模擬水流通過含硫礦土之反應化學傳輸

Modeling of Fluid Flow and Reactive Chemical Transport through Toxici Mine Spoil

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摘　要

污染物在非飽和層中受不穩定水流帶動之反應化學傳輸模式，FRCT，發展完成。此模式考慮地下水流、化學輸送及化學反應相互之對偶效應，其中化學反應包括酸鹼反應、氧化還原反應、水溶性錯合物、溶解沉澱反應及不平衡礦物溶解動力反應，使其足以模擬現場實際之問題。模式應用於探討水流通過含硫礦土產生酸化之影響。三種情況納入考慮，包括以現地土壤覆蓋含硫礦土，以石灰石混合含硫礦土，及以低透水性黏土包圍含硫礦土。模擬結果顯示，以石灰石混合含硫礦土之方法最佳，能夠有效降低酸性流體之產生，然而在實際執行上，操作成本也是重要考量之因素。

ABSTRACT

A numerical model for transient fluid flow and reactive chemical transport through partially saturated media, FRCT, is developed. The model considers the coupled processes among fluid flow, chemical transport and chemical reactions. The chemical reactions include acid/base reactions, oxidation/reduction, aqueous complexation, precipitation/dissolution and kinetic mineral dissolution to simulate realistic field problem. The model is applied to study the flow through toxic mine spoil. Three cases which include toxic spoil covered with native soil, toxic mine spoil blended with lime stone, and toxic mine spoil covered with clay liner are investigated. Results of simulation suggest that the method of blending with lime stone is much more effective than the method of covering with clay liner to reduce the acid generation. However, the overall operational costs is also a key factor in the choice between these two methods for surface mine reclamation.

I. INTRODUCTION

Acid mine drainage is a major environmental problem in surface mining. During the surface mining operation, pyritic sulfur which generally associated with ore are exposed to and reacted with water and oxygen will generate sulphuric acid and pollute the environment. The federal legislative response to such problems resulting from surface mining is the Public Law 95-87, the Surface Mining Control and Reclamation Act of 1977. It requires that the acid forming materials be selective placement and buried to minimize the toxic effect. One of the method is to cover the toxic material with relative low permeability clay liner. The other method is to blend the toxic material with limestone. Because of the complex nature of the problem, it is difficult to quantify which method is superior. Phelps, et al (1985) considered the effect of permeability on the movement of water through toxic mine spoil. The chemical transport and chemical reactions are completely neglected.

Recently, contamination of groundwater has become one of the most concern environmental problems in the nation. To effectively dealing with this problem, a lot of effort has been focused on the development of the reactive chemical transport model. Several general models have been proposed which describe miscible species reactive chemical transport based on principles of thermodynamics (Grove and Wood, 1979; Reardon, 1981; Dance and Reardon, 1983; Miller and Benson, 1983; Kirkner et al., 1984; Walsh et al., 1984; Cederberg, 1985; Bryant et al., 1986; Lewis et al., 1986; Narasimhan et al., 1986; Carnahan, 1986; Liu, 1988). These models, based on their coupling logic, can be grouped into two numerical categories, namely, two-step method and one-step method. In the two-step method, the transport equations are separated from the chemical reaction equations and solved sequentially at each time step, with or without iterations in between (Grove and Wood, 1979; Reardon, 1981; Walsh et al., 1984; Cederberg, 1985; Bryant et al., 1986; Narasimhan et al., 1986; Ague, 1987; Liu, 1988). In the one-step method, the chemical reaction equations are directly inserted into the transport equations, leading to a set of highly non-linear, simultaneous partial differential equations, which are solved either explicitly or implicitly (Rubin and James, 1973; Jennings et al., 1982; Miller and Benson, 1983; Carnahan, 1986; Willis and Rubin, 1987; Ortoleva et al., 1987a, 1987b).

To date, however, most numerical models dealing with reactive chemical transport require the advective flow rate be known and input explicitly (Miller and Benson, 1983; Cederberg, 1985; Lewies et al., 1986; Narasimhan et al., 1986; Liu, 1988) which are not sufficient to handle realistic problems encountered in the field such as the modeling of flow through toxic mine spoil. It involves transient fluid flow and partially saturated condition where velocity needs to be calculated from the potential gradient and other system properties (e.g. permeability, saturation).

In view of the above, the present work was motivated by a desire to develop a transient fluid flow and transient reactive chemical transport model to study the flow through toxic mine spoil under partially saturated condition. Three cases which include toxic mine spoil cover with native soil, toxic spoil blended with limestone, and toxic mine spoil covered with clay liner are investigated. Two numerical models were used as a base for the present model development. The first is DYNAMIX (Liu, 1988), a multi-dimensional, multiple-species reactive chemical transport model, which solves the chemical transport and chemical reaction under partial equilibrium condition; and the second is CHAMP (Narasimhan et al, 1985), which combines a fluid flow code TRUST (Narasimhan and Witherspoon, 1977) and a transport code TRUMP (Edwards, 1972) with adding of hydrodynamic dispersion.

2. NUMERICAL SIMULATOR FRCT

2.1. General

The computer program DYNAMIX first developed by Narasimhan (Narasimhan, et al., 1986), coupled a chemical speciation code PHREEQE with a transport code TRUMP. The model only considered acid/base reactions and precipitation/dissolution of minerals. Later, Liu (1988) extended DYNAMIX to include acid/base reactions, aqueous complexation, redox reactions, precipitation/dissolution reactions and kinetic mineral dissolution. By adding the fluid flow equation into DYNAMIX, the current model FRCT (Fluid flow and Reactive Chemical Transport) can simulate the transient fluid flow reactive chemical transport under partially saturated conditions.

2.2. Mathematical Model

The basic equations describing transient fluid flow and reactive chemical transport through partially saturated porous media can be derived from the conservation laws of mass, chemical species and chemical thermodynamic. The mass continuity equation for flow through partially saturated media can be expressed in an integral form as

$$\int_W \frac{\partial(\theta\phi_f)}{\partial t} dV_e = -\int_W \nabla\cdot\rho_f v\, dV_e + \int_W q_m dV_e \tag{1}$$

Where θ is water content which is equal to $\phi \times S$ where ϕ is porosity and S is saturation, q_m is mass generation rate per unit volume and v is Darcy's velocity, expresses as

$$v = -K\nabla(Z+\Psi) \tag{2}$$

where Z is elevation head and Ψ is fluid pressure head.

