[i] Find K_{iap} of calcite CaCO$_3$
   No CO$_3^{2-}$ concentration given, so assume equilibrium dissociation of bicarbonate

$$HCO_3^- \Leftrightarrow H^+ + CO_3^{2-}$$
$$K_{HCO_3^-} = \frac{\alpha_H \cdot \alpha_{CO_3^{2-}}}{\alpha_{HCO_3^-}} = 10^{-10.33}$$
$$\alpha_{CO_3^{2-}} = \frac{10^{-10.33}\alpha_{HCO_3^-}}{\alpha_H}$$
$$K_{iap} = \alpha_{Ca^{2+}} \cdot \alpha_{CO_3^{2-}}$$

α_{H^+} = 10^{-pH} pH =   7.8
$\alpha_{CO3^{2-}}$ =   1.60E-05

K_{iap} =   2.24E-08 $\boxed{10}$

[j] Compare Kiap to Ksp K_{sp} =   3.98E-09 < K_{iap} so oversaturated with respect to calcite $\boxed{5}$

[k] Trilinear diagram

Ion	Conc. (meq/L)	Percent of Total
Cations		
Calcium	4.16	59.3
Magnesium	2.00	28.5
Sodium	0.86	12.2
Total	7.02	
Anions		
Sulfate	0.49	7.1
Bicarbonate	6.01	87.7
Chloride	0.35	5.1
Total	6.85	

