

Mathematical Models of Water and Solute Transport in Soil

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Abstract: Improved understanding of water flow and solute transport through the unsaturated zone is important for the sustainable management of soils. As soils are complex and heterogeneous systems, quantification of the transport processes is difficult. More knowledge on the relationship between solute transport process, soil structure, hydrologic initial and boundary conditions, and observation scale is needed here. Modeling unsaturated flow and transport with mathematical or numerical methods is an important tool for predicting the infiltration and redistribution of soil water and the transport of solutes in the unsaturated zone. Flow and transport models are commonly used to support the decision making process in agricultural management, environmental impact assessment, toxic waste control, remediation design, and subsurface cleanup monitoring. The movement of contaminants through porous media describes by the combination of advection, diffusion-dispersion and chemical retardation. The most common model that describes solute transport by convection and dispersion is the convection-dispersion equation (CDE). This equation describes the change in concentration at any point along the flow path as a function of time. This paper is mainly dedicated to a discussion of basic processes for modelling of water flow and contaminant transport in saturated and unsaturated soils. After a brief description of the classical approach for simulating water flow and solute transport in porous media, issues related to water and solute transport equation in soil.

Keywords: Soil water flow and solute transfer, Breakthrough curves (BTCs), Pore water velocity, Dispersivity.

1. INTRODUCTION

Soil is heterogeneous porous medium and an exceedingly complex system composed of three phases: the solid phase consisting of soil particles, the liquid phase consisting of soil water together with dissolved substances, and the gaseous phase consisting of soil air. Each of these three phases has organic and inorganic constituents and possesses both inert and active compounds. The biological and heterogeneous character of soil strongly influences its physical and chemical properties. With regard to solute transport, the interaction of the diverse components in the soil has a direct effect on such phenomena as dispersion, convection, adhesion, adsorption, and ion exchange. The understanding of water flow and solute transport processes through the unsaturated zone is important [1-6]. Fate and transport processes are influenced by soil and environmental conditions, including rainfall, atmospheric pressure, wind, relative humidity, temperature, water content, plant coverage, sun light, and soil type [7]. The behaviour of a chemical in the environment depends on its structure and its physico-chemical characteristics (e.g., water solubility and distribution coefficient; [8]. The soil's organic matter and clay content are important parameters for the sorption of pesticides while the temperature

influences the chemical's degradation. Chemicals that are ineffectively retained or rapidly transported through the vadose zone may reach the groundwater. Shallow groundwater tables are especially vulnerable for pesticide contamination [2]. Various theoretical models, deterministic [9, 10] and [11, 12], have been developed to describe the transport of solute into soil. The stochastic model is important for unsteady-state water-flow situation. But a deterministic approach is commonplace in many scientific and technologic domains, as in hydrology, soil science, biology, and chemical engineering. In this chapter, the flow and transport equations used in the present study are briefly described.

2. BASIC PROCESSES IN SOLUTE TRANSPORT

Understanding processes and modelling transport of solutes in porous media is a critical issue in the environmental protection. When water containing a solute is applied to a soil profile, free of solute, there will be a very sharp front of solute initially near the surface of the soil. As more solution is added, the sharp front becomes more and more dispersed due to the combined effects of convection, diffusion, and mechanical dispersion consequently; the transport of solute through soils consists of these three processes.

2.1. Transport of Solute by Convection (Advection)

Advection is the component of solute movement attributed to transport by the flowing water. This is the

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phenomenon whereby dissolved substances are carried by the moving water. In this case, water and the solute move at the same average rate. As a consequence, mass flow of solute is strongly controlled by the laws determining the transport of water. Hence, the convective flux of solute passing through a unit area of soil expressed as:

$$q_c = qC = -C \left[k(h) \frac{\partial h}{\partial x} \right] \quad (1)$$

where q_c is the solute flux ($L T^{-1}$); q is the water flux ($L T^{-1}$) (Darcy velocity); C is concentration of solute in water (ML^{-3}); $K(h)$ is the unsaturated hydraulic conductivity ($L T^{-1}$); h the pressure head (L) and x the spatial coordinate (L) (positively defined upwards).

To estimate solute travel or arrival times, the mean apparent velocity or pore water velocity (v) is used:

$$V = \frac{q}{\theta} \quad (2)$$

Where θ is total volumetric water content of soil, ($L^3 L^{-3}$).

