Modelling of one-dimensional contaminant migration through unsaturated soils using EFGM

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ABSTRACT

The study of contaminant transport processes in unsaturated soils is necessary to achieve an improved understanding of the contaminant migration in the vadose zone, which differs significantly from that of fully saturated behaviour. In this paper, an attempt has been made to model the contaminant transport through unsaturated porous media using the Element Free Galerkin Method (EFGM). In an EFGM, approximate solution is constructed entirely in terms of a set of nodes and no elements or characterization of the interrelationship of the nodes is needed to construct the discrete equations. The EFGM is used for solving the governing differential equation involving one-dimensional advection-dispersion-sorption-decay process. The weak form of the governing equation is formulated and the Lagrange multiplier method is used for enforcing the essential boundary conditions. The van Genuchten model is used for describing the hydraulic properties of the unsaturated soil. Numerical examples are presented to illustrate the applicability of the proposed method, and the results are compared with those obtained from the finite element method and it is found that they agree well.

1 INTRODUCTION

The frequent use of land for disposal of a wide variety of domestic and industrial wastes accentuates the importance of the unsaturated zone. Contaminants dispersed at the land surface migrate through the unsaturated zone before reaching the saturated zone. A clear understanding of chemical transport in the unsaturated zone including the proper quantification of the relevant transport processes is important for risk assessment and risk management pertinent to subsurface environment (van Genuchten 1982). For unsaturated soils the volumetric water content, the coefficient of hydrodynamic dispersion, and the discharge velocity vary both in space and in time, which make modelling of contaminant transport more difficult.

The use of specialized numerical models in modelling of contaminant transport problems is rapidly increasing, as they are able to accommodate the complexity of the domain and the boundary conditions. Many researchers proposed various numerical models (Zheng & Bennett 1995) for solving the governing equation of contaminant transport. Numerical schemes depend on mesh/grid size, element connectivity and need special methods with artificial viscosity, upwinding, etc. for solving advection dominant problems.

In the past decade, new methods called Meshless methods, i.e. Element Free Galerkin Method (EFGM), Smooth Particle Hydrodynamics (SPH), Reproducing Kernel Particle Method (RPKM), Radial Point Interpolation Method (RPIM) and others have been developed. Among all the meshless methods, the EFGM has been successfully used for solving numerous boundary-value problems related to various fields of study (Rao & Rahman 2000). Numerical models based on the meshless methods are not being extensively used for modelling the transport processes in unsaturated porous media. Hence, there is a need to understand the meshless methods properly and to formulate a numerical model to represent the migration of contaminants through the unsaturated porous media.

The objective of this paper is to propose a methodology for modelling one-dimensional advection-dispersion-sorption equation involving first-order degradation through the unsaturated porous media using the EFGM. Student's t distribution function is used as a weight function in the meshless analysis. Lagrange multiplier method is used to enforce the essential boundary conditions. MATLAB program is developed to implement the procedure of the EFGM for contaminant migration. Results of the analysis are compared with those obtained from the finite element method.

2 EFGM

The EFGM is a meshless method because only a set of nodes and a description of the model's boundary are required to generate the discrete equations. The EFGM employs moving least-square (MLS) approximants formulated by Lancaster & Salkauskas (1981) to approximate the function $C(x)$ with $C^h(x)$ in which the $C(x)$ is the contaminant concentration at x, here x is a position coordinate. The reader can find more details about EFGM in the paper by Dolbow & Belytschko (1998). In this paper, a student's t distribution weight function (Rao & Rahman 2000) is adopted. The weight function is written in terms of normalized radius *r* as

$$w(x-x_I) \equiv w(r) = \begin{cases} \dfrac{(1+\beta^2 r^2)^{-\left(\frac{(1+\beta)}{2}\right)} - (1+\beta^2)^{-\left(\frac{(1+\beta)}{2}\right)}}{1-(1+\beta^2)^{-\left(\frac{(1+\beta)}{2}\right)}} & r \le 1 \\ 0 & r > 1 \end{cases} \quad (1)$$

where

β is the parameter controlling the shape of the weight function and

$$r = \frac{\|x - x_I\|}{d_{\max}\, z_I} \quad (2)$$

in which x_I is the sampling point, $d_{\max}$ is the scaling factor and z_I is the distance to the nearest node in the neighbourhood. As the shape functions of the EFGM do not satisfy the Kronecker delta criterion: $\Phi_I(x_J) \neq \delta_{IJ}$, the Lagrange multiplier technique (Dolbow & Belytschko 1998) is used to enforce the essential (Dirichlet) boundary conditions in this paper.