10 values + plot (next page)
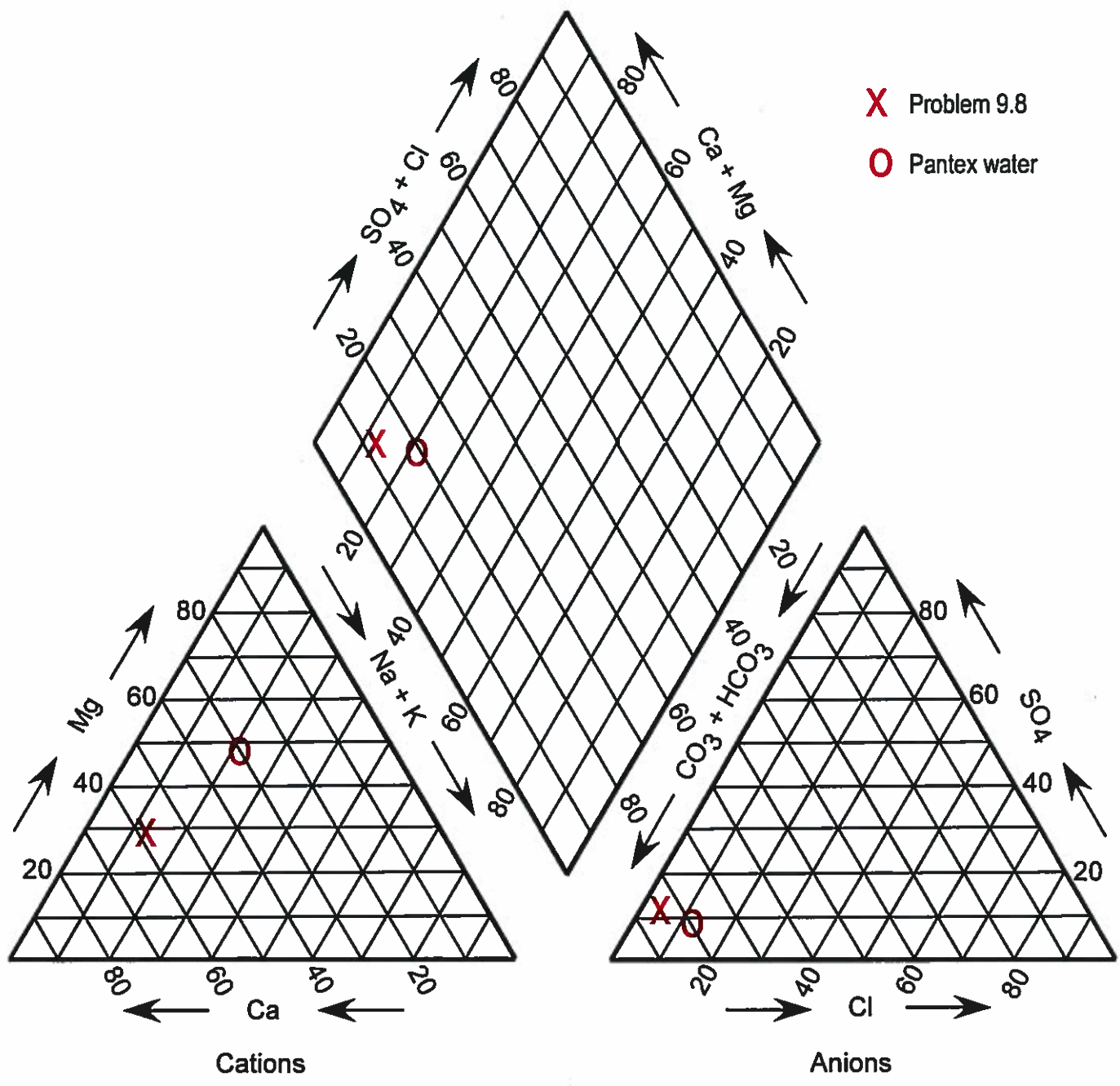
60 total

Problem 3
Given: Pantex perched groundwater, pH = 7.28, T = 15 C
Find: See statements in each section below

You can follow the format recommended on page 382.

[10] *[10]* *[5]*

	Formula Weight (g)	Charge z_i	Ionic Radius a_i	Conc. (mg/L)	m_i (mol/L)	Activity Coef. γ_i	Chemical Activity α_i	Conc. (meq/L)
Ion						[a] [c]	[d]	[e]
Cations								
Calcium	40	2	6	34.6	8.65E-04	0.699	6.04E-04	1.73
Magnesium	24.3	2	8	33.4	1.37E-03	0.711	9.77E-04	2.75
Sodium	23	1	4	26.5	1.15E-03	0.910	1.05E-03	1.15
Potassium	39.1	1	3	5.7	1.46E-04	0.907	1.32E-04	0.15
Total				100.2				5.78
Anions								
Sulfate	96	-2	4	26	2.71E-04	0.685	1.86E-04	0.54
Bicarbonate	61	-1	4	298	4.89E-03	0.910	4.44E-03	4.89
Chloride	35.5	-1	3	24	6.76E-04	0.907	6.13E-04	0.68
Total				348				6.10

[a] Ionic Strength

$$I = \frac{1}{2}\sum m_i z_i^2$$

I =   8.45E-03 *[5]*

[b] Trilinear diagram

Ion	Conc. (meq/L)	Percent of Total
Cations		
Calcium	1.73	29.9
Magnesium	2.75	47.6
Sodium	1.30	22.5
Total	5.78	
Anions		
Sulfate	0.54	8.9
Bicarbonate	4.89	80.0
Chloride	0.68	11.1
Total	6.10	

[10] values + plot (previous page)

[c] Activity Coefficient   Assume T = 15 C

$$-\log \gamma_i = \frac{Az_i^2\sqrt{I}}{1+a_i B\sqrt{I}}$$

A =   0.5
B =   0.3262
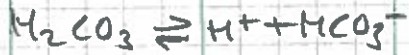
Activity

$$\alpha_i = \gamma_i m_i$$

Continue on hand calculations

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[c] Find P_{CO_2} in aquifer. Only carbonate equilibrium, use activities.

$$CO_2 + H_2O \rightleftharpoons H_2CO_3$$

$$K_{CO_2} = \frac{\alpha_{H_2CO_3}}{P_{CO_2}} = 10^{-1.34} \qquad @ \ T = 15°C \quad \textcircled{1}$$

$$H_2CO_3 \rightleftharpoons H^+ + HCO_3^-$$

$$K_{H_2CO_3} = \frac{\alpha_{H^+}\alpha_{HCO_3^-}}{\alpha_{H_2CO_3}} = 10^{-6.42} \qquad @ \ T = 15°C \quad \textcircled{2}$$

$\boxed{10}$

$$\alpha_{H_2CO_3} = \frac{\alpha_{H^+}\alpha_{HCO_3^-}}{K_{H_2CO_3}} = \frac{(10^{-7.28})(4.44 \times 10^{-3})}{10^{-6.42}}$$

$$= 10^{-3.2} = 6.1 \times 10^{-4} \qquad \text{put in } \textcircled{1}$$

$$P_{CO_2} = \frac{\alpha_{H_2CO_3}}{K_{CO_2}} = \frac{6.1 \times 10^{-4}}{10^{-1.34}}$$

$$\boxed{P_{CO_2} = \quad 0.013 \ bar = 10^{-1.9} \ bar}$$

[b] Water to surface. $P_{CO_2} = 10^{-3.5}$ bar. Find pH.

