

Two-dimensional finite elements model for selenium transport in saturated and unsaturated zones

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Abstract A two-dimensional finite element model was developed to simulate species of selenium transport in two dimensions in both saturated and unsaturated soil zones. The model considers water, selenate, selenite, and selenomethionine uptake by plants. It also considers adsorption and desorption, oxidation and reduction, volatilization, and chemical and biological transformations of selenate, selenite, and selenomethionine. In addition to simulating water flow, selenate, selenite, and selenomethionine transport, the model also simulates organic and gaseous selenium transport. The developed model was applied to simulate two different observed field data. The simulation of the observed data was satisfactory, with mean absolute error of 48.5 µg/l and mean relative error of 8.9%.

Keywords Finite elements method · Unsaturated zone · Selenium (Se) · Selenate · Selenite · Selenomethionine · Organic Se · Gaseous Se · Modeling

Introduction

Selenium (Se) belongs to a group of micronutrient elements required in very small amounts by animals and humans for the basic functions of life. Toxicity and essentiality of selenium have been widely discussed by many authors (Sager 1994a, b; Peters et al. 1997; Zhang et al. 2003; Bujdos et al. 2005; May et al. 2008). The concentration of selenium in plants and animals is strongly correlated with its concentration in soils. Plants and their derivatives transfer selenium from soils to humans (Girling 1984).

Selenium (Se) is considered to be one of the most abundant but toxic elements in the earth's crust. The large quantity of Se in the earth's crust is reported to be about 0.05–0.09 mg/kg (Alloway 1995). Se is a chalcophile element (Goldschmit 1954), and as such is associated with sulfide. As a natural constituent of soil minerals, selenium is normally present in soil at low concentrations ranging from 0.01 to 2 mg/kg (Dungan and Frankenberger 1999). The Se content of soils generally reflects the weathering of parent materials, although in certain conditions, atmospheric and

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more recently anthropogenic inputs may influence their composition. In the natural environment, elevated concentrations of Se in soils are associated primarily with volcanic materials, sulfide ore bodies, black shales, and carbonaceous sandstones (Alloway 1995). Se is most likely to be present in soils in selenate (SeO_4^{2-}) form. In humid regions, selenite (SeO_3^{2-}) appears to be the predominant specie (Adriano 1986). The use of Se as an agrochemical encompasses a variety of areas including its use in pest control and as a dietary supplement for livestock grazed in a Se-deficient area (NAS-NRC 1976). Under the agricultural practice of intense irrigation, Se in these soils can be leached out and further concentrated at locations where drainage water is disposed (Tanji et al. 1986, 1992; Fujii et al. 1988). Since Se contamination in soil and water causes serious damage to wildlife, significant research has been directed at the study of Se fate and its behavior in soil water systems (Frankenberger and Benson 1994; Frankenberger and Engberg 1998).

A number of laboratory and field Se transport studies were carried out to investigate Se transformations and transport (Ahlrichs and Hossner 1987; Alemi et al. 1988; Deveral and Fujii 1988; Deveral and Milliard 1988; Fujii et al. 1988; Sposito et al. 1988; Fio and Fujii 1990; Mirbagheri et al. 2008). In these studies, researchers examined the transport of several species of Se (selenate, selenite, selenomethionine) under a number of different conditions. These conditions ranged from simply steady-state feed of Se in soil columns to the transient transport of Se in the subsurface flow.

Mathematical modeling and simulation of Se transformations and transport were also attempted by several researchers (Deveral and Fujii 1988; Fio et al. 1990; Alemi et al. 1991). In these models, Se transport was mostly treated in one dimension under steady-state conditions. However, there is a need for a more comprehensive model which can treat Se transport in two dimensions under transient conditions and consider all the possible transformations of Se species. For this purpose, in this study, a validated 2-D finite element model (FEM) for water and salts transport in a saturated–unsaturated zone (Nour el-Din

et al. 1987; Karajeh et al. 1994) was extended to consider Se transformations and transport.

The objective of this study is to model selenium transformations and transport in two dimensions by FEM. The model is tested with field data.

