Indian Geotechnical Journal, 38(3), 2008, 363-371

TECHNICAL NOTE

Modelling of 1- D Contaminant Migration through Unsaturated Soils using RPIM

R. Praveen Kumar[*] and G. R. Dodagoudar[**]

Introduction

Interest in the unsaturated zone, which plays an inextricable role in many aspects of hydrology, has dramatically increased in recent years because of growing concern that the quality of the subsurface environment is being adversely affected by the disposal of wide variety of domestic and industrial wastes on the surface. Though significant progress has been made in modelling contaminant transport through unsaturated porous media, it is still a formidable task as the volumetric water content, the coefficient of hydrodynamic dispersion, and the discharge velocity vary both in space and time.

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 Radial Point Interpolation Method (RPIM). The RPIM is a meshfree method and by introducing this method, the potential of meshless methods in the study of migration of contaminants through an unsaturated porous media is highlighted.

In this paper, thin plate spline radial basis functions (TPS-RBFs) proposed by Liu et al. (2005), for solving solid mechanics problems, are made use of in the analysis. MATLAB code is developed for modelling the contaminant migration using the RPIM. Results of the present analysis are compared with those obtained by the finite element method.

Radial Point Interpolation Method

The RPIM is a meshfree method developed using the Galerkin weak form and the radial basis shape functions that are constructed based only on a group of nodes arbitrarily distributed in a local support domain by means of interpolation (Liu et al. 2005). For solving integrals in the weak form formed due to the Galerkin approximation procedure, a background mesh is used. The more details about the RPIM can be found elsewhere (Wang and Liu 2002).

Consider a continuous function $C(x)$ defined on a domain $\Omega \subseteq \mathrm{R}^K$, where K = 1, 2 or 3. Let $\Omega_x \subseteq \Omega$ denote a sub-domain describing the neighbourhood

* Research Scholar, Department of Civil Engineering, Indian Institute of Technology Madras, Chennai, India. Email: praveenkumar.rachakonda@gmail.com

** Assistant Professor, Department of Civil Engineering, Indian Institute of Technology Madras, Chennai, India. Email: goudar@iitm.ac.in

of a point, $x \in \mathrm{R}^K$ located in Ω. According to the RPIM with polynomial reproduction, the function $C(x)$ is expressed as

$$C(x) = \boldsymbol{\Phi}(x)\boldsymbol{C}^e \tag{1}$$

where

$\boldsymbol{C}^e = \left[C_1, C_2, C_3, \ldots, C_N\right]^T$ and

The matrix of shape functions is defined as

$$\boldsymbol{\Phi}(x) = \left[\phi_1(x), \phi_2(x), \ldots, \phi_N(x)\right] \tag{2}$$

in which N is the number of nodes in an influence domain of x.

Discretisation of Governing Equation

A one-dimensional form of the governing equation for contaminant migration through unsaturated porous media is expressed as

$$\frac{\partial}{\partial t}\left(R\,\theta\, C \right) = \frac{\partial}{\partial x}\left(\theta\, D \frac{\partial C}{\partial x} \right) - \frac{\partial}{\partial x}\left(u\, C \right) - \eta\, C \tag{3a}$$

$$R = 1 + \frac{\rho_d\, K_d}{\theta}$$

Initial condition

at t = 0, $C = C_i$ in Ω (3b)

Boundary conditions

$C(0,t) = C_0$, in Γ_s (Dirichlet boundary condition) (3c)

$\dfrac{\partial C}{\partial x} n_s = g$ in Γ_E (Neumann boundary condition) (3d)

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 the 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 the source concentration and concentration gradient are prescribed.

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

$$S = \frac{(\theta - \theta_r)}{(\theta_s - \theta_r)} = \begin{cases} \dfrac{1}{\left[1 + (\alpha\, |h|)^{\chi}\right]^{1-1/\chi}} & if \quad h \le 0 \\ 1 & if \quad h \ge 0 \end{cases} \tag{4a}$$

$$K = K_s (S)^{0.5} \left[1 - \left(1 - S^{(\chi/\chi-1)}\right)^{(1-(1/\chi))}\right]^2 \quad for \ \chi > 1 \tag{4b}$$

and

$$\frac{\partial\theta}{\partial x} = \frac{-\alpha\, \Psi\,(\theta_s - \theta_r)}{1-\Psi} S^{1/\Psi} \left(1 - S^{1/\Psi}\right)^{\Psi} \tag{4c}$$

where $\Psi = 1 - 1/\chi$, 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 the empirical constants determining the shape of the function.

