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USE OF SOLUTE TRANSPORT MODELS FOR PREDICTING THE MOVEMENT OF DISSOLVED CHEMICALS THROUGH THE POROUS MEDIA.

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In recent years wide-spread observation of ground water contamination has focused attention on solute transport through soil. Three widely used solute transport models, namely has convection-dispersion equation (CDE), the mobile-immobile water model (MIM) and the transfer function model (TFM) are reviewed. The CDE model is valid if the residence time of the solute is much longer than the time required for transverse mixing by molecular diffusion. Conversely, if the mean residence time of the solute in the soil is short compared to the transverse mixing time, then the TFM can do a better job for the area-averaged concentration of the solute than the CDE model. The MIM model is good for describing solute transport in aggregated soil but it introduces new parameters into the CDE model which cannot be independently estimated.

The concept

Prediction or measurement of solute movement through the soil is of interest for improving the efficiency of leaching of saline soils and the distribution of surface - applied fertilizers and pesticides. Chemical transport models could be useful for estimating the movement of various dissolved chemicals through the unsaturated zone. Most field solute transport models used in the unsaturated zone are based on the convection-dispersion equation which was developed and tested almost exclusively in laboratory experiments. Convection refers to the average bulk movement of solute within flowing solution while dispersion describes solute spreading and mixing about the mean displacement position caused by local irregular convective displacements. In a system comprised of water and dissolved chemicals, the only mixing occurring is by molecular diffusion which results from collisions occuring at the molecular scale. However, in porous media, convective flow is expressed as an effective flux which has been

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volume averaged over many pores and ignores complex three-dimensional water flow paths resulting from movement around the rigid solid phase. The additional solute spreading caused by these local convective flow paths which are not described as part of the volume-averaged convection is called hydrodynamic dispersion. The classical convection dispersion equation assumes that mechanical mixing caused by local fluctuations in water flow velocity is similar to a large Fickian diffusion process. This CDE model has received many tests in miscible displacement experiments in laboratory and appears to be capable of describing outflow behaviour in saturated and unsaturated homogeneous soil (Biggar and Nielsen, 1967; Yule and Gardner, 1978). It has been pointed out, however, that the evidence that the convection-dispersion equation may be used to describe solute transport through unsaturated porous media is not as strong as in comparable saturated flow experiments (De Smedt and Wierenga, 1984).

The utility of the two-parameter convection-dispersion equation for describing transport through undisturbed soil columns which maintain natural structure has been less satisfactory than when the column structure was broken up and the columns were repacked (Green et al., 1972; Van Genuchten and Wierenga, 1977; Nkedi-Kizza et al., 1983). In these studies, researchers observed asymmetric or non-sigmoid break-through curves characterized by a long, slow decline of the pulse concentration (commonly called tailing) and early arrival of a small quantity of solute. This lack of symmetry in breakthrough curves associated with structure or aggregated soils has been attributed to the presence of mobile and immobile water regions (Van Genuchten and Wierenga, 1977; Nkedi Kizza *et al.*, 1983), the presence of dead end pores (Philip, 1968) or to the existence of bimodal pore size distribution (Green *et al.*, 1972). Each of these alternate hypotheses introduced new parameters into the convection-dispersion model which could not be independently measured or estimated and had to be simultaneously fitted with other parameters when the model was compared to data.

Asymmetric breakthrough curves have also been observed in experiments involving unsaturated flow through homogeneous packed porous media under laboratory conditions (Gaudet *et al.*, 1977; De Smedt and Wierenga, 1984). Most of these experiments have shown that solute movement under unsaturated conditions has characteristics (such as early breakthrough and tailing) which clearly differ from transport under saturated conditions. Gaudet *et al.*, (1977) stated that slow diffusion of solute into or out of stagnant water is probably the main reason for the extensive tailing observed in unsaturated flow experiments. Kirda *et al.*, (1973), Hildebrand and Himmelblau (1977) and Yule and Gardner (1978) successfully used the classical convection-dispersion equation to describe solute transport through unsaturated porous media provided that higher values for the dispersion coefficient were used than in comparable saturated flow studies.

