2. Numerical Simulations of Water Flow and Solute Transport Applied to Acid Sulfate Soils

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Abstract: Field investigations of Rassam et al. in 2001 have highlighted the effects of infiltration, drainage, and evapotranspiration on the dynamics of water flow and solute transport in acid sulfate (AS) soils. In this work, *HYDRUS-2D* is adopted as the modeling tool to elucidate the trends observed in that field experiment. Hypothetical simulations have shown that the relative contribution of drains to lowering the water table is significant only when closely spaced drains are installed in coarse textured soils, evapotranspiration being the main driving force in all other cases. AS soils reaction products that are close to a drain are readily transportable during infiltration and early drainage, but those produced farther away from it near the midpoint between drains are only slowly transported during a prolonged drainage process. Simulating the field trial of Rassam et al. has shown that drain depth and evapotranspiration significantly affect solute fluxes exported to the ecosystem. Managing AS soils should target minimal drain depth and density. Partial or full lining of the drains should be considered as a management option for ameliorating the environmental hazards of AS soils.

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Introduction

Field studies of Rassam et al. (2002) have investigated the hydrology of acid sulfate (AS) soils and pointed out that evapotranspiration (ET) plays a crucial role in driving water-table dynamics in low-conductivity AS soils. The study has also shown unique trends of solute concentration in the drainage water during infiltration and drainage.

Grismer (1989) suggests that intensive field measurements in conjunction with computer modeling might be necessary when designing drainage systems that incorporate water quality. Grismer (1993) adopts numerical techniques to demonstrate the relative effects of drain spacing and depth on water quality.

The interaction of climate, hydrology, and drainage is the most poorly understood aspect of AS soils (White et al. 1996). In this work, numerical simulations are conducted in hypothetical situations to demonstrate the relative importance of drain depth, drain spacing, and ET on the dynamics of water flow and solute transport in soils of various textures. Simulations of solute transport are conducted to simulate the trends observed in the field studies of Rassam et al. (2002). Simulations that use realistic soil parameters and weather data are conducted to show the effects of ET and drain depth on solute fluxes from AS soils. In light of the modeling findings, management options for AS soils are suggested.

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Modeling Tool

HYDRUS-2D (Simunek et al. 1994) was used to investigate water-table dynamics and to simulate solute transport. It uses the finite element program *SWMS-2D* (Simunek et al. 1994) to simulate two-dimensional water movement in variably saturated media. The following modified form of Richards' equation governs water flow:

$$\frac{\partial\theta}{\partial t}=\frac{\partial}{\partial x}\left[k(\psi)\left(\frac{\partial\psi}{\partial x}+1\right)\right]-s \tag{1}$$

where x=spatial coordinate (L); t=time (T); θ=volumetric water content (L^3/L^3); $k(\psi)$=unsaturated hydraulic conductivity (L/T); ψ=pressure head (L); and s=a sink term (L^{-1}). The latter represents the volume of water removed per unit time for a unit volume of soil due to plant water uptake. Feddes et al. (1978) defined s as

$$s(\psi)=a(\psi)s_p \tag{2}$$

where the water stress response function $a(\psi)$=a prescribed dimensionless function and s_p=potential water uptake rate. Water uptake is assumed to be zero both close to saturation ($\psi>h_1$) and beyond the wilting point ($\psi<h_4$). It assumes optimal uptake between intermediate heads h_2 and h_3. The function assumes linear variation between h_1 and h_2 and h_3 and h_4. The Feddes' parameters (h_1, h_2, h_3, and h_4) used for the current simulations are listed in Table 1.

The pressure-saturation relationship is given by van Genuchten (1980)

$$\Theta=\frac{\theta-\theta_r}{\theta_s-\theta_r}=[1+(\alpha\psi)^n]^{-m} \tag{3}$$

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Table 1. Hydraulic and Solute Transport Parameters of Modeled Soils

Hydraulic parameters	K_s (m/s)	θ_s	θ_r	α (m^{-1})	n
Sandy loam	1.228×10^{-5}	0.41	0.065	7.5	1.89
Silt loam	1.25×10^{-6}	0.45	0.067	2	1.41
Silt	6.94×10^{-7}	0.46	0.034	1.6	1.37
Clay loam	7.22×10^{-7}	0.41	0.095	1.9	1.31
Pimpama soil	2.4×10^{-8}	0.54	0.22	0.2093	2.01
Solute transport parameters	Diffusion coefficient[a] (m^2/d)	Longitudinal dispersivity λ_L (m)		Transverse dispersivity Λ_T[b] (m)	
All soils	9.25×10^{-5}	0.1		0.01	
Feddes' parameters[c]	$h_1=-0.01$ m	$h_2=-0.25$ m	$h_3=-2$ m	$h_4=-80$ m	

[a]Diffusion coefficient for SO_4^{2-} (Kemper 1986).

[b]Typically $\lambda_T=\lambda_T/10$ (*HYDRUS-2D* default value).