Thus solute flux may also be characterized as $q_c = v\theta C$. The water flux q represents the flow velocity averaged over an entire cross sectional area. However, because convection occurs in the liquid phase only, ($v > q$) is used to represent the average interstitial flow velocity in the liquid-filled pores.

2.2. Transport of Solutes by Diffusion

Diffusion is the process by which a solute moves from areas of higher chemical potentials to areas of lower chemical potentials. This process is also known as molecular diffusion. It is assumed that the rate of transfer of solute by diffusion through a unit area of a section of soil is proportional to the gradient in concentration normal to the section.

The rate of diffusion (q_d) in bulk water at rest is given by Fick's Law:

$$q_d = -D_c \frac{\partial C}{\partial x} \quad (3)$$

where q_d is the solute flux in soil due to the diffusion process, ($L T^{-1}$); D_c is the diffusion coefficient in bulk water, ($L^2 T^{-1}$) and C is concentration of solute in water (ML^{-3}). The negative sign in equation (3) arises because diffusion occurs in the direction opposite to that of increasing concentration. The diffusion

coefficient in porous media is lower than for bulk water. Because air and solid particles form barriers to liquid diffusion, the apparent soil-liquid diffusivity (D_s [$L^2 T^{-1}$]) is a function of the available path for diffusion determined by the tortuosity $T(\theta)$, resulting from the geometry of the medium (i.e., texture and structure) and the volume water content. An example of the relationship between D_c (bulk water) and D_s (soil) is given by Jury *et al.* [13]:

$$D_s = D_c \theta T(\theta) = D_c \frac{\theta^{10}}{n^2} \quad (4)$$

where n is porosity. An empirical expression proposed by several researchers is given by Bresler *et al.* [14]:

$$D_s = D_c a e^{b\theta} \quad (5)$$

where a and b are empirical parameters ($b=10$, and a ranges from 0.005 to 0.001 for sandy-loam to clay textures). The flux of diffusing solutes in an unsaturated porous medium is thus:

$$q_d = -\theta D_s \frac{\partial C}{\partial x} \quad (6)$$

2.3. Dispersive Solute Transport

Differences in flow velocities at the pore scale (due to different pore sizes and shapes) cause the solute to be transported at different rates and thus lead to mixing (or dispersion) of an incoming solution within an antecedent solution. The process is macroscopically similar to mixing by diffusion (thermal motion); however, it is passive (i.e., not driven by concentration gradients) and is entirely dependent on water flow. The solute flux due to mechanical (or hydrodynamic) dispersion (q_h) is described by an equation similar to Fick's Law for diffusion:

$$q_h = -\theta D_h \frac{\partial C}{\partial x} \quad (7)$$

Where q_h is dispersive flux of solute, ($L T^{-1}$); D_h is the hydrodynamic dispersion coefficient ($L^2 T^{-1}$) and C is concentration of solute in water (ML^{-3}). This coefficient is dependent on the interstitial pore water flow velocity (v [$L T^{-1}$]), and on the dispersivity ($\lambda = [L]$) of the soil (a function of pore sizes and shapes) according to:

$$D_h = \lambda \left(\frac{q}{\theta} \right)^n = \lambda v^n \quad (8)$$

Where n is an empirical factor usually assumed to equal 1 (i.e., a linear dependency of D_h on v). The value of λ may range from 1 cm in small columns to a few meters in field experiments. In most cases the relative effect of hydrodynamic dispersion can exceed that of diffusion. Because of the macroscopic similarity between diffusion and hydrodynamic dispersion, it is common to combine their coefficients (assuming that they are additive) into a diffusion-dispersion coefficient (D_e):

$$D_e(\theta, v) = D_s + D_h \quad (9)$$

Where D_e is longitudinal hydrodynamic dispersion coefficient, $L^2 T^{-1}$.

Usually, D_e is simply referred to as the dispersion coefficient. It is also called the apparent diffusion coefficient [15, 16] or the diffusion- dispersion coefficient [17].

3. WATER FLOW

The movements of water as well as the transport of chemicals in a soil are generally quantified using some fundamental physical and chemical equations.

One-dimensional uniform (equilibrium), steady state water flow under unsaturated conditions is described by the Buckingham-Darcy equation:

$$q = -k(h) \left(\frac{\partial h}{\partial x} + 1 \right) \quad (10)$$

Where q is the water flow ($L T^{-1}$); $k(h)$ the unsaturated water conductivity ($L T^{-1}$); h the pressure head and (L) and x the spatial coordinate (L) (positively defined upwards).