The weak form of Eqn. (3) is written as

$$\int_0^L \delta C^T \left[\frac{\partial}{\partial x}\left(\theta\, D \frac{\partial C}{\partial x}\right) - \frac{\partial}{\partial x}(u\, C) - \eta\, C - \frac{\partial}{\partial t}(R\, \theta\, C)\right] dx = 0 \tag{5a}$$

$$\begin{aligned} &\int_0^L \delta C^T \frac{\partial}{\partial x}\left(\theta\, D\left(\frac{\partial C}{\partial x}\right)\right) dx - \int_0^L \delta C^T \frac{\partial}{\partial x}(u\, C)\, dx \\ &\qquad - \int_0^L \delta C^T \frac{\partial}{\partial t}(R\, \theta\, C)\, dx - \int_0^L \delta C^T \eta\, C\, dx = 0 \end{aligned} \tag{5b}$$

$$\begin{aligned} &-\int_0^L \delta\left(\frac{\partial C^T}{\partial x}\right)\theta D \frac{\partial C}{\partial x} dx + \delta C^T \theta D \frac{\partial C}{\partial x} n_s \Big|_{\Gamma_E} \\ &-\int_0^L \delta C^T \left(\frac{\partial \theta}{\partial x}\right) D \frac{\partial C}{\partial x} dx - \int_0^L \delta C^T \frac{\partial}{\partial x}(u\, C)\, dx \\ &-\int_0^L \delta C^T \frac{\partial}{\partial x}(\eta C)\, dx - \int_0^L \delta C^T \frac{\partial}{\partial t}(R\, \theta\, C)\, dx = 0 \end{aligned} \tag{5c}$$

$$
\begin{aligned}
&-\int_0^L \delta\left(\frac{\partial C^T}{\partial x}\right)\theta D\ \frac{\partial C}{\partial x}\,dx\ +\delta C^T\ \theta D\ g\Big|_{\Gamma_E} \\
&-\int_0^L \delta C^T\left(\frac{\partial \theta}{\partial x}\right)D\ \frac{\partial C}{\partial x}\,dx-\int_0^L \delta C^T\,u\frac{\partial C}{\partial x}\,dx \\
&-\int_0^L \delta C^T\,R\,\theta\frac{\partial C}{\partial t}\,d\Omega-\int_0^L \delta C^T\,\eta\,C\ dx=0
\end{aligned}
\tag{6}
$$

By using divergence theorem, Eqn. (6) can be rewritten as

$$
\begin{aligned}
&\int_0^L \delta\left(\frac{\partial C^T}{\partial x}\right)\theta D\ \frac{\partial C}{\partial x}\,dx\ +\int_0^L \delta C^T\left(\frac{\partial \theta}{\partial x}\right)D\ \frac{\partial C}{\partial x}\,dx \\
&+\int_0^L \delta C^T\ \frac{\partial}{\partial x}\left(\ u\,C\ \right)dx+\int_0^L \delta C^T\ \frac{\partial}{\partial t}\left(\ R\,\theta\,C\ \right)dx \\
&+\int_0^L \delta C^T\ \eta\,C\ \ dx=\delta C^T\ \theta D\frac{\partial C}{\partial x}\,n_s\ \Bigg|_{\Gamma_E}
\end{aligned}
\tag{7}
$$

By using Eqns (1) and (2) in the discretization of Eqn (7), the following relationship can be obtained:

$$
\left[\ \boldsymbol{K}^{(1)}\ \right]_{\mathrm{N}\times\mathrm{N}}\ \{C\}+\left[\ \boldsymbol{K}^{(2)}\ \right]_{\mathrm{N}\times\mathrm{N}}\{C\}_{,t}=\{\ Q\ \}
\tag{8}
$$

where

$$
\boldsymbol{K}_{IJ}^{(1)}=\int_0^L\left[\begin{array}{l}\Phi_{I,x}^T\ \theta D\ \Phi_{J,x}+\Phi_I^T\,u\,\Phi_{J,x}+\Phi_I^T\eta\,\Phi_J \\ +\Phi_I^T\,D\left(\dfrac{-\alpha\ \Psi\left(\ \theta_s-\theta_r\ \right)}{1-\Psi}\ S^{1/\Psi}\left(\ 1-S^{1/\Psi}\ \right)^{\Psi}\ \right)\Phi_{J,x}\end{array}\right]dx
\tag{9a}
$$