[c]Parameters for sugar cane from *HYDRUS-2D* library.

where Θ = relative water content; θ_s = saturated volumetric water content; θ_r = residual volumetric water content; and α (L^{-1}), n, and m = fitting parameters.

The unsaturated hydraulic conductivity function used is that of van Genuchten (1980), who used the statistical pore-size distribution model of Mualem (1976) to obtain the following predictive equation for the special case in which $m=1-1/n$:

$$k(\psi)=K_s\frac{\{1-(\alpha\psi)^{n-1}[1+(\alpha\psi)^n]^{-m}\}^2}{[1+(\alpha\psi)^n]^{m/2}} \tag{4}$$

where K_s = saturated hydraulic conductivity of the soil.

Nonreactive solute transport is governed by the following advection-dispersion equation:

$$\frac{\partial c}{\partial t}=D_h\frac{\partial^2 c}{\partial x^2}-\nu_s\frac{\partial c}{\partial x} \tag{5}$$

where c = concentration of the solute in the liquid phase (M/L^3, M refers to mass expressed in moles); ν_s = average linear velocity of water (L/T); and D_h = hydrodynamic dispersion coefficient (L^2/T), which accounts for mechanical dispersion D_m and molecular diffusion D_o. *HYDRUS-2D* requires separate entries for the diffusion coefficient and dispersivity. The latter is defined as follows:

$$\lambda=\frac{D_m}{\nu_s} \tag{6}$$

where D_m = mechanical dispersion coefficient.

The boundary conditions for the two-dimensional model are illustrated in Fig. 1. Due to symmetry, only half the problem is analyzed (S is half the drain spacing). Both the base and the symmetry line are assumed to be no-flow boundary conditions (the impermeable base is taken as the datum for water-head measurement). The drain is represented by a ditch with a seepage face. The soil surface is an open atmospheric boundary condition through which infiltrative influx or evapotranspirative efflux is allowed.

The governing differential equations are solved using the Galerkin-type linear finite element method applied to a network of triangular elements. Integration in time is achieved using an implicit (backward) finite difference scheme for both saturated and unsaturated conditions.

Modeling of Hydrology

Shallow drains are traditionally introduced into cane fields to prevent water logging and to drain surface runoff. In this section, the effects of drain depth and spacing are investigated. The interdependent effects of evaporation and drainage on the water-table dynamics are closely examined. Two soil types are considered, namely sandy loam (a high-conductivity soil) and clay loam (a low-conductivity soil). The hydraulic properties of these soils, which are listed in Table 1, were obtained from *Rosseta* (Schaap et al. 2001). The simulations assume an initial water table located at the soil surface.

Effect of Drain Depth and Spacing

The steady-state drainage equation of Hooghoudt (1940, in van der Molen and Wesseling 1991) is extensively used to calculate drain spacing

$$S^2=\frac{K_sH}{V}(2d+H) \tag{7}$$

where S = half the drain spacing; H = hydraulic head midway between the drains; d = thickness of an equivalent subsoil layer; and V = steady-state outflow rate (L/T).

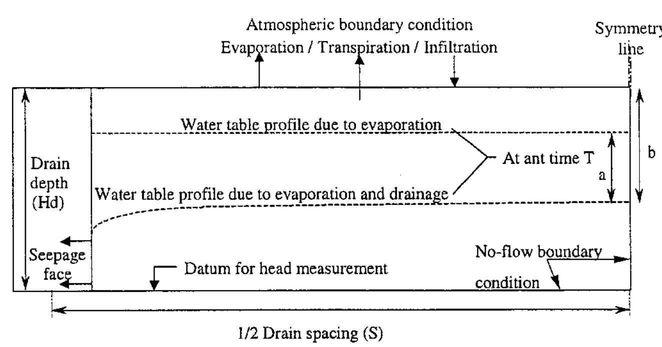

Fig. 1. Vertical cross section showing modeled soil-block and boundary conditions

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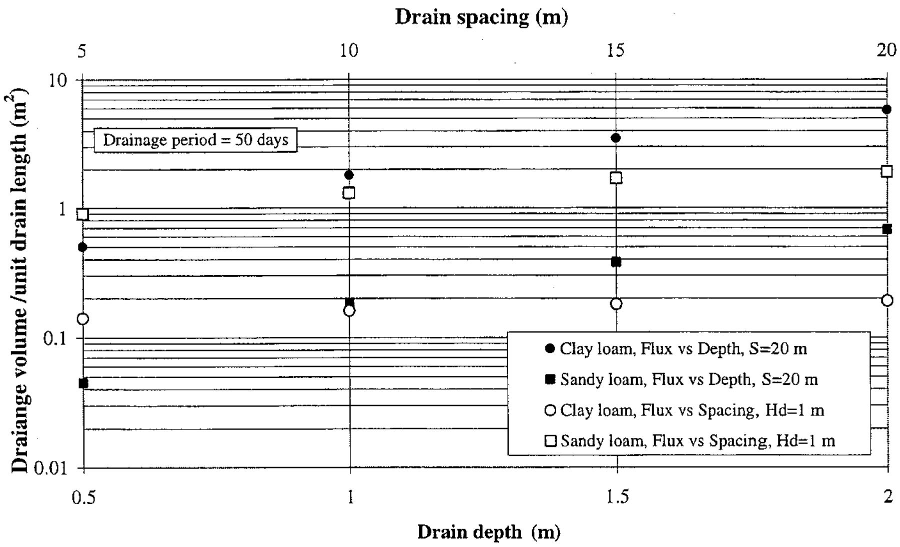