The unsaturated water conductivity is dependent on water content of the soil. The effective soil water content (S_e) itself is a function of the pressure head h . It is often described by the van Genuchten equation:

$$S_e(h) = \frac{1}{\left[1 + (-\alpha h)^n \right]^m} \quad (11)$$

where α and n are fitting parameters and $n > 1$. The definition of m is:

$$m = 1 - \frac{1}{n} \quad (12)$$

To transfer the actual soil water content θ into the effective soil water content (S_e). The definition of S_e is:

$$S_e = \frac{\theta(h) - \theta_r}{\theta_s - \theta_r} \quad (13)$$

Where θ_s ($L^3 L^{-3}$) is the saturated water content and θ_r ($L^3 L^{-3}$) is the residual water content. For Equation (13) the predictive capillary bundle model of Mualem has the following analytical solution for the unsaturated water conductivity (k):

$$k(S_e) = k_s S_e^l \left[1 - \left(1 - S_e^{\frac{1}{m}} \right)^m \right]^2 \quad (14)$$

where l is a parameter taking into account tortuosity and connectivity. The saturated water conductivity is k_s .

4. SOLUTION TRANSPORT EQUATION

The transport of solute through the soil is governed by the combined effects of three main solute transport mechanisms, convection, diffusion, and dispersion. By adding the convective (Eq. 1), diffusive (Eq. 2), and dispersive (Eq. 7) fluxes of solute, the total flux of solute, moving along the direction of flow is expressed by:

$$q_t = qC - \theta D_s \frac{\partial C}{\partial x} - \theta D_h \frac{\partial C}{\partial x} \quad (15)$$

During the transport of reactive solute, the particles of the soil adsorb some solute and retain it on their surfaces.

The rate of change of concentration of the solute or the gradient of the total flux of solute is equal to the amount of solute remaining in a unit volume of the bulk soil. Thus, the mass balance of solute during the transport through the soil is expressed by the continuity equation as:

$$\frac{\partial}{\partial t} (\theta C + \rho_b S_m) = - \frac{\partial q_t}{\partial x} \quad (16)$$

Where ρ_b is bulk density of soil ($kg m^{-3}$); S_m is mass of adsorbed solute per unit mass of soil ($kg kg^{-1}$); t is variable time (sec); θ is total volumetric water content of soil ($L^3 L^{-3}$) and C is concentration of solute in soil-water (ML^{-3}).

Substituting Equation (15) into (16) and using Equation (9) yields the transport equation as:

$$\frac{\partial}{\partial t}(\theta C + \rho_b S_m) = \frac{\partial}{\partial x} \left(\theta D \frac{\partial C}{\partial x} - qC \right) \quad (17)$$

The left-hand side of Equation (17) accounts for the changes in the concentrations of solute associated both with the liquid and solid phases. The actual relation between S_m and C is complicated. However, this relation has been simplified by assuming an instantaneous equilibrium between the liquid and solid phases. The criteria for this equilibrium have been developed [18-21] and the assumption is valid at low concentrations of the solute. At equilibrium, the adsorption of solute by the soil is assumed to be linear and S_m and C are related by a linear equilibrium isotherm of the form:

$$S_m = kC \quad (18)$$

Where k is empirical distribution coefficient of solute between the liquid and solid phases, m^3 (H₂O) kg⁻¹

If, in addition to linear equilibrium adsorption, steady water flow in a homogeneous soil profile is assumed, Equation (17) can be simplified to:

$$R_f \frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} - V \frac{\partial C}{\partial x} \quad (19)$$

Where R_f is retardation factor, dimensionless.

The retardation factor is given by:

$$R_f = 1 + \frac{\rho_b k}{\theta} \quad (20)$$

Where k is a coefficient representing distribution of the contaminant between the solid and liquid phases (e.g., sorption).

If there are no interactions between the solute and soil particles, k becomes zero and R_f reduces to unity. With exclusion (negative adsorption) of solute occurs R_f becomes less than unity. Equation (19) assumes that the solute is not subject to any production or decay processes. But for many organics, nitrogen species, or radionuclides, these processes are involved and Equation 19 is modified as:

$$R_f \frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} - V \frac{\partial C}{\partial x} \mu_d C + \mu_p \quad (21)$$

Where μ_d is rate coefficient for first-order is decay (T^{-1}) and μ_p is rate coefficient for zero-order production (s^{-1}).