3 DISCRITISATION OF GOVERNING EQUATION

A one-dimensional form of the governing equation for contaminant migration through the unsaturated porous media can be written as

$$\frac{\partial}{\partial t}(R\,\theta\,C) = \frac{\partial}{\partial x}\left(\theta\,D\,\frac{\partial C}{\partial x}\right) - \frac{\partial}{\partial x}(u\,C) - \eta\,C$$

$$R = 1 + \frac{\rho_d\,K_d}{\theta} \quad (3)$$

Initial condition

at $t = 0$, $C = C_i$ in Ω (4a)

Boundary conditions

$C(0, t) = C_0$, in Γ_s (Dirichlet boundary condition) (4b)

$\frac{\partial C}{\partial x} n_s = g$, in Γ_E (Neumann boundary condition) (4c) where x is the spatial coordinate, θ is the volumetric water content of the soil, ρ_d is the bulk density of the soil, η is the decay constant, K_d is the distribution coefficient, C is the concentration of contaminant, C_i is the initial concentration of contaminant, D is the dispersion coefficient, R is the retardation factor, u is the discharge (Darcy) velocity, C_0 and g are the concentration of contaminant at the source and concentration gradient at the exit boundary respectively, n_s is a unit normal to the domain Ω and, Γ_s and Γ_E are the portions of the boundary Γ where source concentration and concentration gradient are prescribed.

The hydrodynamic properties of the soil are described by the functions of the van Genuchten model (1980):

$$S = \frac{(\theta - \theta_r)}{(\theta_s - \theta_r)} = \begin{cases} \dfrac{1}{\left[1 + (\alpha\,|h|)^{\chi}\right]^{1-1/\chi}} & if \;\; h \le 0 \\ 1 & if \;\; h \ge 0 \end{cases} \tag{5a}$$

$$K = K_s (S)^{0.5}\left[1 - \left(1 - S^{(\chi/\chi-1)}\right)^{(1-(1/\chi))}\right]^2 \quad for \;\; \chi > 1 \tag{5b}$$

and

$$\frac{\partial\theta}{\partial x} = \frac{-\alpha\,\Psi\,(\theta_s - \theta_r)}{1-\Psi}\, S^{1/\Psi}\left(1 - S^{1/\Psi}\right)^{\Psi}$$
$$where \quad \Psi = 1 - 1/\chi \tag{5c}$$

where θ_r and θ_s are the residual and saturated volumetric water contents of the soil respectively, S is the degree of saturation of the soil, K and K_s are the hydraulic conductivities of the soil at pressure head h and at saturation respectively and, α and χ are empirical constants determining the shape of the function.

The weak form of equation (3) with boundary conditions can be written as

$$\int_0^1 \delta C^T \frac{\partial}{\partial x}\left(\theta D\left(\frac{\partial C}{\partial x}\right)\right)dx - \int_0^1 \delta C^T \frac{\partial}{\partial x}(u\,C)\,dx - \int_0^1 \delta C^T \frac{\partial}{\partial t}(R\,\theta\,C)\,dx$$
$$-\int_0^1 \delta C^T \eta\, C\, dx - \delta\lambda^T (C - C_0)\big|_{\Gamma_s} - \lambda^T \delta C\big|_{\Gamma_s} = 0 \tag{6}$$

where λ is a Lagrangian multiplier for enforcing the essential boundary condition. By using the divergence theorem, equation (6) can be written as

$$\delta C^T \theta D \frac{\partial C}{\partial x} n_s \Big|_{\Gamma_E} - \int_0^1 \delta\left(\frac{\partial C^T}{\partial x}\right)\theta D \frac{\partial C}{\partial x}\,dx - \int_0^1 \delta C^T\left(\frac{\partial\theta}{\partial x}\right) D \frac{\partial C}{\partial x}\,dx$$
$$-\int_0^1 \delta C^T \frac{\partial}{\partial x}(u\,C)\,dx - \int_0^1 \delta C^T \frac{\partial}{\partial t}(R\,\theta\,C)\,dx - \int_0^1 \delta C^T \eta\, C\,dx$$
$$-\delta\lambda^T (C - C_0)\big|_{\Gamma_s} - \lambda^T \delta C\big|_{\Gamma_s} = 0 \tag{7}$$