The equation for conservation of chemical species i in partially saturated media can be expressed

$$\int_W \frac{\partial}{\partial t}(\theta\rho_f C_i^T) dV_e = -\int_W \nabla\cdot\rho_f v(\sum_{j=1}^{J} h_{ij}C_j) dV_e$$
$$+\int_W \nabla\cdot\rho_f D_{diff,i}\nabla(\sum_{j=1}^{J} h_{ij}C_j) dV_e + \int_W \nabla\cdot\theta\rho_f D_{lm}$$
$$\nabla(\sum_{j=1}^{J} h_{ij}C_j) dV_e dV_e + \int_W g_m C_{m,i} dV_e \tag{3}$$

where C_i^T is the total concentration of the chemical component i, C_j is the concentration of chemical species j in aqueous phase ($j = 0...J$), h_{ij} is the stoichiometric coeffiiceint of the i^{th} component in the j^{th} aqueous chemical species, $D_{diff,i}$ is the molecular diffusion coefficient of chemical component i, D_{lm} is the dispersion coefficient (second order tensor), $C_{m,i}$ is the concentration of the chemical component i in the fluid sources. The total concentration of chemical component i, C_i^T includes contribution from both aqueous phase and mineral p in the solid phase

$$C_i^T = \sum_{j=1}^{J} h_{ij}C_j - \sum_{p=1}^{P} b_{ip}\alpha_p \tag{4}$$

where b_{ip} is the stoichiometric coefficient of i^{th} chemical component in the p^{th} mineral phase and α_p is the net mass transfer of p^{th} mineral (+ for dissolution, – for precipition).

The distribution of aqueous chemical species and minerals is governed by chemical thermodynamic which is determined by solving a set of non-linear algebraic equations. These equations include the charge balance equation (for H),

$$\sum_{j=1}^{J} z_j C_j = 0 \tag{5}$$

where z_j is the charge on the j^{th} aqueous chemical species; the electron balance equation (for O),

$$\sum_{j=1}^{J} v_j C_j = RS^T + \sum_{p=1}^{P} u_p\alpha_p \tag{6}$$

where RS^T is the Redox State of the operational valences of the initial solution, and v_j and u_p are the operational valence of j^{th} chemical species and p^{th} mineral respectively; the mass conservation equation of each chemical component i (except for H and O),

$$\sum_{j=1}^{J} h_{ij}C_j = C_i^T + \sum_{p=1}^{P} b_{ip}\alpha_p,\ i = 1,2,3..I \tag{7}$$

where C_i^T is the sum of the initial total aqueous concentration of component i; and mass action equation of each mineral p,

$$\prod_{j=1}^{I} a_i^{b_{ip}} = K_p \tag{8}$$

where a_i is the thermodynamic activity of i^{th}

component which is equal to its activity coefficient γ_i times C_i. The detail formulation of the thermodynamic equations can be found in Liu (1988).

2.2.1. Numerical Solution

FRCT uses a sequential-step approach to solve the equations of fluid flow, chemical transport and chemical equilibrium. At each time step the fluid flow equation, Eq (1), is first solved for pressure field. Darcy's law, Eq (2), can then be applied to obtain the velocity field, which is used to solve chemical transport equation for each chemical component, Eq (3). The equilibrium chemistry calculations are then carried out to determine the chemical speciation and reaction mass transfer in each volume element (grid block) from Eqs (5)-(8).

The solution technique for solving the fluid flow equation and transport equations of each chemical component *i* are the Integral Finite Difference Method (IFDM) (Edwards, 1972; Narasimhan and Witherspoon, 1977). A fully upwind method is used to ensure that the numerical solution of the transport equations by explicit time difference scheme is stable.

To solve the system of non-linear thermodynamic algebraic equations in the equilibrium calculation, the continuous fraction method and the Newton-Raphson method are employed (Parkhurst et al., 1980). At each iteration, the changes in the hydrogen and electron activities and mass transfer of mineral phases are added to the current estimates to form new estimates while the new estimated activities of other aqueous master species are calculated by the continuous fraction method. The iteration process will continue until the convergence criterion is satisfied

$$\left(\frac{\Delta C_i^T}{C_i^T}\right)_N < \varepsilon \qquad (9)$$

where ε is the prescribed tolerance.

3. NUMERICAL SIMULATION

3.1. Problem Definition

The computer program for transient fluid flow and reactive chemical transport through partially saturated media, FRCT, is used to simulate the fluid flow through toxic mine spoil. Three cases are investigated:

(i) toxic mine spoil covered with native soil.
(ii). toxic mine spoil blended with limestone, and
(iii).toxic mine spoil covered with clay liner.

Figure 1 shows a schematic diagram of the system to be modeled. A simplified two-dimensional domain as shown in Figure 2 is used in the simulation. The area simulated is 1000 meters long by 25 meters deep by 1 meter thick. Constant hydraulic heads are applied to both the left and right edges. At the left edge the hydraulic head is 1 meter higher than that of the right edge such that the regional ground water flow is from left to right. The effective annual precipitation is approximately by a constant normal flux of 6.342×10^{-10} m/sec entering all across the top, representing an infiltration of 0.002 m/year. The toxic mine spoil is buried above water table which is approximated by 4 grid blocks. The clay liner is cover along the toxic mine spoil except the bottom which is approximated by 8 grid blocks for the case 3. No flow boundary condition is prescribed along the bottom. The initial water table is set at 10 meter below the ground surface. The relationship for permeability and saturation versus pressure head is given in Table 1. Other physical parameters are:

Diffusion Coefficient of each component, $D_{diff,i} = 1.6 \times 10^{-10}\ m^2/sec$

Dispersivity, $\alpha = 1\ m$

Porosity, $\phi = 0.2$

The computational domain was divided into 40x10 equal size grid of total 400 grids. Each gird has dimension 25 meters long by 2.5 meters wide by 1 meter thick. The initial aqueous compositions for the saturated soil, unsaturated soil, toxic mine spoil without lime, toxic mine spoil with lime, clay liner and rain water are given in Table 2. The mine spoil water is assumed to be more acidic than rain water. The initial ground water is under alkaline reduced conditions. The initial mineral phases and their