Fig. 2. Effect of drain depth and spacing on seepage flux without evaporation

Numerical simulations show that a deeper drain has similar effects on low- and high-conductivity soils (Fig. 2). For both soils, the cumulative seepage flux increases by about an order of magnitude when the drain depth is increased fourfold when there is no evaporation. Referring to Fig. 2, a higher drainage flux from the sandy loam is noted when the drain spacing is increased. It will be shown in the next section that the effects of increasing the drain spacing are offset by evaporation, especially in the case of fine-grained soil.

Interaction of Evaporation and Drainage

The interaction of evaporation and drainage is investigated for a constant evaporation rate of 2 mm/d. The effect of evaporation on seepage from low-conductivity soils for two drain spacings $S=5$ and 20 m is shown in Fig. 3. Fig. 3 demonstrates that for low-conductivity soils regardless of drain spacing, seepage is lowered when evaporation is accounted for in the simulation (curve 1 shows a cumulative discharge lower than curves 2 and 3). In contrast, the effect of S is more significant in high-conductivity soils [the results shown in curves 4 and 5 are different from those in curves 6 and 7 (Fig. 3)]. The effect of evaporation is evident early in the simulation for the case of a low-conductivity soil (Fig. 3, curves 1 and 2), however it exhibits a time lag in the case of a high-conductivity soil (Fig. 3, curves 6 and 7 coincide up to 15 days of simulation time).

The relative significance of seepage and evaporation may be interpreted in terms of the ratio of cumulative evaporative flux to cumulative seepage flux ($\Sigma E_a/\Sigma S$). A simulation is carried out to compare the fluxes from a fine-textured soil with a shallow drain of 1 m (minimize drainage) to those from a coarse-textured soil with a deep drain of 2 m (maximize drainage). Fig. 4 shows a difference in $\Sigma E_a/\Sigma S$ of more than an order of magnitude between the two cases, which later in the simulation increases to more than two orders of magnitude. At the end of the simulation, the slope of $\Sigma E_a/\Sigma S$ has not yet flattened in the case of the fine-textured soil. This is due to the fact that the actual evaporative flux is still close to its potential value (E_p). On the other hand, actual evaporative flux from the coarse-textured soil has