Equation (7) can be split into two parts

$$\int_0^1 \delta\left(\frac{\partial C^T}{\partial x}\right)\theta D\,\frac{\partial C}{\partial x}\,dx+\int_0^1 \delta C^T\left(\frac{\partial\theta}{\partial x}\right)D\,\frac{\partial C}{\partial x}\,dx+\int_0^1 \delta C^T\,\frac{\partial}{\partial x}(\,u\,C\,)\,dx \tag{8a}$$

$$+\int_0^1 \delta C^T\,\frac{\partial}{\partial t}(\,R\,\theta\,C\,)\,dx+\int_0^1 \delta C^T\,\eta\,C\,\,dx+\delta C^T\,\lambda\,\Big|_{\Gamma_s}=\delta C^T\,D\,\frac{\partial C}{\partial x}\,n_s\,\Big|_{\Gamma_E}$$

$$\delta\lambda^T(\,C-C_0\,)\Big|_{\Gamma_s}=0 \tag{8b}$$

The δC and $\delta\lambda$ are arbitrary values and by using MLS approximates in the discretisation of equation (8), the following relationship is obtained [equation (9)]:

$$\begin{gathered}\left[\,\boldsymbol{K}^{(1)}\,\right]\{C\}+\left[\,\boldsymbol{K}^{(2)}\,\right]\{C\}_{,t}+[\,G\,]\{\,\lambda\,\}=\{\,Q\,\}\\ \left[\,G^T\,\right]\{\,C\,\}=\{\,q\,\}\end{gathered} \tag{9}$$

where

$$\boldsymbol{K}_{IJ}^{(1)}=\int_0^1\left[\begin{array}{l}\Phi_{I,x}^T\,\theta D\,\Phi_{J,x}+\Phi_I^T\,u\,\Phi_{J,x}+\Phi_I^T\eta\,\Phi_J\\ +\Phi_I^T\,D\left(\dfrac{-\alpha\,q\,(\,\theta_s-\theta_r\,)}{1-q}\,S^{1/q}\left(\,1-S^{1/q}\,\right)^q\right)\Phi_{J,x}\end{array}\right]dx \tag{10a}$$

$$\boldsymbol{K}_{IJ}^{(2)}=\int_0^1\left[\,\Phi_I^T\,\theta\,R\,\Phi_J\,\right]\,dx \tag{10b}$$

$$\boldsymbol{G}_{IK}=\Phi_K\,\Big|_{\Gamma_s I} \tag{10c}$$

$$\boldsymbol{Q}_I=\Phi_I\,\theta D\,g\,\Big|_{\Gamma_E} \tag{10d}$$

$$\boldsymbol{q}_K=C_{0\,K} \tag{10e}$$

where $\Phi_I\,(x)$ is the EFGM Shape function.

Using the Crank-Nicholson method for time approximation, equation (9) can be written as

$$\begin{bmatrix}\boldsymbol{K}^{(1)*}+\boldsymbol{K}^{(2)} & \boldsymbol{G}\\ \boldsymbol{G}^{\boldsymbol{T}} & \boldsymbol{0}\end{bmatrix}\begin{Bmatrix}\boldsymbol{C}_n\\ \boldsymbol{\lambda}\end{Bmatrix}=\begin{Bmatrix}\boldsymbol{R}_n\\ \boldsymbol{q}\end{Bmatrix} \tag{11}$$

where

$$\boldsymbol{R}_n=\left(\left[\,\boldsymbol{K}^{(2)}\,\right]-(1-\varepsilon)\,\Delta t\left[\,\boldsymbol{K}^{(1)}\,\right]\right)\{\,C\,\}_{n-1}+\varepsilon\,\Delta t\,\{\,\boldsymbol{Q}\,\}_n+(1-\varepsilon)\,\Delta t\,\{\boldsymbol{Q}\}_{n-1} \tag{12a}$$

$$\boldsymbol{K}^{(1)*}=\varepsilon\,\Delta t\left[\,\boldsymbol{K}^{(1)}\,\right] \tag{12b}$$

in which ε is the constant varying between 0 and 1, C_n and C_{n-1} are the nodal concentrations at the start and end of the time increment and, $\boldsymbol{Q}_n$ and $\boldsymbol{Q}_{n-1}$ are the nodal mass fluxes at the start and end of the time increment.