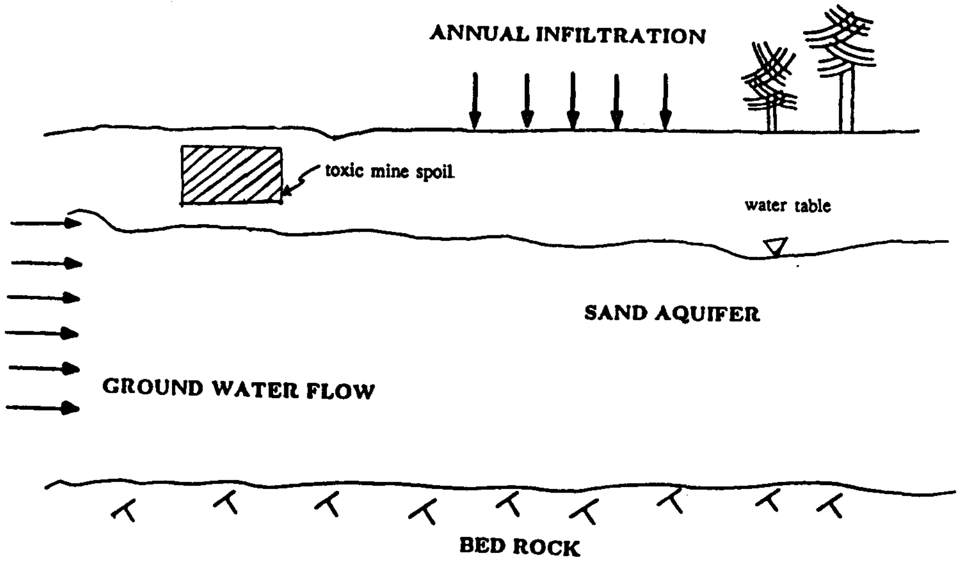

Figure 1. Schematic description of the flow through toxic mine spoil.

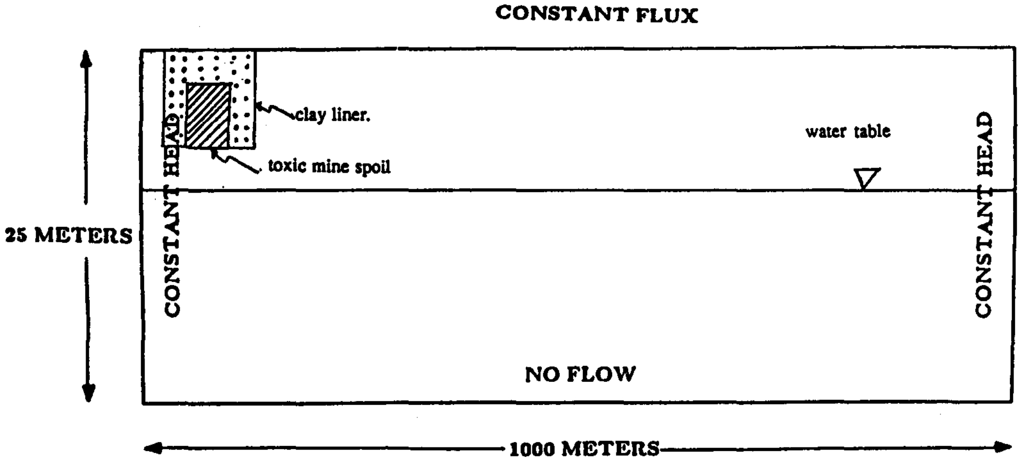

Figure 2. Problem domain and flow boundary conditions used in simulation.

Table 1. Relations of permeability and saturation versus pressure head in the simulation of through toxic min spoil.

Pressure	Saturation		Permeability(m^2)	
Head(M)	Native Soil & Spoil	Clay Liner	Native Soil & Spoil	Clay Liner
30	1.0	1.0	1×10^{-13}	1×10^{-15}
0	1.0	1.0	1×10^{-13}	1×10^{-15}
–0.5	1.0	1.0	1×10^{-13}	1×10^{-15}
–10	0.3	0.3	5×10^{-15}	5×10^{-17}
–20	0.15	0.15	1×10^{-15}	1×10^{-17}
–30	0.15	0.15	1×10^{-15}	1×10^{-17}

Table 2. Initial aqueous chemical composition in the simulation of flow through toxic min spoil.

Chemical	Concentration, mole/m^3				
Components	Saturated Soil	Unsaturated Soil	Spoil, No Lime	Spoil, Lime	Rain Water
p^H	8.9	7.0	1.4	5.75	5.2
p^E	8.9	–2.0	–2.16	–2.6	13
Ca	1.0	1.0	4.0	57.0	5×10^{-3}
Mg	1.0	1.0	16.0	15.0	1×10^{-3}
Na	5.0	5.0	50.0	50.0	7×10^{-3}
K	1.0	1.0	6.0	3.9	1×10^{-3}
Fe	3.2×10^{-7}	1×10^{-3}	59.5	55.0	1×10^{-4}
Al	1.6×10^{-4}	3.1×10^{-5}	8.0	1.79×10^{-7}	1×10^{-3}
Si	0.1	0.098	0 088	0.088	1×10^{-3}
Cl	9.8	7.9	293.0	293.0	2×10^{-2}
C	2.0	2.0	5×10^{-3}	53.0	1×10^{-4}
S	0.2	0.2	9.0	5.8×10^{-8}	1×10^{-3}

Table 3. Initial mineral phases and their volume percents in the simulation of flow through toxic min spoil.

Mineral	Volume Percent			
	Native Soil	Spoil, Lime	Spoil, No Lime	Clay Liner
Quartz	100.0	80.0	90.0	0.0
Illite	0.0	0.0	0.0	100.0
Pyrite	0.0	10.0	10.0	0.0
Calcite	0.0	10.0	0.0	0.0

volume percentage for different materials are given in Table 3. The aqueous complexes derived from the 13 chemical components are listed in Table 4. The mineral phases of interest and their stability constants are listed in Table 5.

3.2. Results and Discussions

Figure 3 and Figure 4 show the simulated hydraulic head contours at 20 years for case 1 and case 3. Only sight difference of hydraulic head around the left edge which suggested that the clay liner has a little effect on the hydraulic head distribution. Figure 5 and Figure 6 show the simulated saturation contours at 20 years for case 1 and case 3. The saturation contours for 20 years in both cases exhibit similar distribution which indicate the ground water table is relatively stable. A similar effect as shown in Figure 4 of clay linear around the left edge can be also found in Figure 6. Figure 7 to Figure 9 show the simulated pH contours at 20 years for case 1, case 2, and case 3 respectively. The movement

Table 4. Intra-aqueous reactions and their equilibrium constants at 25°C for species in the simulation of flow through toxic min spoil.

