Sulfate Generation - Cell 2W Fine

Material used in unsaturated zone: LTVSMC coarse tailings

$K_s := 1.1 \cdot 10^{-4} \cdot \frac{cm}{sec}$	Saturated hydraulic conductivity of LTV fine (Table 1-12b)	
$n := 1.6$	vanGenuchten parameter for LTV fine (Table 1-12a)	
$\theta_r := 0.059$	Residual volumetric water content for LTV fine (Table 1-12a)	
$\phi := 0.493$	Porosity of LTV fine (Table 1-12a)	
$G := 2.9$	Specfic gravity of LTV fine solids (Table 1-12a)	
$\rho_w := 1 \cdot \frac{gm}{cm^3}$	Water density (standard value)	
$A := 3027344 \cdot m^2$	Map area of Cell 2E embankment (Table 1-33)	$A = 748.073 \cdot acre$
$q := 15.93 \cdot \frac{in}{yr}$	Percolation flux (from Fred's seepage spreadsheet with CDA edits)	
$\tau := 0.273$	Tortuosity (Table 1-1, sheet 5)	
$D_a := 1.8 \cdot 10^{-5} \cdot \frac{m^2}{sec}$	Free diffusion coefficient of oxygen in air (Table 1-1, sheet 5)	
$c := 3.28$	Empirical constant (Table 1-1, sheet 5)	
$D_w := 2.2 \cdot 10^{-9} \cdot \frac{m^2}{sec}$	Free difussion coeff of oxygen in water (Table 1-1, sheet 5)	
$K_H := 33.9$	Henry's constant for oxygen (Table 1-1, sheet 5)	
$C_o := 8.89 \cdot \frac{mol}{m^3}$	O2 concentration in air (Table 1-1, sheet 5)	
$W_{SO4} := 96.07 \cdot \frac{gm}{mole}$	Molecular weight of sulfate (standard value)	
$W_S := 32.066 \cdot \frac{gm}{mole}$	Molecular weight of sulfur (standard value)	
$R_{SO4} := 1.95186 \cdot \frac{mg}{kg \cdot 7 \cdot day}$	P50 SO4 distribution paramater for LTVSMC tailings (Table 1-19)	
$CF_{fine} := 0.360$	Calibration factor for LTV coarse tailings (Table 1-1, sheet 5)	
$TF := 0.228589$	Temperature factor (computed in GS using numerous inputs)	
$FF := \frac{3.4}{12}$	Freeze factor (from Table 1-1, sheet 3)	$FF = 0.28333$
$moleratio := \frac{4}{9}$	mole SO4 / mole O2 = mole S / mole O2 (Table 1-1, sheet 6)	$moleratio = 0.444$
$DTW := 85.5 \cdot ft$	Depth to water table in cell 2E during closure (value in Table 1-34 is 51.0 ft; GS value used in calcs is 52.3 ft)	$DTW = 26.06\,m$
$Cont_S := 46.1 \cdot \frac{mg}{kg}$	Sulfur content. Mass of S per unit mass of LTV tailings. (Table 1-22)	

