APPENDIX E

CALCULATIONS - ELBON MINE

$I = 1/2 \sum [M_{anions} \times Z^2 + M_{cations} \times Z^2]$

$M_{SO_4} = 0.00982$

$M_{cations} = 0.01251$ (estimated cations - assumed mostly bi-valent)

$I = 1/2 \ [0.00982 \times 2^2 + 0.01251^2]$

$I = .04555$

$\sqrt{I} = 0.211$

Activity Coefficients by Debye - Huckel Equation

$$-\log \gamma = \frac{AZ^2 \sqrt{I}}{1 + a^{\circ}B \sqrt{I}}$$

$A_{(10^{\circ}c)} = 0.4960$

$B = 0.3258 \times 10^{-8}$

$a^{\circ}_{Fe} \times 10^8 = 6 \times 10^8$

$Z_{Fe} = 2$

$$-\log \gamma_{Fe^{++}} = \frac{0.4960 \times 2^2 \times 0.211}{1 + [6 \times 10^8 \times 0.3258 \times 10^{-8} \times 0.211]}$$

$$-\log \gamma_{Fe^{++}} = \frac{0.4960 \times 2^2 \times 0.211}{1 + 6 \times .3258 \times 0.211} = \frac{0.418}{1 + .412} = \frac{0.418}{1.412} = 0.2960$$

$\gamma_{Fe^{++}} = 0.506$

$Fe^{++} + 3 H_2O \rightleftharpoons Fe(OH)_3 + 3H^+ - e^-$

$$K = \frac{[Fe(OH)_3] \ [H^+]^3}{[Fe^{++}] \ [H_2O]^3} = \frac{[H^+]^3}{[Fe^{++}]}$$

$\Delta F^{\circ} = \Delta F^{\circ}_{f_{Fe(OH)_3}} + 3 \Delta F^{\circ}_{f_{H^+}} - \Delta F^{\circ}_{f_{Fe^{++}}} - 3 \Delta F^{\circ}_{f_{H_2O}}$

$= 166.0 + 3(0) - (-20.30) - 3(-56.69)$

$= -166.0 + 190.37$

$= +24.37$

$E^o = \frac{Fr^o}{(23.06)n} = \frac{24.37}{23.06} = +1.055$ volts

$Eh = E^o + 0.0566 \log \frac{[H^+]^3}{[Fe^{++}]}$

Using $\gamma_{Fe^{++}} = 0.506$ we obtain:

$[Fe^{++}] = \gamma_{Fe^{++}} \times M_{Fe^{++}} = 0.506 \times \frac{52.4}{55.85} = 0.475$

$\log [Fe^{++}] = 1.677$

$Eh = 1.055 + 0.0566 [(3x -4.31) + 1.677]$

$Eh = 1.055 - 0.638$

$Eh = +0.417$

$K_w = 10^{-14.46}$ (@12°C)

$K_{OH^-} = \frac{[H_2O]}{[H^+]} = \frac{10^{-14.46}}{10^{-4.31}} = 10^{-10.15}$

$[Fe^{+++}] = 10^{-7.85}$

$pQ = [Fe^{+++}] [OH^-]^3$

$\log pQ = -7.85 + 3 (-10.15)$

$-\log pQ = +38.30$ (This is still in the amorphous range for ferric oxyhydroxides)

ELK MINE - Fe^{++} ACTIVITY

Hydroxide Equilibrium

$$Fe^{++} + 3\,H_2O \qquad Fe(OH)_3 + 3H^+ + e^-$$

$$K = \frac{[Fe\,(OH_3)]\,[H^+]^3}{[Fe^{++}]\,[H_2O]^3} = \frac{[H^+]^3}{[Fe^{++}]}$$

$$\Delta F^o_r = \Delta F^o_{f_{Fe(OH)_3}} + 3\Delta F^o_{f_{H^+}} - \Delta F^o_{f_{Fe^{++}}} - 3\,\Delta F^o_{f_{H_2O}}$$

$$\Delta F^o_r = -166.0 + 3(0) - (-20.30) - 3(-56.69)$$

$$\Delta F^o_r = +\,24.37$$

$$E_o = \frac{\Delta Fr^o}{23.06n} = \frac{24.37}{23.06} = 1.055 \qquad [Fe^{++}] = 0.614 \times \frac{29.0}{55.85} = .319$$

$$\log [Fe^{++}] = 1.5038$$

$$Eh = E^o + \frac{RT}{nF} \log \frac{[H^+]^3}{[Fe^{++}]}$$

$$\frac{RT}{nF} = \frac{0.001987 \times 285 \times 2.303}{1 \times 23.06} = 0.0566$$

$$Eh = 1.055 + 0.0566\ \frac{(3 \times -5.83)}{-1.504}$$

$$= 1.055 + 0.0566\,(-15.99) = 1.055 - 0.905$$

Eh = 0.150 volts (as opposed to .247 obtained experiementally)

$$pQ = [Fe^{+++}]\,[OH^-]^3$$

$$pQ = 10^{-10.7} \times 2 \times 10^{-8.63}$$

$$-\log pQ = 36.59$$

Ionic Strength + Activity Coefficient

$I = 1/2 \quad [M_{anions} \times Z^2 + M_{cations} \times Z^2]$

$M_{SO_4^-} = \frac{429}{96.06} \times 10^{-3} = 4.47 \times 10^{-3}$

$I = 4.47 \times 10^{-3} \times 2^2$ (Assuming $I_{cations}$ eq. I_{anions})

$I = 0.01788$

$\sqrt{I} = 0.134$

$$- \log \gamma_{Fe^{++}} = \frac{A Z^2 \sqrt{I}}{1 + a^o B \sqrt{I}}$$

$A_{12} = 0.4978$

$B = 0.3260 \times 10^{-8}$

$a^o = 6 \times 10^8$

$$- \log \gamma_{Fe^{++}} = \frac{0.4978 \times 4 \times 0.134}{1 + 6 \times 10^8 \times 0.3260 \times 10^{-8} \times 0.134} = \frac{0.267}{1.262} = 0.2115$$

$\gamma_{Fe^{++}} = 0.614$

CALCULATION OF REGRESSION EQUATION

Acid Load vs. Flow - Discharge No. 1 - Elbon Mine

X Flows (MGD)	Y Acid (lbs/day)	XY	X^2
.453	862	390	.205
.502	921	462	.252
.485	1085	526	.235
.421	1081	455	.179
.421	772	325	.179
.502	1005	504	.252
.479	960	459	.229
.329	660	217	.108
.310	621	192	.096
.301	552	166	.090
.275	572	157	.076
.275	819	225	.076
.340	511	173	.115
.582	1166	678	.338
5.990	12,254	5,118	

$\bar{X} = 0.399$ $\bar{Y} = 816$ $XY = 5112$ $X^2 = 2.504$

$$b = \frac{XY}{x^2} = \frac{5112}{2.504} = 2044$$

$Y = a + bx$

$816 = a + 2044 \times .399$ $816 - 815 = a$

$a = 1$

$Y = 1 + 2044\ x$ (Regression Equation)

Calculation of Coefficient of Variance

$$r = \frac{x\ y}{15\ S_x\ S_y} \qquad S_x = \frac{2.504}{15} = 0.170 = 0.412$$

$$Sy = \frac{10,654.126}{15} = 710.276 = 844$$

$$r = \frac{x\ y}{15 s_x\ s_y} = \frac{5118}{15 \times 844 \times 0.412} = \frac{5118}{5216} = 0.9812$$

$r = 0.9812$ $r^2 = 0.9628$