Chemical Reactions	Log of Equilibrium Constant
$H_2O-H^+ = OH^-$	13.99
$H^+ + CO_3^{2-} = HCO_3^-$	10.34
$2H^+ + CO_3^{2-} = H_2CO_3$	16.70
$H_+ + SO_4^{2-} = HSO_4^-$	1.987
$SO_4^{2-} + 8H^+ + 8e^- - 4H_2O = S^{2-}$	20.735
$SO_4^{2-} + 9H^+ + 8e^- - 4H_2O = HS^-$	33.652
$SO_4^{2-} + 10H^+ + 8e^- - 4H_2O = H_2S$	40.644
$Ca^{2+} + H_2O - H^+ = CaOH^+$	–12.598
$Ca^{2+} + CO_3^{2-} = CaCO_3$	3.153
$Ca^{2+} + CO_3^{2-} + H^+ = CaHCO_3^+$	11.345
$Ca^{2+} + SO_4^{2-} = CaSO^4$	2.309
$Mg^{2+} + H_2O - H^+ = MgOH^-$	–11.794
$Mg^{2+} + CO_3^{2-} = MgCO_3$	2.98
$Mg^{2+} + CO_3^{2-} + H^+ = MgHCO_3$	11.396
$Mg^{2+} + SO_4^{2-} = MgSO_4$	2.25
$Na^+ + CO_3^{2-} = NaCO_3^-$	1.268
$Na^+ + CO_3^{2-} + H^+ = NaHCO_3$	10.08
$Na^+ + SO_4^{2-} = NaSO_4^-$	0.700
$K^+ + SO_4^{2-} = KSO_4^-$	0.85
$Fe^{2+} + H_2O - H^+ = FeOH^+$	–9.50
$Fe^{2+} + 2H_2O - 2H^+ = Fe(OH)_2$	–20.57
$Fe^{2+} + 3H_2O - 3H^+ = Fe(OH)_3^-$	–31.00
$Fe^{2+} + SO_4^{2-} = FeSO_4$	2.25
$Fe^{2+} + 2SO_4^{2-} + 18H^+ + 16e^- - 8H_2O = Fe(HS)_2$	76.25
$Fe^{2+} + 3SO_4^{2-} + 27H^+ + 24e^- - 12H_2O = Fe(HS)_3$	111.937
$Fe^{2+} - e^- = Fe^{3+}$	–13.032
$Fe^{2+} + H_2O + H^+ - e^- = Fe(OH)^{2+}$	–15.22

Chemical Reactions	Log of Equilibrium Constant
$Fe^{2+} + 2H_2O - 2H^+ - e^- = Fe(OH)_2^+$	–18.70
$Fe^{2+} + 3H_2O - 3H^+ - e^- = Fe(OH)_3$	–26.63
$Fe^{2+} + 4H_2O - 4H^+ - e^- = Fe(OH)_4^-$	–34.63
$2Fe^{2+} + 2H_2O - 2H^+ - 2e^- = Fe_2(OH)_2^{4+}$	–29.01
$3Fe^{2+} + 4H_2O - 4H^+ - 3e^- = Fe_3(OH)_4^{5+}$	–45.4
$Fe^{2+} + Cl^- - e^- = FeCl^{2+}$	–11.55
$Fe^{2+} + 2Cl^- - e^- = FeCl_2^+$	–10.90
$Fe^{2+} + 3Cl^- - e^- = FeCl_3$	–11.90
$Fe^{2+} + SO_4^{2-} - e^- = FeSO_4^+$	–9.11
$Fe^{2+} + 2SO_4^{2-} - e^- = Fe(SO_4)_2^-$	–7.61
$Al^{3+} + H_2O - H^+ = Al(OH)^{2+}$	–4.99
$Al^{3+} + 2H_2O - 2H^+ = Al(OH)_2^+$	–10.11
$Al^{3+} + 3H_2O - 3H^+ = Al(OH)_3$	–16.0
$Al^{3+} + 4H_2O - 4H^+ = Al(OH)_4^-$	–23.0
$Al^{3+} + SO_4^{2-} = Al(SO_4)_2^-$	3.02
$Al^{3+} + 2SO_4^{2-} = Al(SO_4)_2^-$	4.92
$Si(OH)_4 - H^+ = H_3SiO_4^-$	–9.929
$Si(OH)_4 - 2H^+ = H_2SiO_4^{2-}$	–21.617

Table 5. Mineral solubility reactions and their equilibrium constants at 25°C for minerals in the simulation in the simulation of flow through toxic min spoil.

Chemical Reactions	Log of Equilibrium Constant
$SiO_2 = Si(OH)_4^4 - 2H_2O$	–4.006
$K_{0.6}Mg_{0.25}Al_{2.3}Si_{3.5}H_2O_{12} = 2H_2O + 0.6K^+$ $+ 0.25Mg^{2+} + 2.3Al^{3+} + 3.5Si(OH)_3 - 8H^+$	9.8046
$FeS_2 = Fe^{2+} + 2HS^- - 2H^+ - 2e^-$	–18.48
$CaCO_3 = Ca^{2+} + CO_3^{2-}$	–8.47
$CaSO_3 \cdot 2H_2O = Ca^{2+} + SO_4^{2-} + 2H_2O$	–4.848
$Fe(OH)_3 = Fe^{3+} + 3H_2O - 3H^+$	4.891

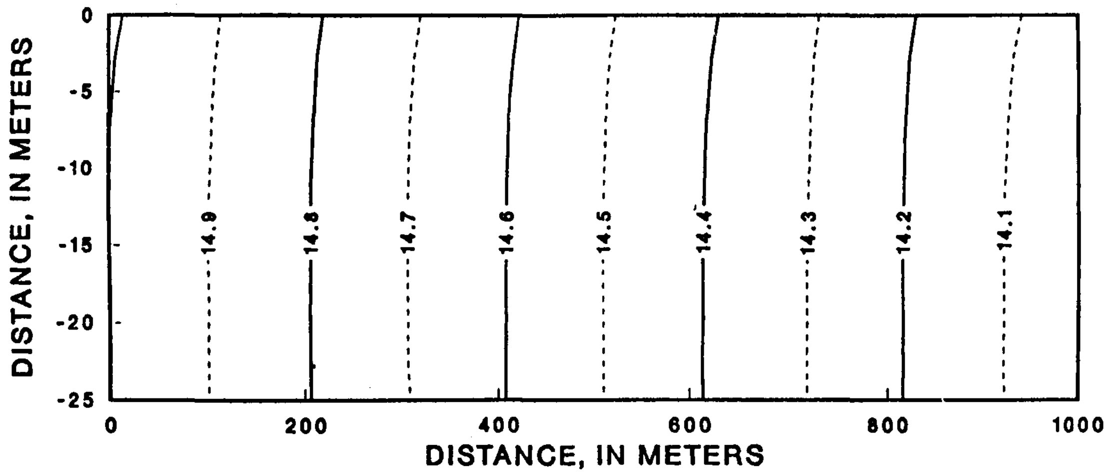

Figure 3. Hydraulic head contour at 20 years for case 1.

