

II-15 A MOBILE-IMMOBILE MODEL OF UNSATURATED WATER AND ION FLOW

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1. Introduction

Solute movement studies are important tools in the field of subsurface hydrology especially in predicting the movement of pesticides, nitrates, heavy metals, leached salts from the surface layers of the soil and other solutes through the soil. Studies of this type provide information not only on the characteristics of the chemical being transported but also information about the medium itself. Presently, most of the formulations are based on the equations of continuity of water flow and the convective-dispersive equation of mass balance (equation 1 for steady state uniform flow). In equation (1) C is the concentration of the flow (g/cm^3), D_d is the dispersion coefficient (cm^2/day) and v_o is the pore water velocity (Darcy flux divided by the volumetric water content q ; cm/day). Also, z is the distance of flow (cm), and t is the time (days).

The use of equation (1) however, produces symmetrical concentration distributions both with depth and as effluent outflow profiles or BTCs. Experiments on the other hand have consistently shown that concentration distributions are generally non-symmetrical or nonsigmoid in character. This phenomenon is usually called *tailing* and was shown to occur during unsaturated flow, during flow in aggregated media, and during flows with low water velocity.

2. Previous Formulations

In order to account for the tailing phenomenon, several researchers have made modifications of equation (1) to include mobile and immobile water or dynamic and stagnant water zones with transfer or diffusion between the two zones. Most of these models consider the immobile part of the soil water to be created from the existence of dead-end pores and trapped air inside the soil, and the adsorption between the soil and the water is usually described by an instantaneous linear Freundlich relationship. Later models also include solute decay in the form of degradation terms for both the water and the soil.

Although these kind of relationships have been successfully used in modeling, most researchers admit that the determination of the numerous parameters becomes a big burden. For one, the separation of the soil water into mobile and immobile zones alone is a big assumption in itself. If the basis of the separation of the zones is the trapped water in dead-ended pores as the immobile part, then the quantification of θ_m and θ_{im} would be very difficult especially during unsteady state flows. Another problem is the assumption that the sorption reactions are instantaneous. This would present problems for variable water velocities especially during transient states of the soil. If the rate of adsorption is slow compared to the rate by which the chemicals move through the soil, then a kinetic approach towards equilibrium would be more appealing.

3. Proposed Model

To overcome some of the limitations of the above formulations, a new model is proposed. Considering the flow of chemicals through an unsaturated, aggregated, sorbing porous media, four regions can be identified as follows: a) air spaces trapped between soil particles, b) mobile water located inside pore spaces both large and small (solute flux occurs through advection and diffusion in this region), c) immobile water which envelopes the soil particles (this enveloping water is the irreducible water film as described by θ_i in the ψ - θ relationship and this region mixes with the mobile region through a kinetic mixing term), d) soil region which is in contact with the immobile region and in some places with the mobile region. The percentage of contact of this region with the mobile part is given by the parameter f . Soil sorption reactions occur in this region with the immobile and mobile water regions. Decay exists in the chemicals in the last three regions described by a first order decay term. For the relationship between the adsorbed and solution concentration, a kinetic approach to equilibrium is proposed.

The equations of continuity for the mobile and immobile regions becomes equations (2) and (3), with the relationship between S and C expressed in non-equilibrium form as equation (4) for the total soil, where linear decay is assumed as equation (5). In the above equations, d_m , d_{im} and d_s are first order decay term for the mobile

$$\left. \begin{aligned} \frac{\partial \theta}{\partial t} + \frac{\partial q}{\partial z} &= 0 \\ \frac{\partial C}{\partial t} &= D_d \frac{\partial^2 C}{\partial z^2} - v_o \frac{\partial C}{\partial z} \end{aligned} \right| \quad (\partial \theta / \partial z = 0) \quad (1)$$

$$\frac{\partial \theta_m C_m}{\partial t} + f \left\{ \frac{\partial \rho S}{\partial t} \right\}_m + \frac{\partial J}{\partial z} + \alpha (C_m - C_{im}) - d_m = 0 \quad (2)$$

$$\frac{\partial \theta_{im} C_{im}}{\partial t} + (1-f) \left\{ \frac{\partial \rho S}{\partial t} \right\}_{im} - \alpha (C_m - C_{im}) - d_{im} = 0 \quad (3)$$

$$\frac{\partial \rho S}{\partial t} = f \rho \beta_{sm} (C_m - S) + (1-f) \rho \beta_{si} (C_{im} - S) - d_s \quad (4)$$

$$(d_m = \xi_m \theta_m C_m, d_{im} = \xi_{im} \theta_{im} C_{im}, d_s = \xi_s \rho S) \quad (5)$$

water, immobile water and soil, respectively ($\text{g}/\text{cm}^3/\text{day}$), β_m , and β_s are kinetic sorption parameters for the soil and the mobile and immobile water (day^{-1}) and ξ_m , ξ_{sm} and ξ_s are decay parameters (day^{-1}). Also, J ($J = \theta_m C_v - \theta D_s \text{grad}(C)$) is the solute flux by advection and dispersion ($\text{g}/\text{cm}^2/\text{day}$).

