Proceedings of ALGORITMY 2000
Conference on Scientific Computing, pp. 309–313

SINGULAR PERTURBATION TECHNIQUES FOR THE SOLUTE TRANSPORT EQUATION IN UNSATURATED POROUS MEDIA

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Abstract. In this paper we formulate a system of partial differential equations that models the contamination of groundwater due to migration of dissolved contaminants through unsaturated to saturated zone. A closed form solution using singular perturbation techniques for the water flow and solute transport equations in the unsaturated zone is given. Indeed, the solution can be used as a tools to verify the accuracy of numerical models of water flow and solute transport.

1. Introduction. Analysis and prediction of solute transport in hydrogeologic systems generally involve the use of some form of the advection-dispersion equation. Dispersivity (i.e., the spreading of a tracer or a solute carried by a fluid flowing in a porous medium) has traditionally been considered and a constant for the entire medium (see, [2]). De Marsily [5] points out that breakthough curves monitored at different distances from the source cannot, in general, be matched optimally with a single dispersivity value, and that optimal dispersivities seem to increase with distance of the observation point from the source.

The movement of water and solutes through the unsaturated zone has been of importance in traditional applications of groundwater hydrology, soil physics, and agronomy. In recent years, the need to understand the behavior of hazardous waste and toxic chemicals in soils has resulted in a renewed interest in this subject. One of the primary concerns is that dissolved contaminants may migrate through the unsaturated zone, reach the saturated zone, and contaminate the groundwater.

Additionally, movement of solutes or pesticides should be identified before their application in agriculture, to prevent any pollution. Therefore, mathematical models are useful tools for a first assessment of the expected concentration in groundwater, which may enable identification of the pesticides with the highest contamination potential.

The search for solutions to model water flow and solute transport continues to be of scientific interest. Typically, water flow and solute transport in unsaturated soils result in transient phenomena, making it a challenging problem. The nature of soil hydraulic conductivity renders the governing flow equation nonlinear.

In recent years, several analytical methods were developed to simulate water movement and solute transport in the unsaturated zone, for more details see [1, 3, 9, 10]. Although much progress has already been made in solving the problems of transient water flow in unsaturated and saturated porous flow media, many new developments have been made by numerical investigations in recent years [6]. A large number of numerical solution are generally approached by a finite-difference approximation [8], or by a finite element methods [11].

The objective of this paper is to capitalize on these features of that analytical flow model and extend its use to simulate contaminant movement in soils to that a complete, closed form approximate solution for solute transport in the unsaturated zone is achieved using singular perturbation techniques.

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In the next section, the solute transport problem is stated mathematically. The solution using the method of singular perturbation techniques is incorporated in section 3. The perturbation solution is tested and the concentration of solute in the soil is determined in section 4.

2. Governing Equations. The traditional approach to describing solute transport through soil is based on the advection-dispersion equation. In one dimension, the theoretical basis for modeling the liquid phase water movement in unsaturated porous media can be described by a combination of the Darcy's law and the equation of continuity, (see, [5, Ch. 10],[3]) as:

$$\frac{\partial}{\partial t}c(x,t) = D\frac{\partial^2}{\partial x^2}c(x,t) - v\frac{\partial}{\partial x}c(x,t) - \lambda c(x,t), \quad x > 0, \quad t > 0. \tag{2.1}$$

where t is the time, x is the horizontal distance taken zero at the soil center and measured positive to the right of the soil center; $c(x,t)$ is the solute concentration (mass of solute over volume of solute) at time t, distance x; D is the soil-water diffusivity; v is the average velocity and λ is the decay coefficient (1/time). The contamination in groundwater can be calculated by means of equation (2.1). July and Roth [7] derived the solution of this equation for a Dirac-δ pulse applied to the soil surface.

We now consider the behavior of contamination in a saturated zone with zero initial concentration, i.e.,

$$c(x,0) = 0, \quad x > 0. \tag{2.2}$$

and at $x = 0$ a periodic infiltration rate is prescribed as:

$$c(0,t) = c_0(1 + \sin \omega t), \quad t > 0. \tag{2.3}$$

where c_0 is the constant concentration at the entrance of the medium ($x = 0$) prescribed from $t = 0$.

3. Perturbation Approximation of the Model. The solute transport equation (2.1) along with the two supplementary conditions (2.2), and (2.3) are the mathematical modeling for the unknown concentration $c(x,t)$. We now scale this mathematical problem by selecting characteristic values for the dependent and independent variables. Consequently, we define dimensionless variables by

$$\bar{t} = \frac{t}{\lambda^{-1}}, \quad \bar{x} = \frac{x}{v/\lambda}, \quad \bar{c} = \frac{c}{c_0}$$

Reformulating the problem in terms of these scaled variables easily gives the scaled problem

$$\frac{\partial}{\partial t}c(x,t) = \epsilon\frac{\partial^2}{\partial x^2}c(x,t) - \frac{\partial}{\partial x}c(x,t) - c(x,t), \quad x > 0, \quad t > 0. \tag{3.1}$$

$$c(x,0) = 0, \quad t > 0. \tag{3.2}$$

$$c(0,t) = 1 + \sin \Omega t, \quad t > 0. \tag{3.3}$$

where $\Omega = \omega/\lambda$ and assumed to be $\mathcal{O}(1)$, and $\epsilon = \lambda D/v^2 << 1$.