$\rho_b := G \cdot \rho_w \cdot (1 - \phi)$	Tailings dry bulk density. Mass of solids per unit bulk volume.	$\rho_b = 1.47 \cdot \frac{gm}{cm^3}$
$mm := 1 - \frac{1}{n}$	Computed vanGenuchten parameter	$mm = 0.375$
$K(ss) := K_s \left(\frac{ss \cdot \phi - \theta_r}{\phi - \theta_r}\right)^{0.5} \cdot \left[1 - \left[1 - \left(\frac{ss \cdot \phi - \theta_r}{\phi - \theta_r}\right)^{\frac{1}{mm}}\right]^{mm}\right]^2$	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	
$SAT := root(f(ss), ss)$	Computed saturation associated with flux (q)	$SAT = 0.6741$
$q - K(SAT) = 1.195 \times 10^{-6} \cdot \frac{in}{yr}$	Confirm root calculation (result should be approx zero)	0.6741
$DD := \tau \cdot D_a \cdot (1 - SAT)^c + \tau \cdot SAT \cdot \frac{D_w}{K_H}$	Effective O2 diffusion coeff used in GS. I believe this diffusion coeff is referenced to void volume,	$DD = 1.243 \times 10^{-7} \frac{m^2}{s}$
$D := \tau \cdot \phi \cdot D_a \cdot (1 - SAT)^c + \tau \cdot \phi \cdot SAT \cdot \frac{D_w}{K_H}$	Effective O2 diffusion coeff referenced to bulk volume	$D = 6.127 \times 10^{-8} \frac{m^2}{s}$
$MRM_{SO4} := R_{SO4} \cdot CF_{fine} \cdot TF \cdot (1 - FF)$	Mass rate of released SO4 per unit mass of tailings solids	$R_{SO4} = 1.952 \cdot \frac{mg}{kg \cdot 7 \cdot day}$
	Effect of three factors	$CF_{fine} \cdot TF \cdot (1 - FF) = 0.059$
$R_{O2} := \frac{MRM_{SO4}}{W_{SO4} \cdot moleratio} \cdot \rho_b$	Molar consumption rate of O2 per unit volume of bulk tailings. (see ERM comment on this equation)	$R_{O2} = 0.00396 \cdot \frac{mol}{m^3 \cdot 7 \cdot day}$
$d := \sqrt{\frac{2 \cdot D \cdot C_o}{R_{O2}}}$	Thickness of sulfate reaction zone if controlled by diffusion	$d = 12.892\,m$
$b := min(d, DTW)$	Actual thickness of sulfate reaction zone. Minimum of diffusion controlled reaction zone or depth-to-water.	$b = 12.892\,m$
$MR_{SO4} := MRM_{SO4} \cdot b \cdot A \cdot \rho_b$	Mass rate of released sulfate	$MR_{SO4} = 943.666 \cdot \frac{kg}{day}$
$MRV_S := R_{O2} \cdot W_S \cdot moleratio$	Mass rate of released S per unit bulk volume	$MRV_S = 9.341 \times 10^{-11} \frac{kg}{m^3 \cdot s}$
$MRA_S := MRV_S \cdot b$	Mass rate of released S per unit map area (m^2)	$MRA_S = 728.302 \cdot \frac{mg}{m^2 \cdot 7 \cdot day}$ 727.95
$Q_{seep} := q \cdot A$	Seepage flow rate	$Q_{seep} = 615.254 \cdot gpm$

$Co_{SO4} := \frac{MR_{SO4}}{Q_{seep}}$ Sulfate concentration in seepage $Co_{SO4} = 281 \cdot \frac{mg}{liter}$

$t_{end} := \frac{Cont_S \cdot \rho_b}{MRV_S} \cdot \frac{DTW}{b}$ Time to deplete all sulfur in the reaction zone if composed of LTVSMC tailings. $t_{end} = 46 \cdot yr$

$V_w := SAT \cdot \phi \cdot A \cdot DTW$ Water volume in unsat zone $V_w = 2.622 \times 10^7 \cdot m^3$

Set up dimensionless equations using m-kg-day units

$tt_{end} := \frac{t_{end}}{day}$ End of sulfate generation in days $tt_{end} = 1.698 \times 10^4$

$MR := \frac{MR_{SO4}}{kg \cdot day^{-1}}$ Mass rate of sulfate generation in kg/day $MR = 943.666$

$M(t) := \begin{vmatrix} MR \text{ if } t < tt_{end} \\ 0 \text{ otherwise} \end{vmatrix}$ Sultate mass generation function

$V := \frac{V_w}{m^3}$ Water volume in m^3 $V = 2.622 \times 10^7$

$Q := \frac{Q_{seep}}{m^3 \cdot day^{-1}}$ Seepage flow rate in m^3/day $Q = 3.354 \times 10^3$

$Co := \frac{Co_{SO4}}{kg \cdot m^{-3}}$ Initial sulfate conc in kg/m^3 $Co = 0.281$

Given $\frac{d}{dt}C(t) = \frac{M(t) - Q \cdot C(t)}{V}$ $C(0) = Co$ $C := Odesolve(t, 100 \cdot 365)$ Governing DEQ and IC

$C_{SO4}(tt) := C\left(\frac{tt}{day}\right) \cdot kg \cdot m^{-3}$ $tt := 0, 1 \cdot yr .. 100 \cdot yr$ Sulfate conc as a function of time