Equation (19) is the basic equation governing the transport of solute through soils and is known as the classical convection-dispersion equation (CDE); however, the CDE is not valid during the early stages of the transport process, because, the hydrodynamic dispersion starts only after a sufficient time has elapsed [22, 23]. Equation (19) assumes that adsorption process is instantaneous and is described by a linear equilibrium isotherm. But since the solid phase of the soil consists of different constituents; a chemical is likely to react with these constituents at different rates and with different intensities. Sorption data exhibit a two-stage approach to equilibrium: a short initial phases of fast uptake, followed by an extended period of much slower uptake. This pattern is followed by sorption reactions. The adsorption of the solute by soil minerals consists of two components, one governed by the equilibrium adsorption and the other by a first-order kinetic non-equilibrium adsorption. The adsorption sites of the soil particles are divided accordingly into two fractions. Adsorption on one fraction is assumed to be instantaneous, and that on the other fraction is thought to be time-dependent. This type of 'two site' adsorption model has been described [24-28] for the transport of solute through the soil. Ignoring any production or decay processes, the 'two site' model is expressed by:

$$\left(1 + \frac{F \rho_b K}{\theta} \right) \frac{\partial C}{\partial t} + \frac{\rho_b}{\theta} \frac{\partial S_k}{\partial t} = D \frac{\partial^2 C}{\partial x^2} - V \frac{\partial C}{\partial x} \quad (22)$$

$$\frac{\partial S_k}{\partial t} = \alpha' [(1-F)KC - S_k] \quad (23)$$

Where F is fraction of adsorption sites of soils occupied by instantaneous adsorption, dimensionless; S_k is mass of adsorption solute per unit mass of soil by the kinetic adsorption sites (kg kg⁻¹) and α' is first-order rate coefficient for kinetic adsorption (s^{-1}).

The non-equilibrium concentration of solute is sometimes assumed to be attributed due to the large heterogeneities in the macroscopic velocities of pore-water. This approach assumes that the water phase of the soil consists of mobile and immobile regions. The convective and dispersive transport of solute is restricted to the mobile phase of soil-water whereas the transfer of solute into and out of the mobile water phase is controlled by diffusion. The transport of solute under these assumptions is described by a two-region mobile-immobile model of the form:

$$(\theta_m + f\rho_b k) \frac{\partial C_m}{\partial t} + [\theta_{im} + (1-f)\rho_b k] \frac{\partial C_{im}}{\partial t} = \theta_m D_m \frac{\partial^2 C_m}{\partial x^2} - V_m \theta_m \frac{\partial C_m}{\partial x} \quad (24)$$

$$[\theta_{im} + (1-f)\rho_b k] \frac{\partial C_{im}}{\partial t} = \alpha^* (C_m - C_{im}) \quad (25)$$

Where θ_m is volumetric water content of soil in the mobile phase ($L^3 L^{-3}$); θ_{im} is volumetric water content of soil in the immobile phase ($L^3 L^{-3}$); f is fraction of the sorption sites in contact with the mobile soil-water phase, dimensionless; C_m is concentration of solute in the mobile soil-water phase ($M L^{-3}$); C_{im} concentration of solute in the immobile soil-water phase ($M L^{-3}$); D_m is dispersion coefficient of the solute for the mobile region ($L^2 T^{-1}$); V_m is velocity of water in the mobile phase ($L T^{-1}$) and α^* is first-order rate constant that governs the rate of exchange of solute between the mobile and immobile regions (s^{-1}).

5. RESIDENT AND FLUX CONCENTRATIONS

In solving transport problems two types of chemical concentrations are usually involved in the transport of solutes through the soils. Depending on the mode of detection, the concentration may be volume-average known as the total *resident* concentration, denoted as c^r , which is the mass of solute per volume of soil or the *flux* concentration, c^f , which is the ratio of the solute mass flux (q_c) and the water flux (q), i.e., $c^f = q_c/q$. The difference between these two concentrations may be illustrated by the outcome of a hypothetical measurement of the effluent leaving a soil column vs. The solution concentration at a given soil volume within the column. This is somewhat analogous to the relationship between changes in volumetric water content and the water flux leaving a soil volume. These concentrations are related through the solute continuity equation (for an inert solute assuming vertical flow along x):

$$\frac{\partial C^r}{\partial t} = - \frac{\partial q_c}{\partial x} \quad (26)$$