A careful examination of the problem (3.1) will show that went wrong and point the way toward a correct, singular perturbation method for obtaining an approximate solution. To get the outer solution, denoted by $c^o(x,t)$, the unperturbed problem found by setting $\epsilon = 0$ is

$$\frac{\partial}{\partial t}c^o(x,t) + \frac{\partial}{\partial x}c^o(x,t) = -c^o(x,t) \tag{3.4}$$

and using the characteristic method, the solution is given by $c^o(x,t) = \eta e^{-t}$ on the lines $x - t = \mathit{constant}$ where $\eta = \mathit{constant}$. To satisfy both the initial condition $c^o(x,0) = 0$ and the boundary condition $c^o(0,t) = 1 + \sin \Omega t = c_b(t)$, it is obviously that for $x > t$, $c^o(x,t) = 0$. For $x < t$, the characteristic back from (x,t) to $(0,\tau)$ is $x = t - \tau$, and so $c^o(x,t) = c_b(\tau)e^{\tau - t}$, i.e., the outer solution is given by

$$c^o(x,t) = \begin{cases} 0, & x > t \\ c_b(t-x)e^{-x}, & x < t \end{cases} \tag{3.5}$$

We should remark that along $x = t$ the solution does not match. We will focus in along $x = t$, where we will put a boundary layer and solve the inner problem, denote the inner solution by $c^i(x,t)$.

In the characteristic coordinates $\tau = t - x$, $\eta = x$ and passing a simple calculations equation (3.1) becomes

$$\epsilon\frac{\partial^2}{\partial \eta^2}c(\eta,\tau) - 2\epsilon\frac{\partial^2}{\partial \eta \partial \tau}c(\eta,\tau) + \epsilon\frac{\partial^2}{\partial \tau^2}c(\eta,\tau) - \frac{\partial}{\partial \eta}c(\eta,\tau) - c(\eta,\tau) = 0 \tag{3.6}$$

where now the layer is along $\tau = 0$. It is easy to show that the layer has width $\sqrt{\epsilon}$. The scale transformation is then $\bar{\tau} = \tau/\sqrt{\epsilon}$, and the partial differential equation (3.6) becomes

$$\epsilon\frac{\partial^2}{\partial \eta^2}c(\eta,\bar{\tau}) - 2\sqrt{\epsilon}\frac{\partial^2}{\partial \eta \partial \bar{\tau}}c(\eta,\bar{\tau}) + \frac{\partial^2}{\partial \bar{\tau}^2}c(\eta,\bar{\tau}) - \frac{\partial}{\partial \eta}c(\eta,\bar{\tau}) - c(\eta,\bar{\tau}) = 0 \tag{3.7}$$

To leading order, set $\epsilon = 0$ we get the diffusion equation

$$\frac{\partial}{\partial \eta}\hat{c}(\eta,\bar{\tau}) = \frac{\partial^2}{\partial \bar{\tau}^2}\hat{c}(\eta,\bar{\tau}) - \hat{c}(\eta,\bar{\tau})$$

which can be solved via the transformation $\hat{c}(\eta,\bar{\tau}) = ue^{-\eta}$ to get

$$\hat{c}(\eta,\tau) = \frac{1}{2}\{1 + erf\left(\frac{\tau/\sqrt{\epsilon}}{2\sqrt{\eta}}\right)\}e^{-\eta}$$

Therefore

$$c^i(x,t) = \frac{1}{2}\{1 + erf\left(\frac{t-x}{\sqrt{4x\epsilon}}\right)\}e^{-x}$$

Finally, to obtain a composite expansion that is uniformly valid in the domain we note that the sum of the outer and the inner approximations is

$$c^o(x,t) + c^i(x,t) = \begin{cases} \frac{1}{2}\{1 + erf\left(\frac{t-x}{\sqrt{4x\epsilon}}\right)\}e^{-x}, & x > t \\ \frac{1}{2}\{1 + erf\left(\frac{t-x}{\sqrt{4x\epsilon}}\right)\}e^{-x} + c_b(t-x)e^{-x}, & x < t \end{cases} \tag{3.8}$$

FIG. 1. *The concentration in the saturated zone.*

Hence, by subtracting the common limit in the overlap domain, which has value 0 for $x > t$, and e^{-x} for $x < t$, we have the approximate solution

$$(3.9) \qquad c(x,t) = \begin{cases} \frac{1}{2}\{1 + erf\left(\frac{t-x}{\sqrt{4x\epsilon}}\right)\}e^{-x}, & x > t \\ \frac{1}{2}\{1 + erf\left(\frac{t-x}{\sqrt{4x\epsilon}}\right)\}e^{-x} + c_b(t-x)e^{-x} - e^{-x}, & x < t \end{cases}$$

Therefore, we have obtained an approximate form of the concentration $c(x,t)$ for $x > 0, \ \ t > 0$.

4. Results and Discussion. In this section, the perturbation solution formulated here is tested, and the solution of Equation (2.1) for the concentration $c(x,t)$ of solute in the soil is determined without iterative steps commonly used in numerical schems. The input requirement for the perturbed simulation includes, the diffusivity D; the average velocity v; the decaying coefficient λ. For the sake of illustration, we choose $D = 0.05m^2/yr$, $v = 1m/yr$, and $\lambda = 9.29yr^{-1}$. The boundary condition is $c(0,t) = 1 + \sin 8t$, and thus $\Omega = 0.861$, $\epsilon = 0.4645$. Figure 1 shows the concentration in the saturated zone as a function of time, calculated with Equation (3.9). The concentration $c(x,t)$ in equation (3.9) accounts for a pulse entering the coupled unsaturated/saturated system as $t = 0$. The results in Figure 1 indicate that the pulse inputs yield a large time limit for which the maximum and minimum concentration do not increase anytime.

5. Conclusion. The preliminary results obtained by the model are encouraging and allow us to be optimistic regarding its application. It has the advantage of being easy to use, because of the relative simplicity of the calculations, easily and needing few resources. The resent approach may be extended to more complex cases, such as three-dimensional flow dispersion of real tracers, and dispersion with radioactive decay or chemical reactions.

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