Mathematical development

Flow transport

The equation which models the transient flow in saturated–unsaturated zone in two dimensions is expressed as (Neuman 1973; Nour el-Din et al. 1987; Karajeh et al. 1994):

$$\left(\lambda S_s + \frac{\partial \theta}{\partial p} \right) \frac{\partial p}{\partial t} = \frac{\partial}{\partial x} \left[K_r \frac{k_{xx}}{\mu} \frac{\partial p}{\partial x} \right] + \frac{\partial}{\partial z} \left[K_r \frac{k_{zz}}{\mu} \left(\frac{\partial p}{\partial z} - \rho g \right) \right] \mp Q \quad (1)$$

where λ = a coefficient taken as unity in the case of saturated flow and zero in the case of unsaturated flow; S_s = the storage coefficient that describes the volume of water released from storage under a unit decline in hydraulic head; θ = volumetric water content; p = soil water pressure; K_r = relative hydraulic conductivity ($0 < K_r < 1$); k_{xx} = saturated hydraulic conductivity tensor in x -direction; k_{zz} = saturated hydraulic conductivity tensor in z -direction; μ = kinematic viscosity; ρ = the density of water; g = the gravitational acceleration; and Q = the strength of all sources and sinks in the system.

Equation 1 is nonlinear since the hydraulic conductivity and soil water content are functions of pressure. In order to solve Eq. 1, initial and boundary conditions need to be specified. Initial spatial distribution of the pressure needs to be specified as the initial condition. The boundary conditions can be either Dirichlet type or Neuman type for specified pressure or specified flux, respectively.

Selenium transport

The Se transport and transformation processes in a soil column under transient flow conditions are

complex. Several complicating factors like pore water velocity gradient, hydraulic conductivity, evaporation and transpiration fluxes, concentration gradient, and seasonal rise and fall of the water table control the transport of different Se species. In general, Se is transported in soil by convection and dispersion which are the result of mass flow and concentration gradient. The Se transformation processes in soil systems are oxidation and reduction, adsorption and desorption, plant uptake, mineralization and immobilization, and volatilization.

Selenate is the most oxidized chemical species of Se with a chemical valence of $6+$ (Se^{6+}). Selenate can be both chemically and biologically reduced into selenite (Se^{4+}), which is then further reduced to elemental (Se^0) or organic Se (Se^{2-}). Methylation of Se is generally considered to occur on reduced Se species with a chemical valence of $\leq 4+$; however, the exact order in which the reaction steps occur is still debated (Dungan and Frankenberger 1999). These simultaneous and sequential Se reactions can be represented by the conceptual model presented in Fig. 1.

The rate of transformation of Se from selenite to selenate and vice versa through oxidation/reduction processes is very slow, but oxidation of elemental Se to selenite is somewhat more pronounced (Cary and Allaway 1969). The rate of oxidation/reduction of different species depends on factors such as the Eh, pH, and oxygen status of soil, soil temperature, microbial activity, and soil water content. In general, in alkaline soils of semiarid areas, Se exists in the selenate form. However, under acidic and reducing conditions, as in humid regions, Se may exist dominantly in the selenite form.

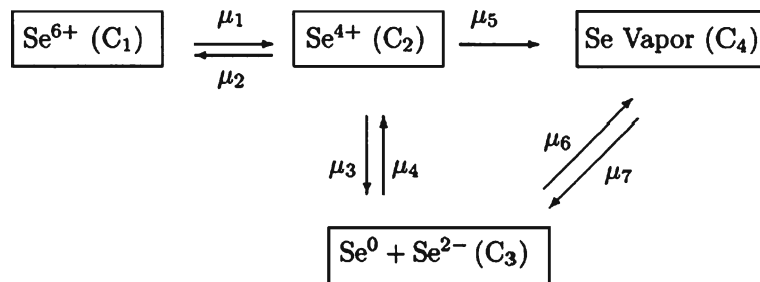
The process of selenate and selenite adsorption and desorption plays a crucial role in governing soil Se mobility in most acidic soils. This, in turn, affects the other Se processes in the soil, especially Se availability for plant uptake and volatilization. Since selenious acid is weaker than selenic acid, selenite is retained more strongly by soils than selenate (Balistrieri and Chao 1987; Neal and Sposito 1989; Fio and Fujii 1990; Shifang 1991). Factors affecting the processes of adsorption and desorption are the properties of adsorbents, the

solution pH, competitive anions such as PO_4^{3-} , and the concentration of soil amendment (CaCO_3 and CaSO_4 ; Hamdy and Gissler-Nielson 1977; Neal et al. 1987). The properties of adsorbents affect Se adsorption and desorption because of specific affinity sites and total surface area. Selenite adsorption was found to be positively correlated with specific areas and organic carbon. pH is very sensitive factor with respect to Se adsorption since it affects both surface electrochemical potential and Se redox potential (Hamdy and Gissler-Nielson 1977).