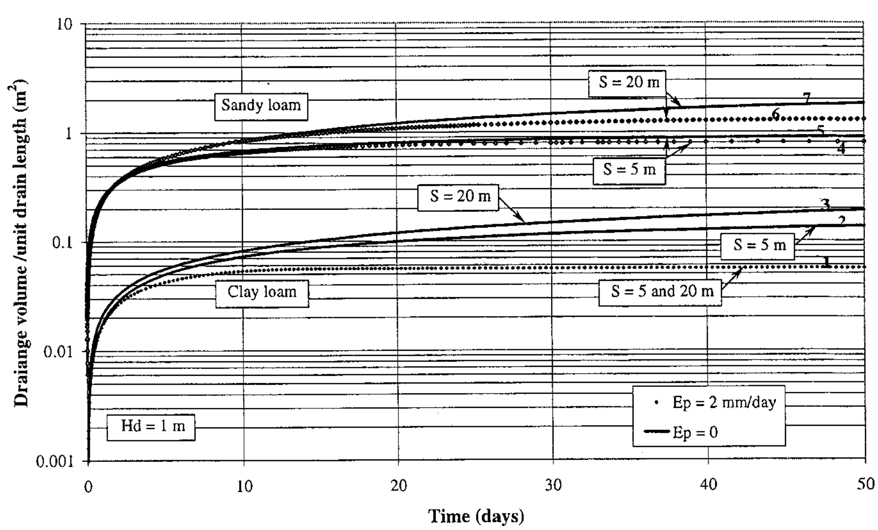

Fig. 3. Interaction of evaporation and drainage

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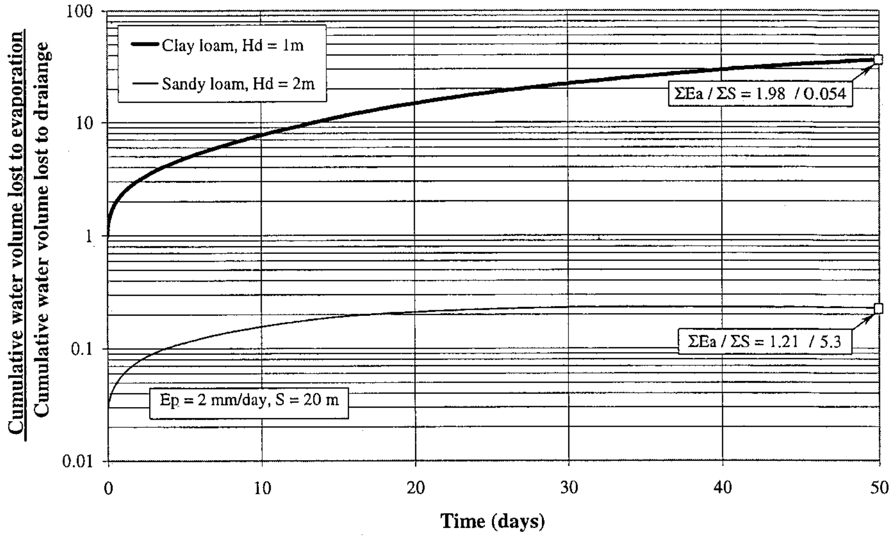

Fig. 4. Relative significance of evaporative and drainage fluxes

fallen to about $0.6E_p$ due a dramatic drop in the unsaturated hydraulic conductivity of the coarse-textured soil. For the case of a fine-textured soil with a shallow drain, ΣS (cumulative drainage) accounts for only 3% (=0.054/[0.054+1.98], see Fig. 4) of the total water balance compared to 81% (=5.3/[1.21+5.3], see Fig. 4) for the case of a coarse-grained soil with a deep drain.

The midpoint water-table depth is an important criterion in drain design (Ayars et al. 1997). Youngs (1985) proposed a simple equation that uses the midpoint water depth to describe the water-table draw-down. Referring to Fig. 1, *b*-*a* and *b* represent the midpoint water-table depths due to evaporation only and the combined evaporation and drainage, respectively. Fig. 5 demonstrates the variation of $[Hd\text{-}(b\text{-}a)]$ and $(Hd\text{-}b)$ with time for $S = 5$ m and the drained soil is a coarse-textured sandy loam. Fig. 6 compares the contribution of drainage to the draw-down of the water table as indicated by the ratio a/b for three different scenarios of drain spacings and soil types. It demonstrates that the contribution of drainage is significant only in the case of narrow drain spacing and coarse-textured soil. In the case in which the drain spacing is narrow, the contribution of drainage peaks very early in the simulation, while a time lag is noticed in the case of the wider drain spacing.

Modeling of Solute Transport

In order to investigate the impact of different hydrologic scenarios and soil types on the export of solutes from AS soils, a hypothetical soil block was assumed to have a uniform solute concentration of 1 mmol/m^3 (in soil's pore water). The assumed solute transport parameters are listed in Table 1. The soil types considered were sandy loam, silt loam, and silt. The hydraulic properties of these soils, which are listed in Table 1, were obtained from *Rosseta* (Schaap 1999, unpublished).

The first set of simulations assumes an initial water-table depth of 1.5 m and hydrostatic equilibrium; other details are shown in Fig. 7. A large infiltration rate of 1 m/d is simulated to investigate concentration patterns at different locations and times. Fig. 7

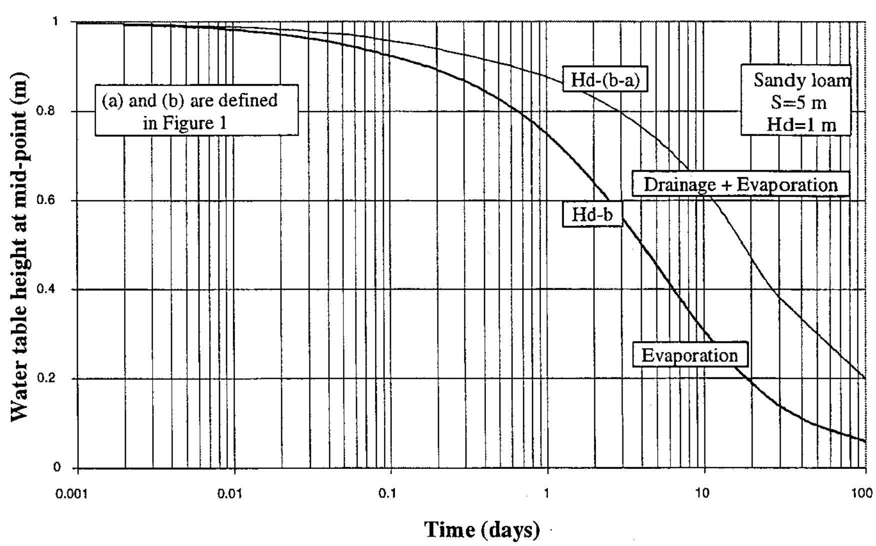

Fig. 5. Water-table draw-down for evaporation alone and combined evaporation and drainage