$$
\boldsymbol{K}_{IJ}^{(2)}=\int_0^L\left[\ \Phi_I^T\ \theta\,R\,\Phi_J\ \right]\,dx
\tag{9b}
$$

$$
\boldsymbol{Q}_I=\ \Phi_I\ \theta D\ g\ \ \Big|_{\Gamma_E}
\tag{9c}
$$

where $\Phi_I\left(x\right)$ is the shape function of the RPIM.

Using Crank-Nicholson method for time approximation, Eqn (8) can be written as

$$\boldsymbol{K}_{new}\,\boldsymbol{C}_n = \boldsymbol{R}_n \tag{10}$$

where

$$\boldsymbol{K}_{new} = \boldsymbol{K}^{(1)*} + \boldsymbol{K}^{(2)} \tag{11a}$$

$$\boldsymbol{R}_n = \{\, C \,\}_{n-1} \begin{pmatrix} \left[\, \boldsymbol{K}^{(2)} \,\right] - \\ (1-\varepsilon)\ \Delta t\ \left[\, \boldsymbol{K}^{(1)} \,\right] \end{pmatrix} + \begin{pmatrix} \varepsilon\ \Delta t\ \{\, \boldsymbol{Q} \,\}_n + \\ (1-\varepsilon)\,\Delta t\ \{\boldsymbol{Q}\}_{n-1} \end{pmatrix} \tag{11b}$$

$$\boldsymbol{K}^{(1)*} = \varepsilon\ \Delta t\ \left[\, \boldsymbol{K}^{(1)} \,\right] \tag{11c}$$

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

Numerical Examples: Results

The proposed methodology using the RPIM 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 source of contaminant as continuous. A few processes occurring in the porous media during transport are considered and four numerical examples are presented to illustrate the applicability of the RPIM. The four examples considered in the study are:

(1) Advection-dispersion,

(2) Advection-dispersion-sorption,

(3) Advection-dispersion-decay, and

(4) Advection-dispersion-sorption-decay.

In the present analysis, a central finite difference scheme (ε = 0.5) is used for time integration. In the RPIM, a linear basis function is used for constructing the shape functions and for the TPS-RBFs, a shape parameter q = 1.15 is chosen in the analysis.

The hydrodynamic and transport parameters along with the boundary conditions that are considered in the analysis are tabulated in Table 1. Analysis has been carried for two Peclet numbers (P_e) for all the example problems presented in the paper. The RPIM model has been divided into 251 uniformly spaced nodes for P_e = 2 and 51 for P_e = 10. The problem domain [0, 50] is divided into 250 and 50 elements, solely for numerical integration purpose. Nodes of the background mesh are chosen such that they coincide with the meshless nodes. A time step (Δt) of 50 s and the total time of simulation of 12 hours is used for all the examples.

In order to study the influence of shape parameter q on the predicted results, a parametric study is attempted by varying the shape parameter q from 1.05 to 1.50. From the results (Figure 1), it is seen that they were almost invariant with respect to q.

Table 1 Parameters Considered in the Analysis

Parameter	*Value*
Initial pressure head (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 (θ_s)	0.368
Residual volumetric water content (θ_r)	0.102
Saturated hydraulic conductivity of soil, K_s (cm/s)	0.00922
α (cm^{-1})	0.0335
χ	2.0
Bulk density of soil (g/cm^3)	1.733
Distribution coefficient (cm^3/g)	0.733
Decay constant (day^{-1})	0.864
Dispersivity of soil (cm)	0.1
Length of vertical column of soil (cm)	50
Initial concentration ($\mu g/cm^3$)	0.0
Concentration at source boundary ($\mu g/cm^3$)	1.0