Se volatilization from soils has often been reported as being a result of microbial processes. The conversion of added Se to volatile gases was enhanced when soils were amended with organic matter (Karlson and Frankenberger 1989; Thompson-Eagle and Frankenberger 1990). Factors affecting the volatilization of soil Se are soil pH, soil temperature, organic matter content, liming and moisture content, microbial activity, and plant growth (Gissler-Nielson 1973, 1976; Hamdy and Gissler-Nielson 1977; Mushak 1985; Thompson-Eagle and Frankenberger 1990; Biggar and Jayaweera 1990). Gissler-Nielson (1976) from their studies concluded that the change in soil moisture content and the increase in liming, organic matter content, temperature, carbon sources, and protein sources increase the volatilization.

Se is absorbed by plants in both the inorganic form, such as selenate and selenite, and the organic form, as selenomethionine (Johnson et al. 1967; Gissler-Nielson 1973; Statman 1974). The factors affecting the Se uptake by plants are: soil moisture content, plant type, soil pH, soil texture, soil solution salinity, organic matter content, competitive anions such as SO_4^{2-} and PO_4^{3-} , tillage, and fertilizer (Carter et al. 1972; Westernman and Robbins 1974; Gissler-Nielson 1973, 1976; Hamdy and Gissler-Nielson 1977). In soils with a high content of organic matter and iron oxides, the selenite is very strongly fixed and thereby unavailable to plants (Gissler-Nielson 1973, 1976; Hamdy and Gissler-Nielson 1977). Sandy soil retains less Se than clay soil but is more available for plant uptake. Low pH favors the fixation of selenite to the clay minerals, while high pH favors the

Fig. 1 Reactions of selenium in soil [μ_i , is the forward or backward reaction rate coefficients among various Se species]



oxidation of selenite to the far more easily extractable selenates. Carter et al. (1972) suggested that plant uptake of selenite might be increased by phosphate (PO_4^{3-}), probably because of adsorbed selenite displacement, increased root growth, and enhanced microbial activities. Se concentration in plants decreases with the addition of SO_4^{2-} because of Se- SO_4^{2-} antagonism effects. Soil solution salinity decreases Se uptake, while tillage and fertilizer increases Se uptake due to soil aeration and stimulation of microbial activities and root growth (Westernman and Robbins 1974).

In the following section, the equations expressing selenate, selenite, and selenomethionine transport in two dimensions are given. Each equation comprises the advection diffusion terms and all the possible sink and source terms resulting from transformations and plant uptake.

Selenate transport

$$\begin{aligned} & \frac{\partial}{\partial t}(R_1 C_1) \\ &= \frac{\partial}{\partial x} \left[\theta D_{1x} \frac{\partial C_1}{\partial x} \right] + \frac{\partial}{\partial z} \left[\theta D_{1z} \frac{\partial C_1}{\partial z} \right] \\ & \quad - \frac{\partial}{\partial x} (C_1 q_x) - \frac{\partial}{\partial z} (C_1 q_z) - (\lambda_{a1} \alpha_1 U C_1) \\ & \quad - [(K_{r1} + K_{v1} + K_{b1}) \theta C_1] + (\rho_s K_{m1} S_o) \end{aligned} \quad (2)$$

where

$$R_1 = [\theta + \rho_s (K_{a1} n C_1^{n-1})] \quad (3)$$

where C_1 = selenate concentration (mg/l); R_1 = retardation factor for selenate; ρ_s = bulk density of the porous medium (kg/m^3); K_{a1} = adsorption coefficient for selenate (l/kg); n = nonequilibrium exponent for selenate; D_{1x} = total diffusion coefficient for selenate in x -direction (cm^2/day);

D_{1z} = total diffusion coefficient for selenate in z -direction (cm^2/day); θ = volumetric water content; q_x = Darcy flux in x -direction ($q_x = \theta v_x$, where v_x = pore water velocity in x -direction; cm/day); q_z = Darcy flux in z -direction ($q_z = \theta v_z$, where v_z = pore water velocity in z -direction; cm/day); λ_{a1} = root absorption coefficient for selenate; α_1 = coefficient for SO_4^{2-} antagonism effect for selenate; U = root water extraction (1/day); K_{r1} = transformation rate constant for reduction of selenate (1/day); K_{v1} = volatilization rate constant of selenate (1/day); K_{b1} = transformation rate constant for immobilization of selenate (1/day); K_{m1} = transformation rate constant for mineralization of selenate (1/day); and S_o = organic selenium concentration (mg/kg).