And under steady state flow conditions:

$$\frac{\partial C^r}{\partial t} + q \frac{\partial C^f}{\partial x} = 0 \quad (27)$$

An alternative representation was given by [29]:

$$C^f = C^r - \frac{D}{V} \frac{\partial C^r}{\partial x} \quad (28)$$

The inlet boundary condition for the analytical solution of the CED differs with the type of concentration. Improper use of the mode of concentration leads to the erroneous estimate of the solute-transport parameters [30] from the solution of CDE, because some of the solutions describe the resident concentrations adequately while others describe the flux concentrations. When the initial distribution of the solutes through the column of soil is uniform, a flux concentration is usually used to solve the CDE [31, 32], otherwise a resident concentration is used.

The dimensionless column Péclet number P_L , a ratio between solute convection and molecular diffusion [33], for a given column segment with length L , is defined as:

$$P_L = \frac{VL}{D} \quad (29)$$

However, for high values of the Peclet number, P_L , which occur for long columns of soil and/or at high velocities of pore-water, the mode of concentrations is not important. This is because the resident and flux concentrations becomes nearly identical for a semi-infinite system when P_L is greater than 5 [32].

6. INITIAL AND BOUNDARY CONDITION

In order to obtain a unique solution to the differential equation it is necessary to specify the initial and the boundary conditions that apply. The initial conditions describe the values of the variables under consideration (concentration) at some initial time equal to 0 and it is expressed as:

$$C(x, 0) = C_{in}(x) \quad x \geq 0 \quad (30)$$

Proper formulation of the boundary condition are important, because an incorrect choice of the solute-transport parameters for short soil column [34]. The boundary conditions specify the interaction between the area under investigation and its external environments. Three types of boundary condition are normally used in transport (1) Dirichlet, (2) Neumann and (3) Cauchy boundary condition. The first kind condition, Dirichlet specifies the concentration along a boundary segment. It is also referred as a concentration-type boundary and can be expressed as follow:

$$C(0, t) = f(t) \quad t \geq 0 \quad (31)$$

Where the expression $f(t)$ is an arbitrary function that describes the concentration of the influent. The

second-kind condition, Neumann, specifies the concentration gradient along a boundary segment setting dispersive flux equal to zero. It is also referred as a fixed-gradient boundary and can be expressed as follows:

$$\left. \frac{\partial C}{\partial x} \right|_{x=0} = f(t) \quad (32)$$

The third-kind condition, Cauchy, also referred as a mixed or as the flux-type condition, prescribes total contaminant flux in a linear combination of concentration (convection) and concentration gradient (dispersion along the boundary [35]. Mass conservation along the boundary requires:

$$\left(-D \frac{\partial C}{\partial x} + VC \right) \Big|_{x=0} = Vf(t) = VC_0 \quad t \geq 0 \quad (33)$$

Where the expression $f(t)$ is also an arbitrary function that describes the concentration of the influent. The right side of the equation represents the flux entering the model area, while the left side gives the mass flux just inside the boundary. This boundary condition is valid if the concentration in the outside region adjacent to the model boundary is perfectly mixed. In this case the concentration across the inlet boundary are discontinuous in contrast to the first-type boundary.

7. CONCLUSION

The mobility and persistence of contaminant in soils are controlled by fate and transport processes involving advection, dispersion, mass transfer, and various physical, chemical, and biological reaction processes. Advective and dispersive processes relate to the movement of the chemicals with and within the bulk fluids (water, air), and control the direction and magnitude of this movement. Chemical, physical, and biological reactive processes influence the fate of the chemicals and overall transport. Mathematical models can be used effectively as a tool for predicting the extent of solute in the environment and their adverse effects on natural resource systems. Fate and transport processes affecting the mobility of solute in soils are incorporated into fate and transport equations that can be applied to describe and predict the spatial and temporal distribution of chemical concentrations in soils. The most common model that describes solute transport by convection and dispersion is the convection-dispersion equation (CDE). This equation describes the change in concentration at any point

along the flow path as a function of time. The accuracy of the distribution of solute obtained with the CDE depends on concentration of the initial and boundary condition. These reduce the physical complexity of the flow and transport of solute near or across the inlet or outlet boundary and simplify the transport process. So proper formulation of the initial and boundary condition are important.

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Received on 11-03-2017

Accepted on 10-07-2017

Published on 31-10-2017

DOI: <https://doi.org/10.6000/1929-5030.2017.06.03.2>