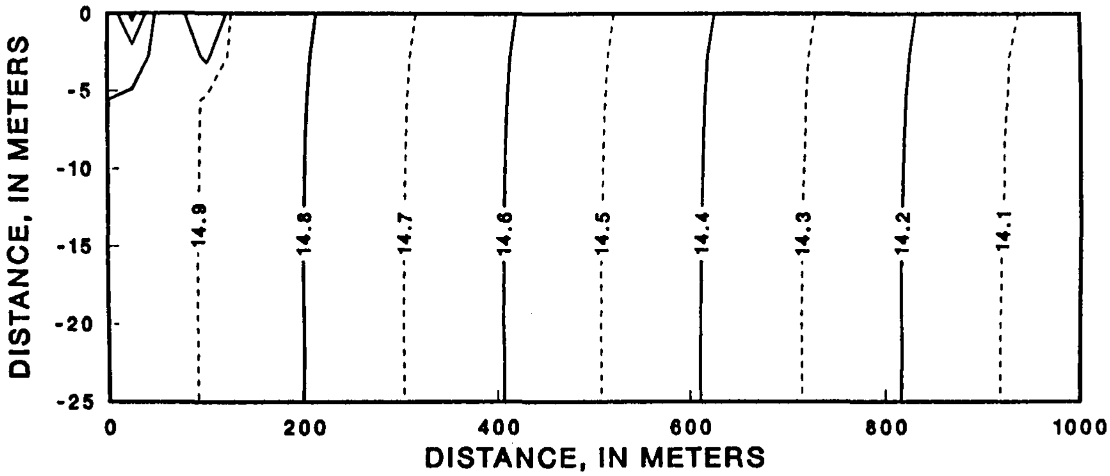

Figure 4. Hydraulic head contour at 20 years for case 3.

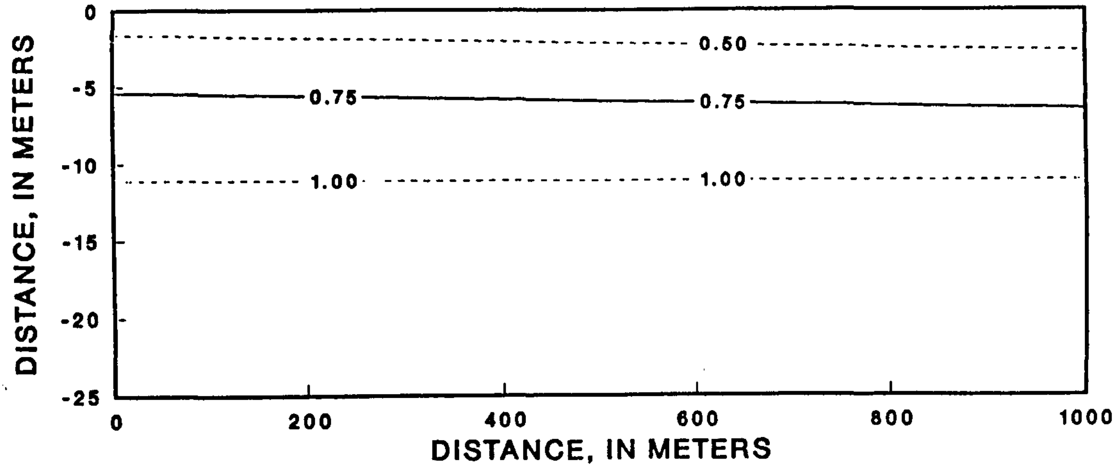

Figure 5. Saturation contour at 20 years for case 1.

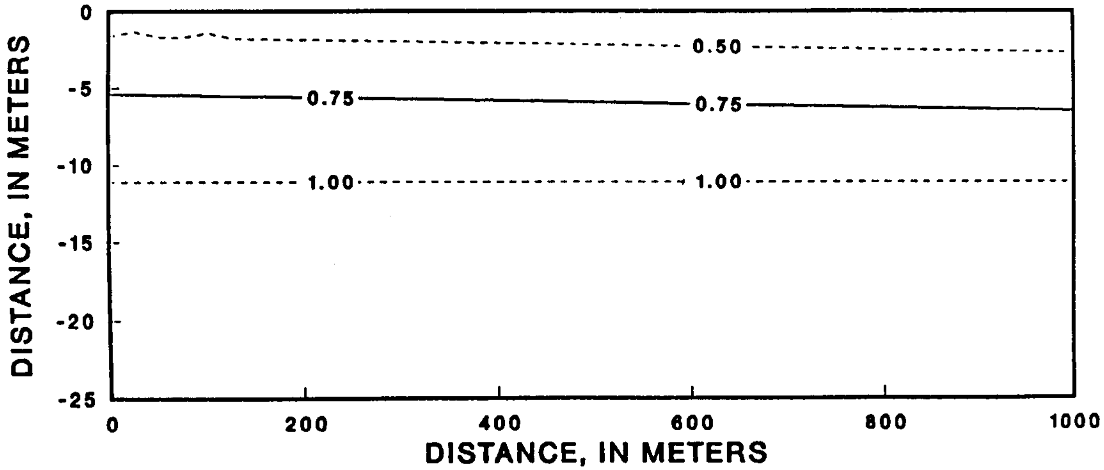

Figure 6. Saturation contour at 20 years for case 3.