Selenite transport

$$\begin{aligned} & \frac{\partial}{\partial t}(R_2 C_2) \\ &= \frac{\partial}{\partial x} \left[\theta D_{2x} \frac{\partial C_2}{\partial x} \right] + \frac{\partial}{\partial z} \left[\theta D_{2z} \frac{\partial C_2}{\partial z} \right] \\ & \quad - \frac{\partial}{\partial x} (C_2 q_x) - \frac{\partial}{\partial z} (C_2 q_z) - (\lambda_{a2} \alpha_2 U C_2) \\ & \quad - [(K_{r2} + K_{v2} + K_{b2}) \theta C_2] + (\rho_s K_{m2} S_o) \\ & \quad + (K_{r1} \theta C_1) \end{aligned} \quad (4)$$

where

$$R_2 = [\theta + \rho_s (K_{a2} w C_2^{w-1})] \quad (5)$$

where C_2 = selenite concentration (mg/l); R_2 = retardation factor for selenite; K_{a2} = adsorption coefficient for selenite (l/kg); w = nonequilibrium exponent for selenite; D_{2x} = total diffusion coefficient for selenite in x -direction (cm^2/day); D_{2z} = total diffusion coefficient for selenite in

z -direction (cm^2/day); λ_{a2} = root absorption coefficient for selenite; α_2 = coefficient for SO_4^{2-} antagonism effect for selenite; K_{r2} = transformation rate constant for reduction of selenite (1/day); K_{v2} = volatilization rate constant of selenite (1/day); K_{b2} = transformation rate constant for immobilization of selenite (1/day); and K_{m2} = transformation rate constant for mineralization of selenite (1/day).

Selenomethionine transport

$$\begin{aligned} & \frac{\partial}{\partial t}(R_3 C_3) \\ &= \frac{\partial}{\partial x} \left[\theta D_{3x} \frac{\partial C_3}{\partial x} \right] + \frac{\partial}{\partial z} \left[\theta D_{3z} \frac{\partial C_3}{\partial z} \right] \\ & - \frac{\partial}{\partial x} (C_3 q_x) - \frac{\partial}{\partial z} (C_3 q_z) - (\lambda_{a3} \alpha_3 U C_3) \\ & - (K_{v3} \theta C_3) + (\rho_s K_{m3} S_o) \end{aligned} \tag{6}$$

where

$$R_3 = \left[\theta + \rho_s \left(K_{a3} l C_3^{l-1} \right) \right] \tag{7}$$

where C_3 = selenomethionine concentration (mg/l); R_3 = retardation factor for selenomethionine; K_{a3} = adsorption coefficient for selenomethionine (l/kg); l = nonequilibrium exponent for selenomethionine; D_{3x} = total diffusion coefficient for selenomethionine in x -direction (cm^2/day); D_{3z} = total diffusion coefficient for selenomethionine in z -direction (cm^2/day); λ_{a3} = root absorption coefficient for selenomethionine; α_3 = coefficient for SO_4^{2-} antagonism effect for selenomethionine; K_{v3} = volatilization rate constant of selenomethionine (1/day); and K_{m3} = transformation rate constant for mineralization of selenomethionine (1/day).

The rate of change in organic selenium can be expressed as:

$$\begin{aligned} \frac{\partial S_o}{\partial t} &= \frac{\theta}{\rho_s} K_{b1} C_1 + \frac{\theta}{\rho_s} K_{b2} C_2 - K_{m1} S_o \\ & - K_{m2} S_o - K_{m3} S_o \end{aligned} \tag{8}$$

The rate of change in gaseous selenium can be expressed as:

$$\frac{\partial G}{\partial t} = \frac{\theta}{\rho_s} K_{v1} C_1 + \frac{\theta}{\rho_s} K_{v2} C_2 + \frac{\theta}{\rho_s} K_{v3} C_3 \tag{9}$$

where G is gaseous selenium concentration ($\mu\text{g}/\text{kg}$). Numerical solution of the transport equations requires initial and boundary conditions. As an initial condition, zero concentrations along the soil profile are specified. The boundary conditions can be specified as Dirichlet type, Neuman type, and Cauchy type for specified concentration, zero flux, and prescribed flux, respectively. The details can be obtained from Nour el-Din et al. (1987) and Karajeh et al. (1994) where the flow part of the model was already tested and validated.