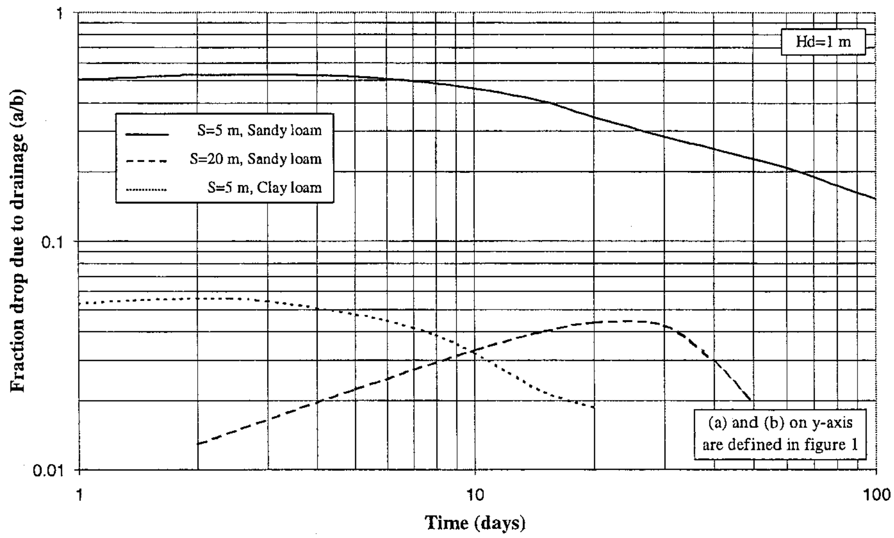

Fig. 6. Relative contribution of drainage to water-table draw-down

shows that the solute concentration in the soil close to the surface commences to decrease earlier and faster compared to the soil located at a greater depth. Solutes are diluted as the volumetric water content of the soil increases up to saturation, hence the kinks apparent at time $T1$, which are associated with soil saturation (Fig. 7, OP1 and OP2). The higher volume fraction of the pore air space associated with a lower soil potential near the surface explains the higher dilution noted closer to the soil surface (OP3 drops to a concentration lower than OP2). This demonstrates the significance of the initial soil conditions when modeling solute transport. The kink is not seen clearly close to the drain (Fig. 7, OP1) because of the replenishment action of the infiltrating water in such a high conductivity soil, which continues to dilute the solutes and readily carries them into the drain [Fig. 8(b), see velocity vectors close to the drain]. At 0.8 m from the drain (Fig. 7, OP1), the concentration drops to zero after 2.5 d. On the other extreme, the concentration during the period $T2$-$T1$ remains almost unchanged at 10 m from the drain (Fig. 7, OP2 and OP3). Fig. 8(a) demonstrates how the concentration contours move during the infiltration period close to the drain while they remain stationary at a distance farther from the drain [Fig. 8(b), see velocity vectors with very low magnitude >6 m from the drain].

During drainage ($T>20$ d), a notable drop in concentration occurs at a depth of 0.6 m, 10 m from the drain (Fig. 7, OP2). The phenomenon is less notable closer to the soil surface (Fig. 7, OP3). Shortly after drainage commences, a rise in concentration is notable close to the drain (Fig. 7, OP1). This phenomenon may be attributable to the transverse movement of water having a high solute concentration towards the drain [Fig. 8(c), see velocity vectors; note movement of concentration contours during drainage in Fig. 8(a)].

The velocity vectors shown in Figs. 8(b and c) show that the pore-water (and hence dissolved solutes) located close to a drain is more quickly transported during a rainfall event. In contrast, the pore-water located farther away from a drain is more slowly transported during the drainage stage that follows the cessation of rainfall.

The impact of varying drain depth, drain spacing, and evaporation rate on the cumulative solute seepage flux (total export to

