Sulfate Generation - Cell 2W Fine

Material used in unsaturated zone: LTVSMC coarse tailings

\[ K_s := 1.1 \times 10^{-4} \text{ cm/sec} \]

\[ n := 1.6 \]

\[ \theta_r := 0.059 \]

\[ \phi := 0.493 \]

\[ G := 2.9 \]

\[ \rho_w := 1 \frac{\text{gm}}{\text{cm}^3} \]

\[ A := 3027344 \text{ m}^2 \]

\[ q := 15.93 \frac{\text{in}}{\text{yr}} \]

\[ \tau := 0.273 \]

\[ D_a := 1.8 \times 10^{-5} \frac{\text{m}}{\text{sec}} \]

\[ c := 3.28 \]

\[ D_w := 2.2 \times 10^{-9} \frac{\text{m}^2}{\text{sec}} \]

\[ K_H := 33.9 \]

\[ C_o := 8.89 \frac{\text{mol}}{\text{m}^3} \]

\[ W_{SO4} := 96.07 \frac{\text{gm}}{\text{mole}} \]

\[ W_S := 32.066 \frac{\text{gm}}{\text{mole}} \]

\[ R_{SO4} := 1.95186 \frac{\text{mg}}{\text{kg} \cdot \text{day}} \]

\[ CF_{fine} := 0.360 \]

\[ TF := 0.228589 \]

\[ FF := \frac{3.4}{12} \]

\[ \text{moleratio} := \frac{4}{9} \]

\[ DTW := 85.5 \text{ ft} \]

\[ \text{Cont}_S := 46.1 \frac{\text{mg}}{\text{kg}} \]

Saturated hydraulic conductivity of LTV fine (Table 1-12b)
vanGenuchten parameter for LTV fine (Table 1-12a)
Residual volumetric water content for LTV fine (Table 1-12a)
Porosity of LTV fine (Table 1-12a)
Specific gravity of LTV fine solids (Table 1-12a)
Water density (standard value)
Map area of Cell 2E embankment (Table 1-33)
Percolation flux (from Fred's seepage spreadsheet with CDA edits)
Tortuosity (Table 1-1, sheet 5)
Free diffusion coefficient of oxygen in air (Table 1-1, sheet 5)
Empirical constant (Table 1-1, sheet 5)
Free diffusion coeff of oxygen in water (Table 1-1, sheet 5)
Henry's constant for oxygen (Table 1-1, sheet 5)
O2 concentration in air (Table 1-1, sheet 5)
Molecular weight of sulfate (standard value)
Molecular weight of sulfur (standard value)
P50 SO4 distribution parameter for LTVSMC tailings (Table 1-19)
Calibration factor for LTV coarse tailings (Table 1-1, sheet 5)
Temperature factor (computed in GS using numerous inputs)
Freeze factor (from Table 1-1, sheet 3)
\[ FF = 0.28333 \]

\[ \text{moleratio} = 0.444 \]

\[ DTW = 26.06 \text{ m} \]

\[ \text{Cont}_S = 46.1 \frac{\text{mg}}{\text{kg}} \]

Sulfur content. Mass of S per unit mass of LTV tailings. (Table 1-22)
\[ \rho_b := G \rho_w (1 - \phi) \]

Tailings dry bulk density. Mass of solids per unit bulk volume.

\[ \rho_b = 1.47 \text{ gm cm}^{-3} \]

Compressed vanGenuchten parameter

\[ mm := 1 - \frac{1}{n} \]

Unsaturated hydraulic conductivity as a function of saturation (ss) based on vanGenuchten relationship

\[ f(ss) := q - K(ss) \quad ss := 0.6 \]

Root equation and saturation guess

\[ SAT := \text{root}(f(ss), ss) \]

Computed saturation associated with flux (q)

\[ q - K(SAT) = 1.195 \times 10^{-6} \text{ in yr} \]

Confirm root calculation (result should be approx zero)

\[ DD := \tau \cdot D_a (1 - SAT)^c + \tau \cdot SAT \cdot \frac{D_w}{K_H} \]

Effective O2 diffusion coeff used in GS. I believe this diffusion coeff is referenced to void volume,

\[ D := \tau \cdot \phi \cdot D_a (1 - SAT)^c + \tau \cdot \phi \cdot SAT \cdot \frac{D_w}{K_H} \]

Effective O2 diffusion coeff referenced to bulk volume

\[ MRM_{SO4} := R_{SO4} \cdot CF_{fine} \cdot TF \cdot (1 - FF) \]