Model application to field data

The extended model was applied to simulate two different data sets obtained from the Mendota site, CA, USA. In the USA, various anthropogenic activities have greatly increased the mobilization and transport of selenium into aquatic ecosystems. From the 1960s through the 1980s, selenium mobilization on a regional and national scale largely was a result of two causes: (1) procurement, processing, and combustion of fossil fuels and (2) irrigation of seleniferous soils for crop production in arid and semiarid regions (Lemly et al. 1993; May et al. 2001).

A critical agricultural and environmental problem emerged in California’s San Joaquin Valley in the 1980s when saline subsurface drainage waters from 17,000 ha of waterlogged croplands were impounded in the Kesterson Reservoir. Cooke and Bruland (1987) identified various soluble Se species in surface waters at Kesterson Reservoir and San Joaquin River. Discharge of drainage water with high Se concentration was identified as the primary source of Se in the Kesterson National Wildlife Refuge (Deverel et al. 1984). The evapoconcentration of drain waters containing about 300 $\mu\text{g}/\text{l}$ of selenium (Se) and its subsequent biomagnification and bioaccumulation in the aquatic food chain resulted in the reduced reproduction, deformity, and death of waterbirds (NRC 1989).

The 1984 discovery of Se toxicosis in birds at the Kesterson National Wildlife Refuge triggered a massive federal/state investigation known as the San Joaquin Valley Drainage Program (SJVDP). Upon completion of a 6-year investigation, the SJVDP (1990) recommended a broad array of management options to solve the drainage related

Table 1 Soil characteristics parameters for soil type I (silty clay) and soil type II (clay)

Soil type	θ_r	θ_s	α	n	Se	K_s (cm/day)	ρ_b (gr/cm ³)
I	0.02530	0.425	0.0250	1.65	0.0002	13.3	1.385
II	0.02525	0.425	0.0129	1.98	0.0002	13.3	1.385

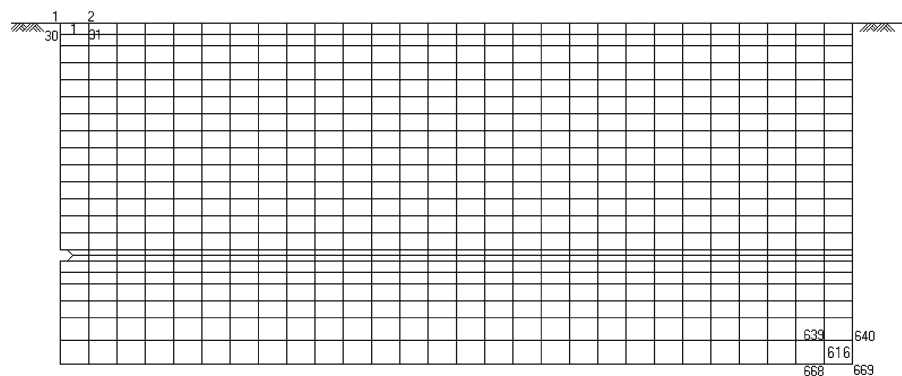
θ_s and θ_r are the saturated and residual field volumetric water contents, respectively; K_s is the saturated hydraulic conductivity; n and α are statistical parameters to be found by the least-square fitting for the specific soil type using the model of van Genuchten, and S_e is the reduced water content (see Nour el-Din et al. (1987) and Karajeh et al. (1994))

problems in the 0.9 million hectares of croplands of which 39% are waterlogged. One management option recommended was the reuse of drain waters in agroforestry systems comprised of salt-tolerant trees and shrubs. Drain water reuse was one of the few viable options available in those areas of irrigated croplands where there was little or no opportunity for discharge of irrigation return flows. This particular management option reduced the volume of unusable waters and concentrated salinity and trace elements for easier disposal and/or treatment. Moreover, reuse of drain water in agroforestry systems was also a remedial measure in itself because a portion of the salts and selenium participated in sink mechanisms.