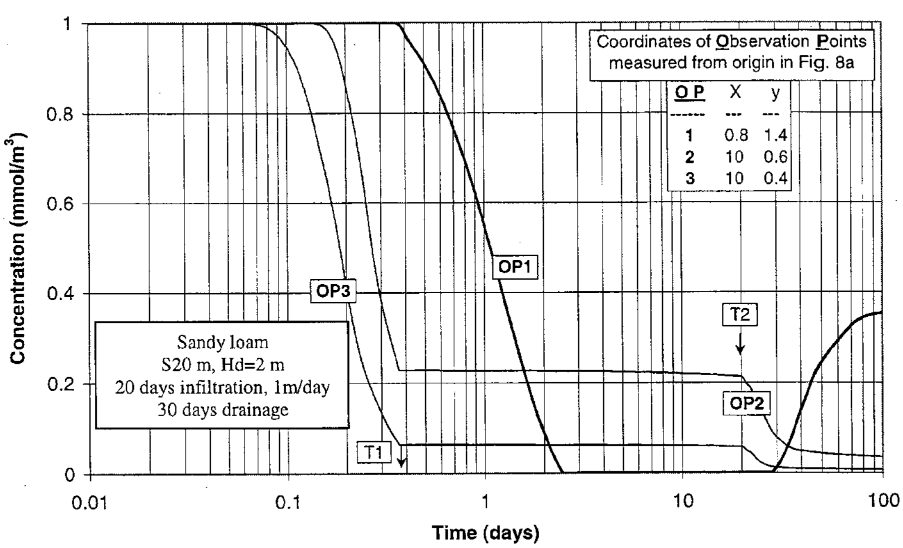

Fig. 7. Solute concentration versus time at various locations relative to drain

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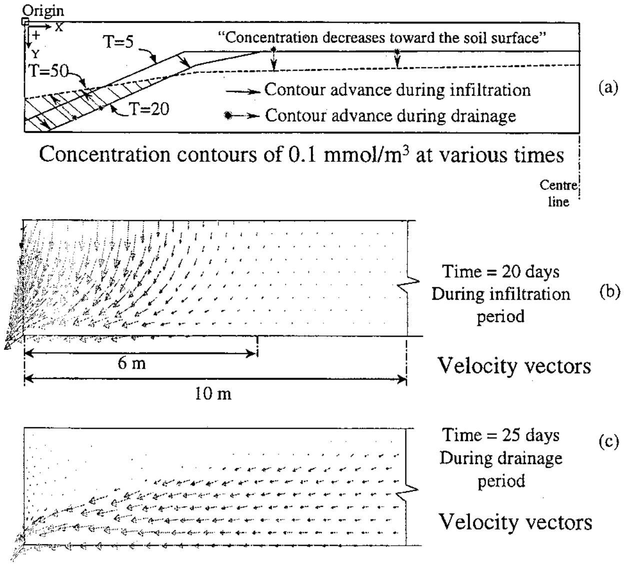

Fig. 8. Solute concentration contours and velocity vectors during infiltration and drainage

ecosystem) is shown in Fig. 9. It is notable that during infiltration (time $< T1$), drain spacing has little effect (Fig. 9, curves 2–5 coincide). This is attributable to the fact that most solutes during the infiltration stage are transported from the soil in the vicinity of the drain (hence drain spacing is irrelevant). Cook et al. (1998) used a stream-tube model to demonstrate that solutes are unlikely to arrive from a distance of more than 10 m from the drain during a storm event. A marginal long-term increase of total solutes, in the case of wider drain spacing, is attributed to the transverse solute flux that takes place over a long period of time (Fig. 9, curves 2 and 5). This increase is offset when evaporation is incorporated into the simulation. Evaporative flux drops the hydraulic gradient, but unlike water flux, it does not contribute to increasing the total solute mass (Fig. 9, compare curves 5, 4, and 3). However, drain depth has an effect on the total solute export at all stages (Fig. 9, compare curve 1 with the rest). It is worth mentioning that the simulation assumes a sandy loam soil for which the effects of the drains are magnified.

Measuring ion concentration in the drainage water is one of the most common tools adopted to monitor AS soils. The variation of ion concentration during infiltration and drainage events is an indicator of the impact that the contaminated water is having on the environment. The simulations assume 10 days of infiltration, during which a steady-state infiltrative condition is established (corresponding to constant seepage flux during the infiltration period, Fig. 10), followed by 90 days of drainage. During the infiltration period, the concentration dramatically decreases [as demonstrated when studying the velocity vectors, Fig. 8(b)]. The longer the infiltration period, the lower the resulting concentration. A higher saturated conductivity results in a steeper drop in concentration (Fig. 10, compare silt $K = 0.1$ and 0.5 m/d). However, a surge in concentration is notable during drainage, a trend noted in the field experiment of Rassam et al. (2002). Since fluxes during drainage run mainly in the horizontal direction [see velocity vectors, Fig. 8(c)], it is postulated that a higher initial solute concentration (in soil's pore-water) away from the drain would affect the steepness of the concentration surge. A simulation was conducted in which the grid was discretized into three equal zones in the horizontal direction. The initial solute concentration C (in soil's pore-water) away from the drain was assigned values of 1, 3, and 5 mmol/m^3. Fig. 10 (empty squares) shows that the steepness of the concentration surge is mainly controlled by the initial solute concentration, though the water retention parameters of the soil play a minor role too (Fig. 10, solid triangles).

Effect of Drain Depth and Envapotranspiration on Solute Fluxes from an Acid Sulfate Soil Field

It has been shown that drain depth and ET have a significant impact on solute export from low-conductivity soils. The effects of those two factors will be further demonstrated by adopting the measured soil parameters listed in Table 1 and weather data reported in the field trial of Rassam et al. (2002). The initial concentration in the soil's pore-water is assumed to be 1 mmol/m^3.