Mass rate of released SO4 per unit mass of tailings solids

\[ R_{SO4} = 1.952 \text{ mg kg}^{-1} \text{ day}^{-1} \]

Effect of three factors

\[ CF_{fine} \cdot TF \cdot (1 - FF) = 0.059 \]

Molar consumption rate of O2 per unit volume of bulk tailings. (see ERM comment on this equation)

\[ R_O2 := \frac{MRM_{SO4}}{W_{SO4} \cdot \text{moleratio}} \cdot \rho_b \]

\[ R_O2 = 0.00396 \text{ mol m}^{-3} \text{ day}^{-1} \]

Thickness of sulfate reaction zone if controlled by diffusion

\[ d := \sqrt{\frac{2 \cdot D \cdot C_o}{R_O2}} \]

Actual thickness of sulfate reaction zone. Minimum of diffusion controlled reaction zone or depth-to-water.

\[ b := \text{min}(d, DTW) \]

\[ MRSO4 := MRM_{SO4} \cdot b \cdot A \cdot \rho_b \]

Mass rate of released sulfate

\[ MRSO4 = 943.666 \text{ kg day}^{-1} \]

\[ MRV_S := R_O2 \cdot W_S \cdot \text{moleratio} \]

Mass rate of released S per unit bulk volume

\[ MRV_S = 9.341 \times 10^{-11} \text{ kg m}^{-3} \text{ s}^{-1} \]

\[ MRA_S := MRV_S \cdot b \]

Mass rate of released S per unit map area (m²)

\[ MRA_S = 728.302 \text{ mg m}^{-2} \text{ day}^{-1} \]

\[ Q_{seep} := q \cdot A \]

Seepage flow rate

\[ Q_{seep} = 615.254 \text{ gpm} \]
\[ \text{Co}_\text{SO}_4 := \frac{\text{MR}_\text{SO}_4}{Q_{\text{seep}}} \]

Sulfate concentration in seepage

\[ \text{Co}_\text{SO}_4 = 281 \text{ mg/liter} \]

\[ t_{\text{end}} := \frac{\text{Cont}_{\text{S}} P_b DTW}{\text{MRV}_\text{S} b} \]

Time to deplete all sulfur in the reaction zone if composed of LTVSMC tailings.

\[ t_{\text{end}} = 46 \text{-yr} \]

\[ V_w := \text{SAT} \phi A DTW \]

Water volume in unsat zone

\[ V_w = 2.622 \times 10^7 \text{ m}^3 \]

Set up dimensionless equations using m-kg-day units

\[ \text{tt}_{\text{end}} := \frac{t_{\text{end}}}{\text{day}} \]

End of sulfate generation in days

\[ \text{tt}_{\text{end}} = 1.698 \times 10^4 \]

\[ \text{MR} := \frac{\text{MR}_\text{SO}_4}{\text{kg day}^{-1}} \]

Mass rate of sulfate generation in kg/day

\[ \text{MR} = 943.666 \]

\[ \text{M}(t) := \begin{cases} \text{MR} & \text{if } t < \text{tt}_{\text{end}} \\ 0 & \text{otherwise} \end{cases} \]

Sulfate mass generation function

\[ \text{V} := \frac{V_w}{m^3} \]

Water volume in \( m^3 \)

\[ \text{V} = 2.622 \times 10^7 \]

\[ \text{Q} := \frac{Q_{\text{seep}}}{m^3 \text{-day}^{-1}} \]

Seepage flow rate in \( m^3/\text{day} \)

\[ \text{Q} = 3.354 \times 10^3 \]

\[ \text{Co} := \frac{\text{Co}_\text{SO}_4}{\text{kg m}^{-3}} \]

Initial sulfate conc in kg/m\(^3\)

\[ \text{Co} = 0.281 \]

Given

\[ \frac{d}{dt} C(t) = \frac{M(t) - \text{Q} C(t)}{V} \]

\[ C(0) = \text{Co} \]

\[ \text{C} := \text{Odesolve}(t, 100, 365) \]

Governing DEQ and IC

\[ \text{C}_\text{SO}_4(t) := C(t) \left( \frac{t}{\text{day}} \right) \text{kg m}^{-3} \]

Sulfate conc as a function of time

\[ \text{tt} := 0, 1 \text{-yr.. 100 \text{-yr}} \]

\[ \text{SO}_4 \text{ conc (mg/L)} \]

\[ \frac{\text{C}_\text{SO}_4(t)}{\text{mg/L}} \]

Time (yrs)

\[ \frac{\text{tt}}{\text{yr}} \]