Solute dispersivity and the scale effect

The dispersivity parameter, which is a measure of the dispersive properties of a system, has commonly been regarded as a specific single-valued property of the entire medium (Bear, 1972). In recent years it has been realized that field-measured values for dispersivity or dispersion coefficient values obtained from fitting the CDE model to tracer tests are scale dependent. This means that the size of the apparent dispersion coefficient or dispersivity increases tremendously with the size of the averaging volume in the field (Pickens and Grisak, 1981). In addition to the larger values of apparent dispersion parameters required to explain field behaviour, the apparent dispersion coefficient or dispersivity required to achieve agreement with consecutive observations of a tracer has been noted to increase with increasing travel distance from the source of the solute (Gelhar and Axness, 1983). Many of these large-scale observations of soult movement have come from ground water tracer experiments. In summary, these findings suggest that dispersion cannot be described as a Fickian-type mixing process prior to the asymptotic state, and the non-uniqueness of dispersivity or the so-called scale effect problem may limit the predictive value of numerical models of solute transport based on the CDE (Gelhar *et al.*, 1979).

Mobile-Immobile Water Model

Several methematical models have been proposed to describe asymmetrical solute breakthrough curves obtained in structured soil. A common characteristic of most of these models is the assumption that there are two distinct soil water zones in the system: one zone designated as the 'mobile' water region where solute tranport takes place by convection and dispersion, and another zone designated as the 'immobile' region where solute transfer takes place by diffusion only. Highly asymmetric breakthrough curves with pronounced effluent tailing have been attributed to the slow diffusion of solute in or out of immobile water (Gaudet *et al.*, 1977). Various models have been presented to explain the exchange of solute between mobile and immobile water regions. One of the simplest and more practical approach assumes that the transfer of solute in and out of the immobile water regions is described by the first-order exchange process (Van Genuchten and Wierenga, 1976; Gaudet *et al.*; 1977). Transfer between the two liquid regions is assumed to be proportional to the concentration difference between the mobile and immobile soil water phases.

Van Genuchten and Wierenga (1977) reported that the first-order rate model provided an excellent description of the experimental effluent data and showed that tailing observed during tritium transport through a unsaturated, aggregated Glendale clay loam soil could be explained satisfactorily by this model. This model also presented a good description of the extensive tailing of the chloride concentration distributions measured at several depths inside and the end of a 94-cm sand column (Gaudet *et al.*, 1977), and through columns of various-sized aggregates of an Ion oxisol soil (Nkedi-Kizza *et al.*, 1983).

Transfer Function Model.

Jury (1982) proposed the use of a transfer function model for describing solute movement through soil when sufficient solute leaching is occurring to move solute from an inflow boundary to an exit boundary. In this approach, which may be applied to any three-dimensional solute transport volume, all solute transport mechanisms are implicitly characterized by measuring the distribution of travel times from the inflow boundary to the exit boundary. The distribution function, expressed as a probability density function of travel times, is then used in a convolution integral to predict exit concentrations for arbitrary surface input concentrations. This model was successfully applied on the field scale to describe leaching of a bromide pulse over a 0.64 ha surface area (Jury *et al.*, 1982.).

White (1985) applied the transfer function model to nitrate leaching through cracking clay soils, both below crop rooting zones and to the effluent of tile-drains. He reported that the transfer function model fitted the data from soil column experiments well for moist or prewetted cores but was inadequate for very dry soils irrigated at high water inflow rates. Recently, Jury *et al.*, (1986) generalized the transfer function model to describe the movement of a solute which may undergo physical, chemical or biological transformations as it moves through a natural soil unit. In a second paper (White *et al.*, 1986), these authors successfully analyzed the results of both field and laboratory studies of solute transport through unsaturated soil, and developed guidelines for its general use in solute transport experiments.

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