Use Eqs. from [c] — don't have to write them again

$\textcircled{1}$
$$CO_2 + H_2O \rightleftharpoons H_2CO_3$$

$$K_{CO_2} = \frac{\alpha_{H_2CO_3}}{P_{CO_2}} = 10^{-1.34} \ @ \ T = 15°C$$

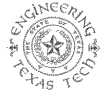$$\alpha_{H_2CO_3} = K_{CO_2} \ P_{CO_2} = (10^{-1.34})(10^{-3.5}) = 10^{-4.84} = 1.4 \times 10^{-5}$$

$\textcircled{2}$
$$H_2CO_3 \rightleftharpoons H^+ + HCO_3^-$$

$$K_{H_2CO_3} = \frac{\alpha_{H^+}\alpha_{HCO_3^-}}{\alpha_{H_2CO_3}} = 10^{-6.42} \ @ \ 15°C$$

$\boxed{10}$

$$\alpha_{H^+} = \frac{K_{H_2CO_3} \ \alpha_{H_2CO_3}}{\alpha_{HCO_3^-}} = \frac{(10^{-6.42})(10^{-4.84})}{4.44 \times 10^{-3}}$$

$$\alpha_{H^+} = 1.3 \times 10^{-9} = 10^{-8.9}$$

$$pH = -\log_{10}\alpha_{H^+} = -\log_{10}(10^{-8.9})$$

$$\boxed{pH = 8.9}$$

10-1 | Given: $C_0 = 1823 \, mg/L$, Column $L = 2m$, $C_i = 0 \, mg/L$.

Injection $V_x = 1.45 \, m/d$, $a_L = 15 cm$

Find: $C(L, 0.7d)$

$$C(L,t) = \frac{C_0}{2}\left[erfc\left(\frac{L - V_x t}{2\sqrt{D_L t}}\right) + exp\left(\frac{V_x L}{D_L}\right) erfc\left(\frac{L + V_x t}{2\sqrt{D_L t}}\right)\right]$$

$$D_L = a_L V_x + D^{*^{\,2o}} = 15cm \,(1.45\,m/d)\left(\frac{1m}{100cm}\right)$$

$$D_L = 0.214 \, m^2/d$$

10

$$C(2m, 0.7d) = \frac{1823 \frac{mg}{L}}{2}\left[erfc\left\{\frac{2m - 1.45\frac{m}{d}(0.7d)}{2\sqrt{(0.214\frac{m^2}{d})(0.7d)}}\right\} + exp\frac{1.45\frac{m}{d}(2m)}{0.214\frac{m^2}{d}} \, erfc\left\{\frac{2m + 1.45\frac{m}{d}(0.7d)}{2\sqrt{(0.214\frac{m^2}{d})(0.7d)}}\right\}\right]$$

$$= 911\frac{mg}{L}\left[\underset{(0.068)}{erfc(1.29)} + \underset{(C^{13.36})}{exp(13.36)}\underset{(0.0)}{erfc(3.877)}\right]\text{— from Table}$$

$$\boxed{C = 62 \frac{mg}{L}}$$

if you use Excel for erfc $\overline{C = 86 mg/L}$

10.5 Given: $K_d = 83 \frac{mL}{g}$, $\rho_b = 2.12 \frac{g}{cm^3}$, $\theta = 0.26$

Find: relative velocity

$$v_c = \frac{v_x}{1 + \frac{\rho_b}{\theta} K_d}$$

$$= \frac{v_x}{1 + \frac{2.12 \frac{g}{cm^3}}{0.26} \left(83 \frac{mL}{g}\right) \frac{1 cm^3}{1 mL}}$$

$$v_c = 0.0015 \, v_x \qquad \boxed{R = 678}$$

10.7 Given: Capture well $Q = 37000 \, ft^3/d$, confined aquifer, $K = 925 \, ft/d$

$i = 0.0027$, $b = 40 ft$

Find: [a] maximum width of capture zone
[b] distance from well to stagnation point

[a] $$y_{max} = \pm \frac{Q}{2bKi}$$

$$= \pm \frac{37000 \, ft^3/d}{2(40 ft)(925 ft/d)(0.0027)}$$

$$= 185 \, ft$$

Max width = 370 ft

[b] $$x = -\frac{Q}{2\pi K b i}$$

$$= -\frac{37000 \, ft^3/d}{2\pi (40 ft)(925 ft/d)(0.0027)}$$

$$x = -59 \, ft$$