A drainage event is simulated to demonstrate the effect of ET on solute fluxes from the Pimpama AS soil. The average ET values for the dry and wet seasons in the Pimpama region are 3.6 and 1 mm/d, respectively (Rassam et al. 2002). The impact of the seasonal variation of ET on solute export is shown in Fig. 11. It is

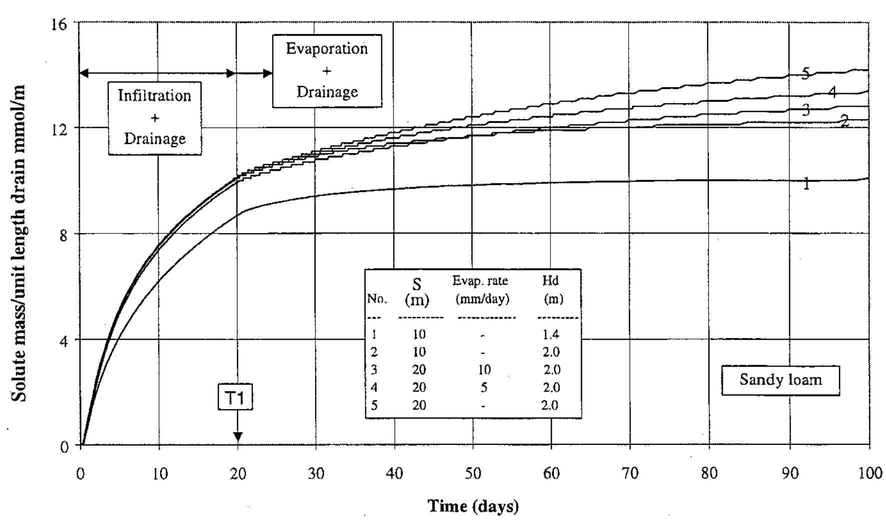

Fig. 9. Effect of S, Hd, and E_p on solute mass export to drain

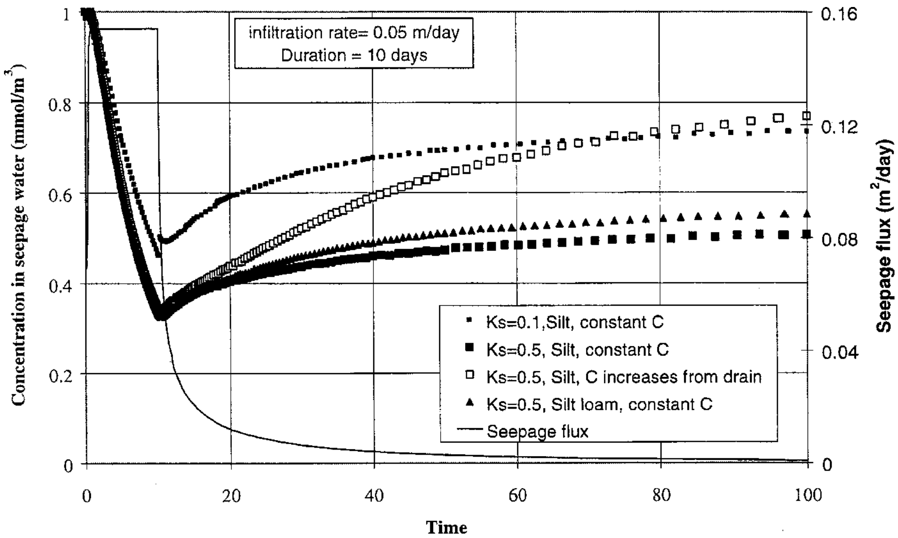

Fig. 10. Effect of initial solute concentration and soil type on ion concentration in seepage water with time

also revealed that excluding ET from the simulation results in a magnified estimate of solute export.

The weather data reported in the field trail of Rassam et al. (2002) were incorporated as atmospheric boundary conditions to investigate the effect of reducing drain depth on the cumulative solute flux. A series of 180-day simulations covering the period between January and June of 1999 were carried out. Fig. 12 clearly shows a significant drop (logarithmic decay pattern) in solute fluxes as a result of reducing drain depth in such AS soil fields.

Conclusions

Field and laboratory observations of Rassam et al. (2002) have shed some light on water-table dynamics and solute transport in acid sulfate (AS) soils. Numerical modeling helps us to understand the mechanisms involved in such complex systems and hence leads to better management options.

Hypothetical numerical simulation using *HYDRUS-2D* has shown that in low-conductivity AS soils, drains are responsible for lowering the water table and exposing the pyrites only in their close vicinity. The main factor responsible for lowering the water table away from the drain is evapotranspiration. That is, drains make an appreciable contribution to the phenomenon only when closely spaced drains are installed in high-conductivity soils. The interaction of drainage and evaporation, which depends upon soil type and drain spacing, plays a key role in the hydrology of AS soils.