4. Application

The differential equation was solved using an alternative predictor-corrector *finite difference scheme* which retains all the advantages of a Crank-Nicolson approach but slightly increases the truncation error to $O((\Delta x)^2 + (\Delta t)^{3/2})$. To determine the performance of the model, the numerical results were fitted with the analytical and experimental data. Model comparison with the analytical data can be seen in figure 1. The analytical results were for the mobile-immobile model by van Genuchten and Wierenga (1976), where the soil-water sorption was estimated using the Freundlich isotherm. From figure 1 it can be seen that for almost the same model parameters, the numerical and analytical results vary by a lag of about 0.2 pore volumes. This can be explained by the fact that the Freundlich isotherm produces instantaneous sorption reactions between the soil and the water causing a faster distribution of chemicals between the water and the soil thus the delay of the concentration breakthrough. However, besides the lag, it can be seen that the two curves are similar in shape and are acceptable considering the differences between the sorption terms of the two model approaches.

For the experimental data fitting, the curves can be seen in figure 2. Details of the experimental procedure can be found in Taniguchi and Sharma (1990) and Shimojima and Sharma (1993). From figure 2, it can be seen that the numerical calculations predict well the experimental data. The result of the fitting shows that the fraction of the soil exposed to the mobile water zone does not greatly affect the effluent profile (BTC), mainly due to the very low sorption terms required for the estimated fitting. The dispersion coefficient was also very low which can be explained by the very steep BTC of the experiment. The assumption of this model to use the irreducible moisture content as the immobile zone of the water produces very good results.

4. Conclusions

As can be seen in figures 1 and 2, the numerical results show good correspondence with the analytical and experimental data, showing the non-sigmoid characteristics that regular mobile-only mass flow modeling yields. This means that the numerical model is as accurate in predicting the actual BTCs as the analytical solution. Even though the analytical solution used by van Genuchten and Wierenga (1976) may also produce accurate results in predicting the effluent BTC, model assumptions on how to predict the amount of the immobile zone and the speed of the sorption reactions would make their solution less desirable. Generally, although this model can predict the lumped concentration BTCs as well as the distributed concentration with depth curves, the real use of the model would be to fit the numerical curves with actual concentration with depth data. In this way more information can be gained compared to just the characteristics of the outflow concentration.

References

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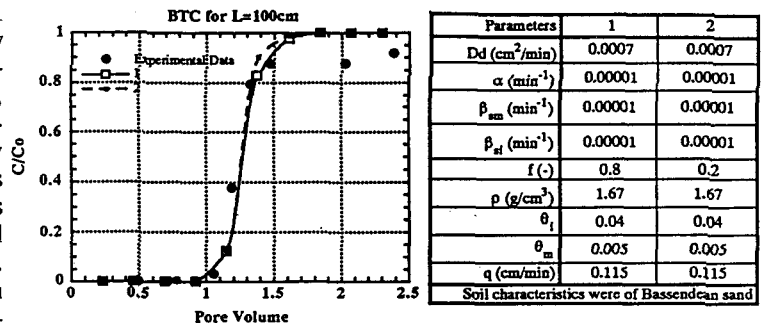


Figure 1. Comparison of the BTCs generated by the numerical solution of this model and van Genuchten and Wierenga's (1976) analytical solution.

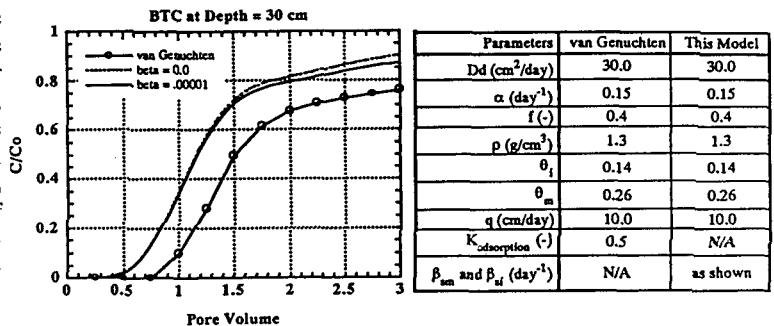


Figure 2. Comparison of the BTCs generated by the numerical solution of this model and the experimental data of Shimojima and Sharma (1993).