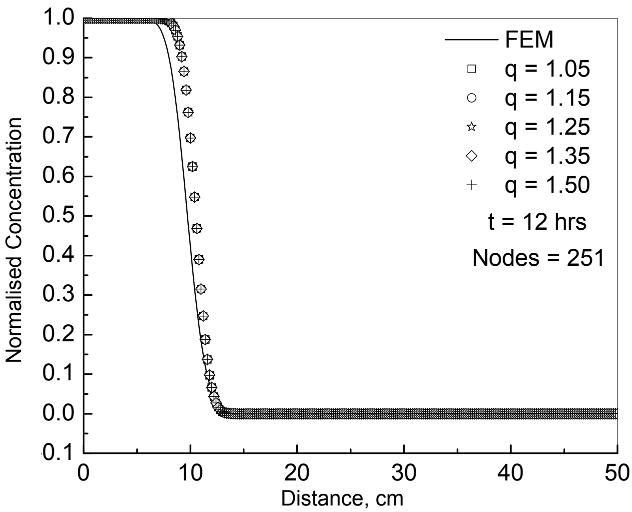

Fig. 1 Normalised Concentration Profiles for Different q Values

The results of the RPIM are compared with those obtained by the Hydrus-1D model (Simunek et al. 1998), a finite element software (indicated as

FEM in the figures). The results of both the RPIM and FEM are presented in Figures 2 to 5.

From the figures, it is observed that for the grid Peclet number of 2, both the models provide similar results and for grid Peclet number of 10, the results of the FEM show oscillations at the level face of concentration, whereas the RPIM model does not show any such oscillations. For high values of the Peclet number, i.e. when advection dominates, special techniques must be developed to obtain accurate solutions of the advection-diffusion equation in finite element analysis (Donea and Huerta 2003).

As the RPIM generates a fully populated matrix, the computational speed is slower than the FEM, which generates a symmetric tridiagonal matrix. However, when comparing the two methods for a given accuracy, the RPIM is much faster and stable than FEM.

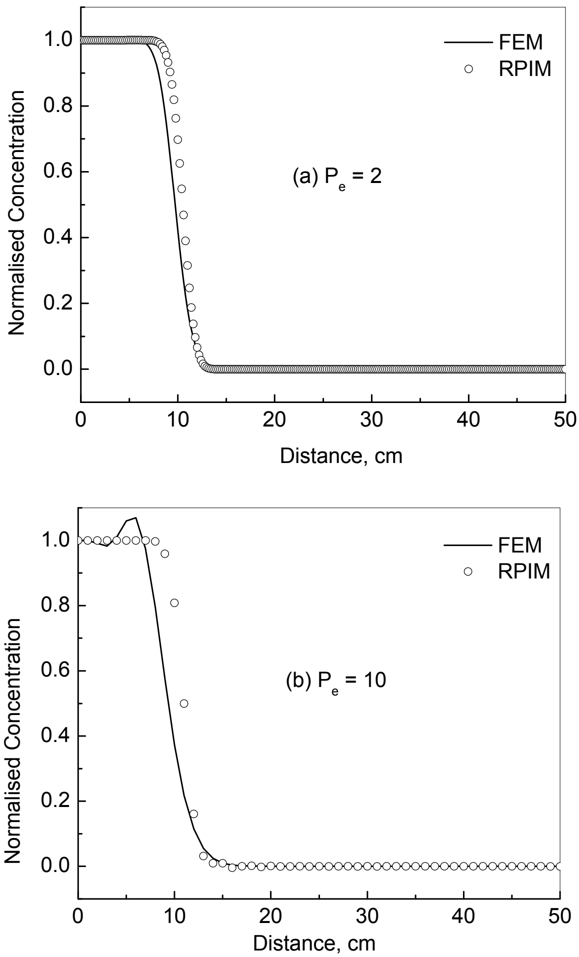

Fig 2 Comparison of RPIM Results with FEM Results (Advection-Dispersion)

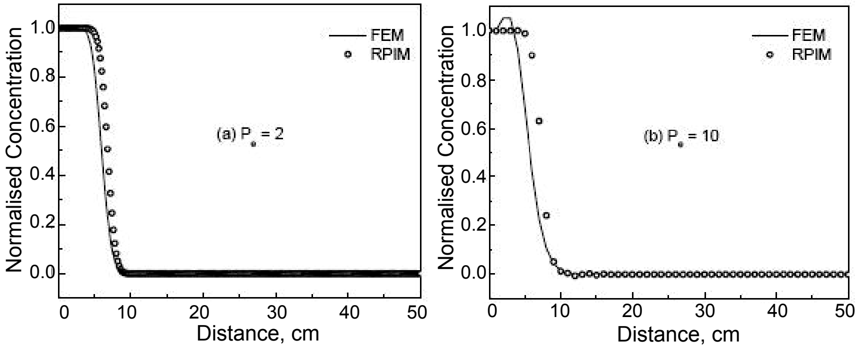

Fig. 3 Comparison of RPIM Results with FEM Results (Advection-Dispersion-Sorption)