4 NUMERICAL EXAMPLE: RESULTS

The proposed methodology using the EFGM is applied to the problem of one-dimensional contaminant transport modelling. The porous medium in which the contaminants move is homogenous with unsaturated condition assuming the continuous contaminant source. The processes occurring in the porous media during transport are considered and three numerical examples are presented to illustrate the applicability of the method. In the present analysis, a central finite difference scheme (ε = 0.5) is used for time integration. In the EFGM, a linear basis function is used for constructing the shape functions. As the shape functions are linear one it is required to take the weight function, β = 2. Based on the parametric study, it is found that $d_{\max}$ = 1.15 for the present analysis and the same value is used in the EFGM.

The parameters that are considered for the analysis are tabulated in table 1. For all the example problems, the EFGM model has been divided into 251 (P_e = 2) uniformly spaced nodes. The problem domain [0, 50] is divided into 250 elements, solely for numerical integration purpose. Nodes of the background mesh are chosen such that they coincide with the meshless nodes. For all the examples, the total time of simulation is 12 hours. A time step (Δt) of 50 s is adopted for all the examples studied in the paper.

Comparison between the EFGM and finite element results for advection–dispersion, advection-dispersion–sorption and advection-dispersion-decay cases are presented in figures 1-3. From the figures, it is depicted that both the EFGM and the finite element results are almost identical with one another.

Table 1: Parameters considered in the analysis

Parameter	Values
Initial condition for flow (cm)	- 300.0
Boundary condition for flow at upper surface (cm)	- 75.0
Boundary condition for flow at lower surface (cm)	- 300.0
Saturated volumetric water content	0.368
Residual volumetric water content	0.102
Saturated hydraulic conductivity of soil (cm/s)	0.00922
α (cm^{-1})	0.0335
χ	2.0
Distribution coefficient	0.073
Decay constant	1E-05
Total duration of simulation (hours)	12.0
Length of the reach (cm)	50.0
Initial concentration ($\mu g/cm^3$)	0.0
Concentration at source boundary ($\mu g/cm^3$)	1.0

5 CONCLUSIONS

In the present study, a truly meshless EFGM is obtained for modelling the one-dimensional contaminant transport through the unsaturated soils. The results of the EFGM are compared with those obtained using the finite element method for the three types of one-dimensional contaminant transport processes that occur in the unsaturated porous media. It is concluded that the EFGM generates excellent results for almost all the types of transport processes thus encouraging its potential usage to the more complex transport processes involving higher dimensions and complex boundaries.

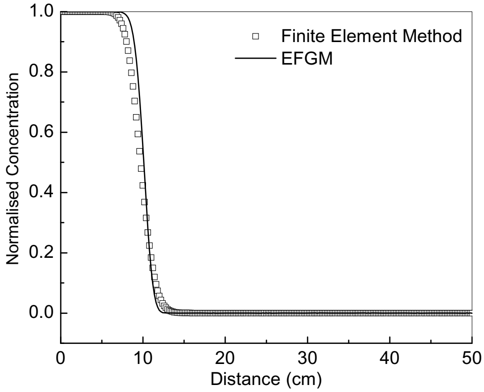

Figure 1: Normalised concentration profiles for advection-dispersion

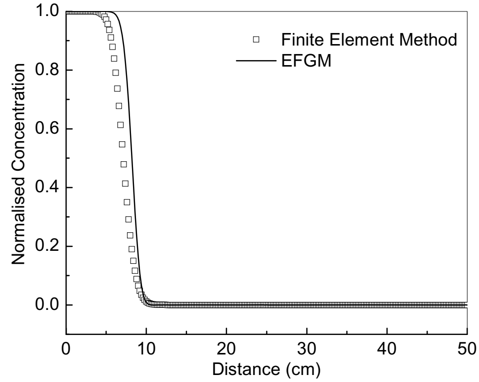

Figure 2: Normalised concentration profiles for advection-dispersion-sorption

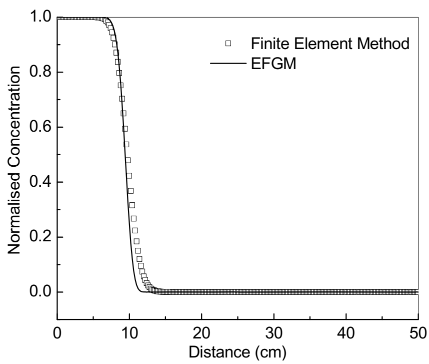

Figure 3: Normalised concentration profiles for advection-dispersion-decay

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