The California Department of Food and Agriculture (CDFA) and USDA's Soil Conservation Service initiated trial tree plantings in the valley to lower the shallow groundwater and use saline drain waters as irrigation of trees such as *Eucalyptus* and *Atriplex* (Cervinka 1987). By 1990, over 0.5 million trees had been planted on 226 ha in 41 farms. Most of this effort was directed toward selection of salt-tolerant eucalyptus trees and their growth performance in saline soil environments. One of these farms was located

in Mendota, CA, USA. Saline drain waters from nearby croplands, having an average electrical conductivity (EC) of 10 dS/m and Se concentration of 400 $\mu\text{g/l}$, were being used to irrigate the *Eucalyptus camaldulensis*. Tile effluents from this tree plantation had an average EC of 32 dS/m and Se concentration of 700 $\mu\text{g/l}$. The tile effluents were then collected in evaporation tanks for salt harvest. From 1987 to 1990, there was a substantial buildup of soil salinity and Se. There was a need to assess the environmental fate pathways of Se in tree plantations utilizing saline drain waters containing elevated concentrations of Se.

The first data set belongs to the 1985–1990 plantations, and the second one belongs to the 1992 plantations. The Mendota site is the first monitored agroforestry demonstration project established by the Natural Resources Conservation Service and CDFA. The experimental site consists of fine-textured silty clay (0 to 60 cm) to clay soils (60 to 300 cm) underlain by an impermeable clay layer at 3- to 3.7-m depths over the entire plantation. Table 1 shows the soil property parameters for the two soil layers. Several lines of *E. camaldulensis* were planted in 1985 and 1986. The underdrainage system was installed in 1987. The

Fig. 2 Finite-element mesh with 616 elements and 669 nodes

trees were surface-irrigated with saline drainage waters collected from croplands about 2 years after planting. The irrigation was performed from April to November of each year. The total irrigation depths were 370 mm in 1988, 530 mm in 1989, and 1,055 mm in 1990. The irrigation rates were applied almost every 10 days for about 24 h. The irrigation application efficiency, which shows the amount of water stored in the crop root zone compared to the amount of irrigation water applied, was 75%. The average annual crop evapotranspiration depth was about 450 mm. The average Se concentration in the irrigation water was 400 µg/l. The trees performed remarkably well until they suffered killing frost damage in December 1990. Most of the detailed observations were made between the fall of 1987 and the summer of 1990. For model simulation, a finite element mesh with 616 elements and 669 nodes was constructed (Fig. 2). In order to capture the effect of gradients in the solution domain, the number of elements was increased; thereby, the size of elements was kept smaller. The model coefficients of the sink and source terms in the main equations were compiled from Hutson and Wagenet (1989), Fio et al. (1990), Thompson-Eagle and Frankenberger (1990), Biggar and Jayaweera (1990), Alemi et al. (1991), and Shifang (1991). Table 2 shows model predictions of measured data at the Mendota site in 1990. Since there were only four observations along the soil depth, we presented the results in a tabulated format. As seen in Table 2, the model closely predicted measured data. Following the killing frost of 1990 at the Mendota site and subsequent harvest of the trees, several lines of frost-tolerant *Eucalyptus* trees were planted in 1992. The experimental site was redesigned and automated for water flows, and the soils were also leached. Table 3 shows the model predictions of the measured Se concentration data in 1992. As can be seen, the model closely captured the

Table 2 FEM model predictions of Se concentrations at Mendota site (1990 observations)

Soil depth (cm)	53	110	158	210
Observed Se data (µg/l)	500	550	600	800
Model predictions (µg/l)	543.2	550.6	552	557.4

Table 3 FEM model predictions of Se concentrations at Mendota Site (1992 observations)

Soil depth (cm)	53	110	158	210
Observed Se data (µg/l)	59	258	270	326
Model predictions (µg/l)	63.4	267.9	284.5	301.2

measured data. The computed error measures for the results in Tables 2 and 3 are mean absolute error = 48.5 µg/l and mean relative error = 8.9%. These results imply that the model can produce a less than 10% error in predicting measured Se concentration in the soil zone. However, it should be noted the model cannot handle the rapid concentration variations at critical depths which are located at the tile drainage.

Concluding remarks

In this study, the two-dimensional FEM was extended to simulate Se transport in a saturated–unsaturated crop root zone. The model can simulate seasonal variations of soil water content and Se concentration distribution in irrigated and underdrained agroforestry systems. The model considers water, selenate, selenite, and selenomethionine uptake by plants, adsorption and desorption, oxidation and reduction, volatilization, and chemical and biological transformations of selenate, selenite, and selenomethionine. In addition to simulating water flow, selenate, selenite, and selenomethionine transport, the model also simulates organic and gaseous selenium transport.