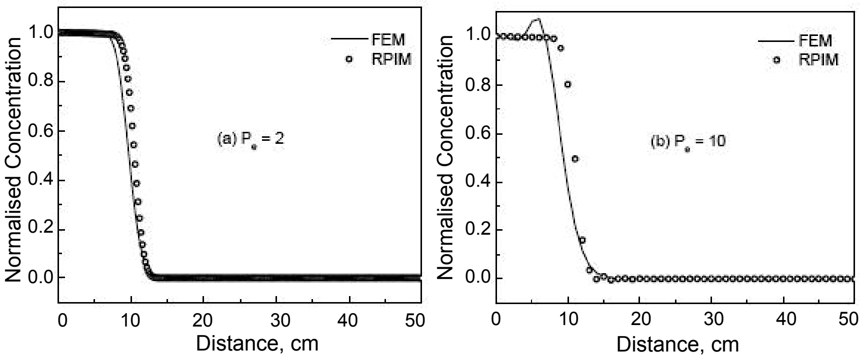

Fig. 4 Comparison of RPIM Results with FEM Results (Advection-Dispersion-Decay)

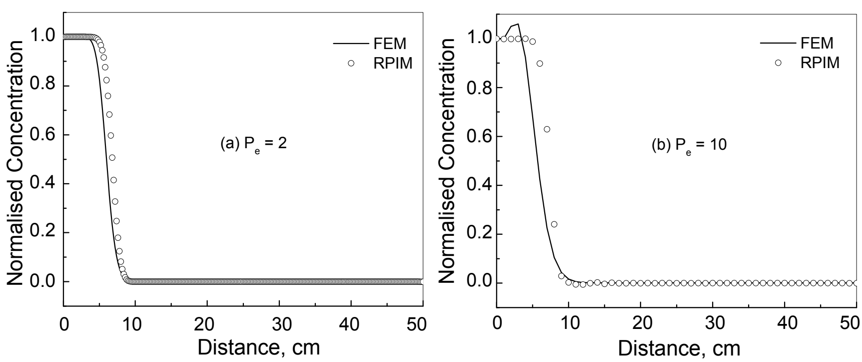

Fig. 5 Comparison of RPIM Results with FEM Results (Advection-Dispersion-Sorption-Decay)

Conclusions

In the present study, a meshless method called, RPIM is presented for modelling the one-dimensional contaminant transport through the unsaturated soils. The results of the RPIM are compared with those obtained using the finite element method for the four types of one-dimensional contaminant transport processes that occur in the unsaturated porous media. It is to be noted that the RPIM produces accurate results for almost all types of transport processes thus ensures the correct formulation of the RPIM. It is possible to extend the potential usage of the RPIM for more complex transport processes involving higher dimensions and complex boundaries. A future work in this direction is currently under investigation by simulating the 2-D and 3-D contaminant migration through the unsaturated porous media.

References

Donea, J. and Huerta, A. (2003): *Finite Element Methods for Flow Problems*, John Wiley and Sons, New York

Liu, G. R., Zhang, G. Y., Gu, Y. T. and Wang, Y. Y. (2005): 'A Meshfree Radial Point Interpolation Method (RPIM) for Three-dimensional Solids', *Computational Mechanics*, 36, pp. 421–430

Šimunek, J., Sejna, M. and van Genuchten, M. Th. (1998): *The Hydrus-1d Software Package for Simulating the One-dimensional Movement of Water, Heat, and Multiple Solutes in Variably Saturated Media*, US Salinity Laboratory, Agricultural Research Service, US Department of Agriculture, Riverside, California

van Genuchten, M. Th. (1980): 'A Closed – formed Equation for Predicting the Hydraulic Conductivity of Unsaturated Soils', *Soil Science Society of America Journal*, 44, pp. 892-898

Wang, J. G. and Liu, G. R. (2002): 'On the Optimal Shape Parameters of Radial Basis Functions Used for 2-d Meshless Methods', *Computer Methods in Applied Mechanics and Engineering*, 191, pp. 2611–2630