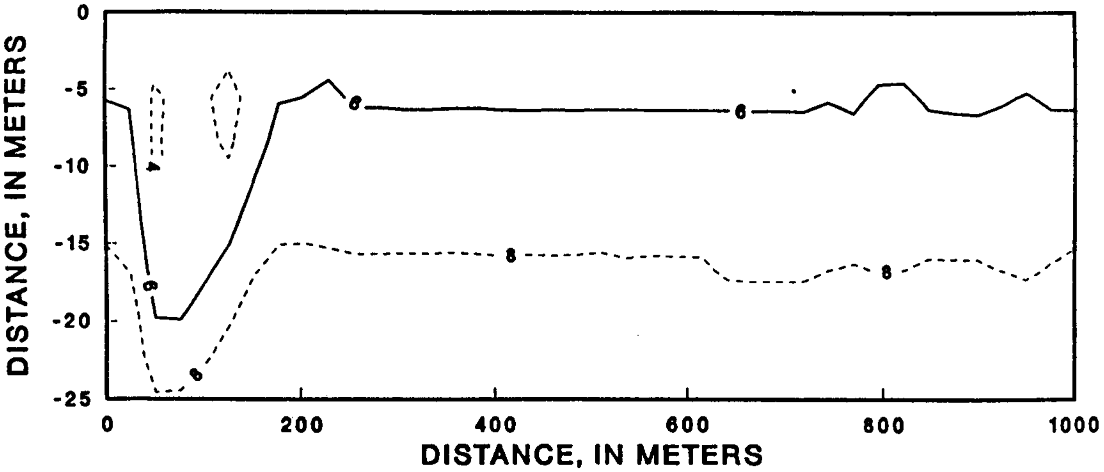

Figure 7. pH contour at 20 years for case 1.

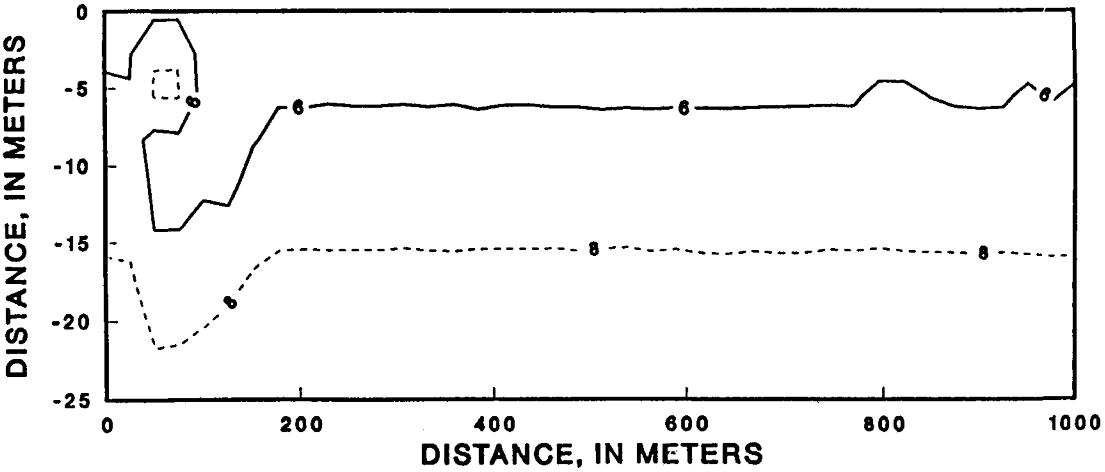

Figure 8. pH contour at 20 years for case 2.

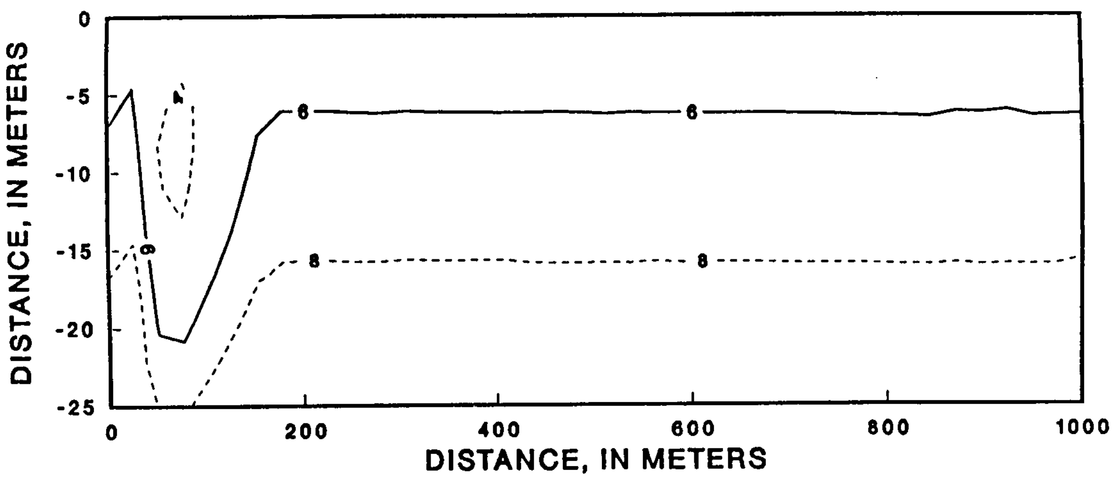

Figure 9. pH contour at 20 years for case 3.

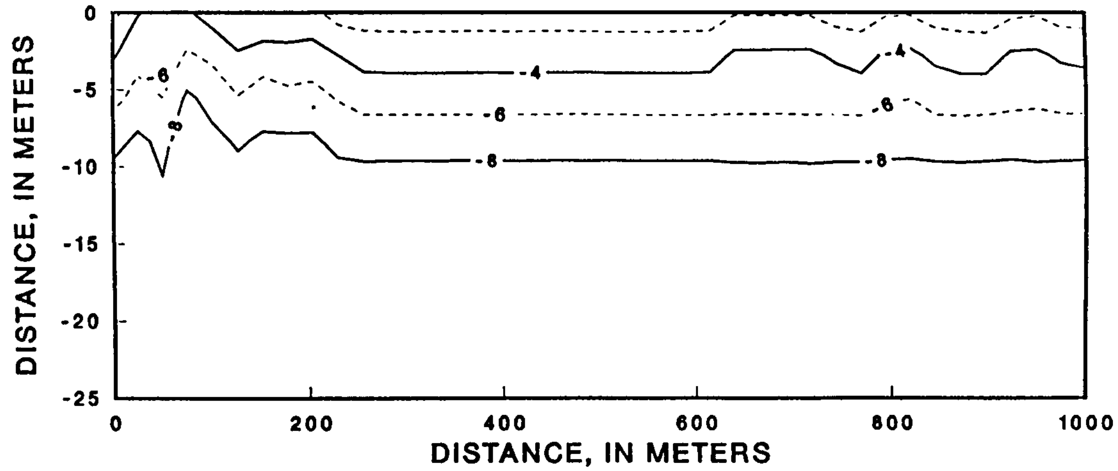

Figure 10. pE contour at 20 years for case 1.