Hypothetical simulations of solute transport have shown that the reaction products that are close to a drain are readily transportable during infiltration, while those produced farther away from it are slowly transported during a prolonged drainage process. Ion concentration in the drainage water exhibited unique trends during the infiltration and drainage periods. A decline in concentration was notable during infiltration, which was controlled by the duration of infiltration and the saturated hydraulic conductivity of the soil. However, a surge in concentration was notable during drainage, which was mainly controlled by the spatial variation of initial solute concentration (in soil's pore-water) and marginally affected by the water retention parameters of the

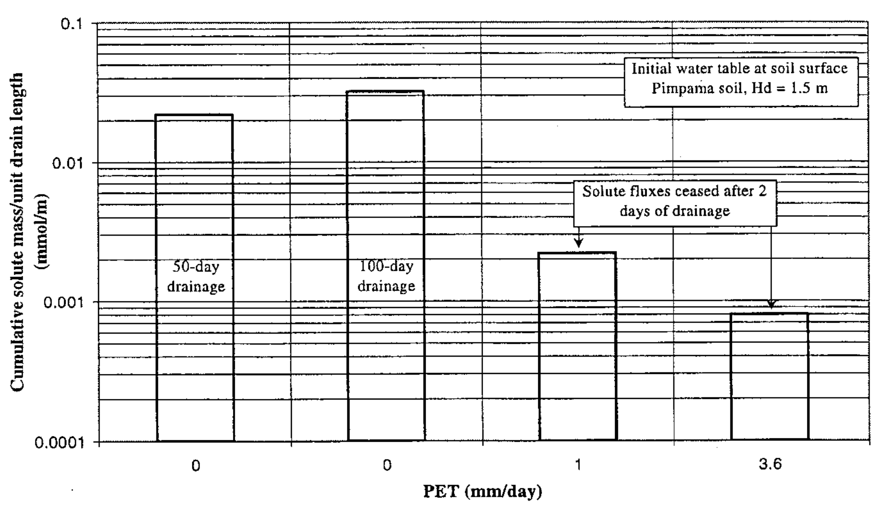

Fig. 11. Effect of potential evapotranspiration on cumulative solute mass export during drainage of Pimpama soil

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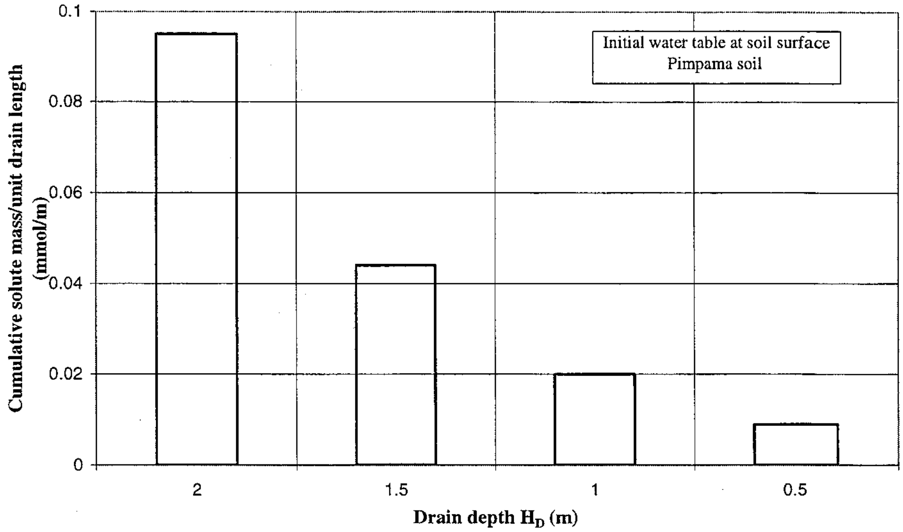

Fig. 12. Effect of drain depth on cumulative solute mass export during wet year in Pimpama region

soil. Simulations that assumed an increasing initial solute concentration away from the drain have resulted in a steep surge in concentration during drainage.

Numerical simulations that incorporated the field data of Rassam et al. (2002) have shown that the seasonal variations in evapotranspiration (ET) have a pronounced effect on solute fluxes from draining AS soils. Excluding ET from the simulations resulted in a magnified estimate of solute fluxes to drains. A 180-day simulation has shown the advantages of reducing drain depth in AS soil fields.

The design of drainage systems in AS soil fields should include a thorough environmental impact study. Modeling results have shown that minimal drain depth and density should be targeted in AS soil fields. Partial lining of existing open-ditch drains should reduce the environmental hazards of AS soils. In areas where the drains' function is mainly for collecting runoff water (e.g., where laser leveling is adopted), it is highly recommended that the sides of the drains be fully lined.

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Notation

The following symbols are used in this paper:

c = solute concentration in liquid phase;
D = dispersion coefficient;
h = pressure head for Feddes' function;
K = saturated hydraulic conductivity;
k = unsaturated hydraulic conductivity;
m = fitting parameter for van Genuchten model;
n = fitting parameter for van Genuchten model;
S = half drain spacing;
s = sink term;
t = time;
V = steady-state outflow rate from drain;
x = spatial coordinate;
α = fitting parameter for van Genuchten model;
Θ = relative water content;
θ = volumetric water content;
λ = dispersivity;
ν = average linear pore-water velocity; and
ψ = pressure head.

Subscripts

h = hydrodynamic;
L = longitudinal;
m = mechanical;
o = molecular;
r = residual;
s = saturation; and
T = transverse.

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