The successful predictions of measured field data sets indicate that the developed model can be employed for the management of selenium transport in agroforestry sites. It is, however, worth noting that the model cannot handle the rapid concentration variations at critical depths (which are located at the tile drainage). When applied to field situations, this shortcoming of the model should be taken into account.

It also needs to be pointed out that the extended model requires extensive field data such as relative and saturated hydraulic conductivities, relative and saturated soil moisture, porosity, bulk density, diffusion coefficients, and parameters and constants for the volatilization, immobilization,

transformation, and mineralization processes for different soils in both horizontal and vertical directions. In addition, it requires the estimation of van Genuchten infiltration parameters and hydrometeorological data for the computation of evapotranspiration. Furthermore, it requires parameter values such as the absorption coefficient and root effectiveness function for different trees. As such, for realistic field applications, the model needs to be provided with the required data on soil, flow, and tree properties. It is, however, well known that it is not usually possible to obtain all the data due to time and budgetary constraints. Instead, representative samples at different locations and different depths can be obtained from the field and subjected to laboratory analysis to provide some of the parameter values. Some parameter values can be compiled from the literature, and some can be estimated through statistical methods.

Notation

C_1	Selenate concentration (mg/l)	K_{m1}	Transformation rate constant for mineralization of selenate (1/day)
C_2	Selenite concentration (mg/l)	K_{m2}	Transformation rate constant for mineralization of selenite (1/day)
C_3	Selenomethionine concentration (mg/l)	K_{m3}	Transformation rate constant for mineralization of selenomethionine (1/day)
D_{1x}	Total diffusion coefficient for selenate in x -direction (cm^2/day)	K_r	Relative hydraulic conductivity ($0 < K_r < 1$)
D_{1z}	Total diffusion coefficient for selenate in z -direction (cm^2/day)	K_{r1}	Transformation rate constant for reduction of selenate (1/day)
D_{2x}	Total diffusion coefficient for selenite in x -direction (cm^2/day)	K_{r2}	Transformation rate constant for reduction of selenite (1/day)
D_{2z}	Total diffusion coefficient for selenite in z -direction (cm^2/day)	K_{v1}	Volatilization rate constant of selenate (1/day)
D_{3x}	Total diffusion coefficient for selenomethionine in x -direction (cm^2/day)	K_{v2}	Volatilization rate constant of selenite (1/day)
D_{3z}	Total diffusion coefficient for selenomethionine in z -direction (cm^2/day)	K_{v3}	Volatilization rate constant of selenomethionine (1/day)
g	Gravitational acceleration	k_{xx}	Hydraulic conductivity tensor in x -direction
G	Gaseous selenium concentration ($\mu\text{g}/\text{kg}$)	k_{zz}	Saturated hydraulic conductivity tensor in z -direction
K_{a1}	Adsorption coefficient for selenate (l/kg)	l	Nonequilibrium exponent for selenomethionine
K_{a2}	Adsorption coefficient for selenite (l/kg)	n	Nonequilibrium exponent for selenate
K_{a3}	Adsorption coefficient for selenomethionine (l/kg)	p	Soil water pressure
K_{b1}	Transformation rate constant for immobilization of selenate (1/day)	Q	Strength of all sources and sinks in the system
K_{b2}	Transformation rate constant for immobilization of selenite (1/day)	q_x	Darcy flux in x -direction
		q_z	Darcy flux in z -direction
		R_1	Retardation factor for selenate
		R_2	Retardation factor for selenite
		R_3	Retardation factor for selenomethionine
		S_o	Organic selenium concentration (mg/kg)
		S_s	Storage coefficient that describes the volume of water released from storage under a unit decline in hydraulic head
		U	Root water extraction (1/day)
		w	Nonequilibrium exponent for selenite
		α_1	Coefficient for SO_4^{2-} antagonism effect for selenate
		α_2	Coefficient for SO_4^{2-} antagonism effect for selenite
		α_3	Coefficient for SO_4^{2-} antagonism effect for selenomethionine
		μ	Kinematic viscosity
		λ	Coefficient taken as unity in the case of saturated flow and zero in the case of unsaturated flow

λ_{a1}	Root absorption coefficient for selenate
λ_{a2}	Root absorption coefficient for selenite
λ_{a3}	Root absorption coefficient for selenomethionine
θ	Volumetric water content
ρ	Density of water
ρ_s	Bulk density of the porous medium (kg/m ³)

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