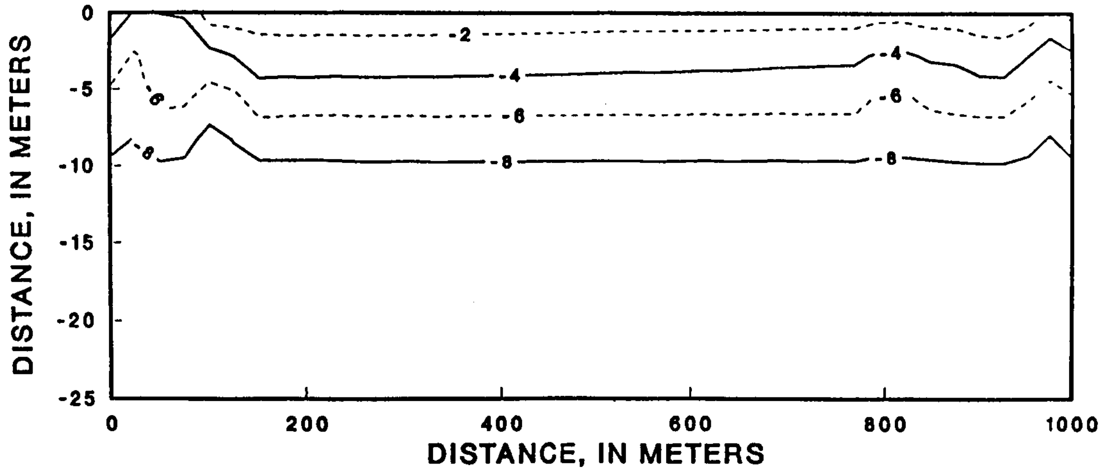

Figure 11. pE contour at 20 years for case 2.

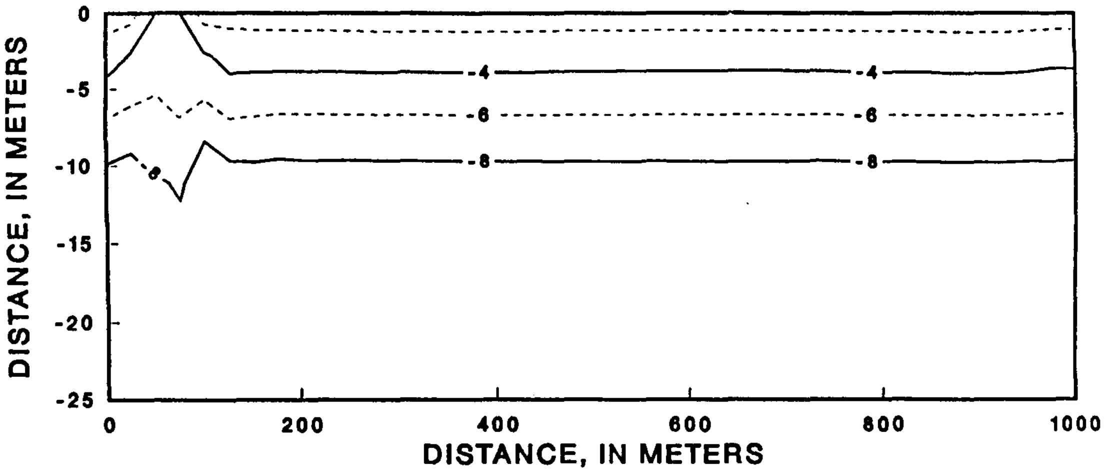

Figure 12. pE contour at 20 years for case 3.

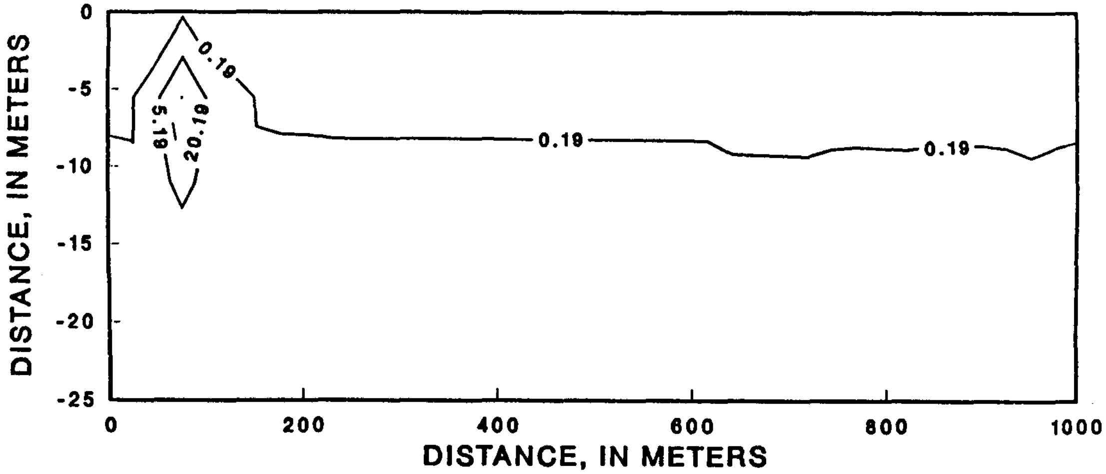

Figure 13. Aqueous sulfur concentration contour at 20 years for case 1.

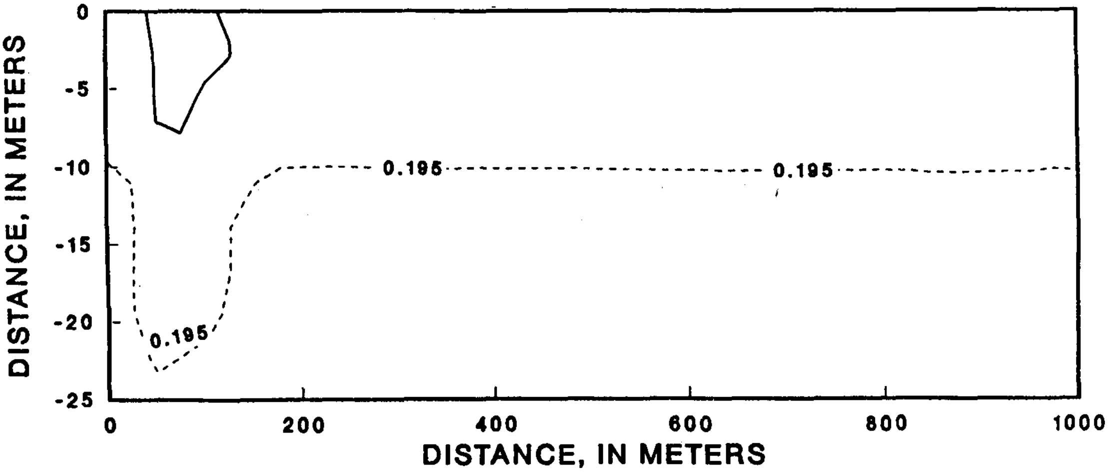

Figure 14. Aqueous sulfur concentration contour at 20 years for case 2.

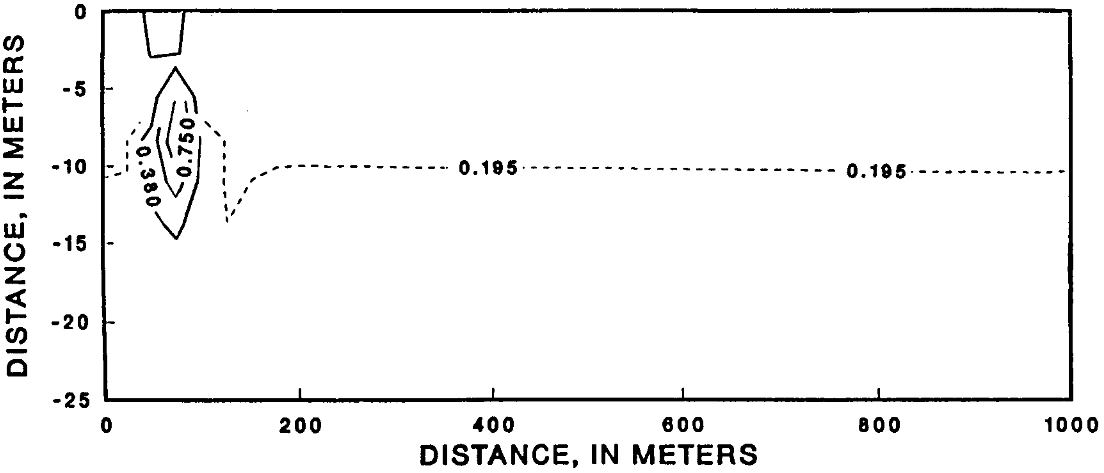

Figure 15. Aqueous sulfur concentration contour at 20 years for case 3.

of acid front for case 2 is relative slow as compare with case 1 and case 3 which suggest that the method of blending with lime stone is much more effective to retard the acid movement. Figure 10 to Figure 12 show the simulated pE contours at 20 years for case 1, case 2, and case 3 respectively. The movements of redox front among three cases are relatively slow and very close each other. Figure 13 to Figure 15 show the simulated aqueous S concentration contours at 20 years for case 1, case 2, and case 3 respectively. Case 1 has the highest aqueous sulfur concentration. Case 3 have the second but is much higher than case 2.

The amount of pyrite dissolution in the toxic mine spoil are 1,000 moles, 30 moles and 130 moles for case 1, case 2 and case 3 after 20 years which also suggest that the lime stone method is much more effective than clay liner to reduce pyrite oxidation and acid generation.

Results of simulation suggest that the method of blending with lime stone is much more effective than the method of covering with clay liner to reduce the acid generation. However, the overall operational cost is also a key factor in the choice between these two methods for surface mine reclamation.

4. SUMMARY

In this paper, a numerical model for multi-dimensional transient fluid flow and reactive chemical transport through partially saturated media, FRCT, is developed. The multi-dimensional nature of the model allows it to simulate realistic field problem. The model is applied to study the flow through toxic mine spoil. Three cases which include toxic spoil covered with native soil, toxic mine spoil blended with lime stone, and toxic mine spoil covered with clay liner are investigated. Results of simulation suggest that the method of blending with lime stone is much more effective than the method of covering with clay liner to reduce the acid generation. However, the overall operational cost is also a key factor in the choice between these two methods for surface mine reclamation.

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NOTATION

Symbol	Description	Dimensions
a_i	Activity of chemical component i	M/M
b_{ip}	Stoichiometry coefficient of i^{th} chemical component in the p^{th} mineral phase	
C	Concentration	M/M
C_i	Concentration of chemical component i	M/M
C_j	Concentration of chemical species j	M/M
C_i^T	Total concentration of chemical component i	M/M
C_{gi}	Fluid source concentration of chemical component i	M/M
$D_{diff,i}$	Molecular diffusion coefficient of chemical component v	L^2/T
D	Dispersion coefficient	L^2/T
g_m	Mass generation rate of fluid per unit volume	M/L^3T
h_{ij}	Stoichiometry coefficient of the i^{th} chemical component in the j^{th} chemical species	
I	Number of chemical components	
i	i^{th} chemical component	
J	Number of chemical species	
j	j^{th} chemical species	
K_p	Thermodynamic equilibrium constant for mineral phase p	
P	Number of mineral phases	
p	p^{th} mineral phase	
p^E	Negative logarithm of the hypothetical electron activity	
p^H	Negative logarithm of the hydrogen ion activity	
RS	Redox state of an aqueous solution	
s	Aqueous phase saturation	
t	time	
v	Operational Valence	
v_j	Operational valence of j^{th} chemical species	
V	Darcy velocity	
v_p	Operational valence of p^{th} mineral phase	
V_e	Volume of element e	
Z_j	Electrical charge of j^{th} chemical species	
α_l	Longuitudinal dispersivity	
α_p	Mass transfer due to dissolution(+) or precipitation(–) of p^{th} mineral phase	M/M
γ_i	Activity coefficient of i^{th} chemical component	
ϕ	Porosity	
ε	Prescribed tolerance	
ρ_f	Fluid density	M/L^3

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