

## **Modelling of Solute Transport in the Unsaturated Zone**

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A numerical model for solute transport in the unsaturated zone has been developed. The model is based on the basic equation for soil water flow in one dimension and the general convection-dispersion equation. These are solved by numerical techniques and coupled under the assumption that the flow equation can be solved independently.

Options for solute-soil reactions are included in the model comprising adsorption, ion exchange and decay. In addition the effect of immobile water may be considered in the calculations.

The model has been applied for simulating field conditions. The model calculations have been compared with measurements of moisture content and the results from a field tracer experiment.

### **Introduction**

The first stage of many groundwater pollution problems takes place in the unsaturated zone. When the pollution source is situated above the water table, the pollutants will move vertically through the partially saturated soil before entering the groundwater zone at the water table.

During this passage the pollutants will be subject to a number of physical and chemical reactions which can change the concentration of pollutants significantly. In addition, a considerable time lag may be experienced during the passage through the unsaturated zone. Hence, this zone is an important link in many

groundwater pollution problems.

Prediction of the transport of pollutants is most appropriately carried out by a numerical simulation model in which all relevant processes are incorporated. The model described in this paper is an attempt to develop an operational model for practical applications. In the model are included the most important physical and chemical processes, which are formulated in terms of basic physical and chemical mechanisms in so far as it seems possible and practical at present.

## **Model Components**

The solute transport model has been designed to suit the overall structure of the European Hydrologic System (SHE), Jensen and Jønch-Clausen (1982). Here it has been assumed that the water flow in the unsaturated zone can be described by independent one-dimensional flow columns. Hence, the solute transport model has been developed from the assumption that the water flow is vertical. Further, it has been assumed that the solute concentrations are small so that density differences are not affecting the water flow process. This implies that the water flow can be calculated independently of the solute transport calculations.

### **Water Flow**

The water flow calculations in SHE are based on a numerical solution to the differential equation for soil water flow

$$C \frac{\partial \psi}{\partial t} = \frac{\partial}{\partial x_3} \left( K \frac{\partial \psi}{\partial x_3} \right) - \frac{\partial K}{\partial x_3} \psi - S \quad (1)$$

where

- $\psi$  – capillary pressure head
- $t$  – time
- $x_3$  – vertical space coordinate (positive downwards)
- $C$  – water capacity
- $K$  – hydraulic conductivity
- $S$  – sink term

In the subsequent solute transport calculations the variation in moisture content and water flux with time and distance is used.

### **Solute Transport**

The solute transport calculations are based on the traditional convection-dispersion equation

$$\frac{\partial (\theta C)}{\partial t} = \frac{\partial}{\partial x_i} \left( \theta D_{ij} \frac{\partial C}{\partial x_j} \right) - \frac{\partial}{\partial x_3} (qC) + \text{CHEM} \quad (2)$$

where

- $\theta$  – moisture content
- $C$  – concentration of the dissolved chemical species
- $x_i$  – space coordinates
- $q$  – water flow in vertical direction
- $D_{ij}$  – coefficient of hydrodynamic dispersion

CHEM – term accounting for chemical reactions

As described above the water flow is assumed strictly vertical and consequently the same restriction applies to the convective transport of the dissolved solutes. On the other hand, allowance is made for both longitudinal and transverse dispersion. The model can in its present version simulate the dispersion process from an area and line source. In addition, a cone-shaped spreading of pollutant from a point source can be calculated by solving the transport equation in polar coordinates.

Eq. (2) is solved by numerical methods in a two-step procedure. The convective transport is solved by displacing the concentration profile according to the velocity field. In this calculation procedure third order polynomial approximations are used. The changes in concentration caused by hydrodynamic dispersion and chemical reactions are subsequently superimposed the convected concentration profile. These changes are calculated by an explicit finite-difference approximation to the dispersion term.

The dispersion coefficient is a function of the intrinsic properties of the soil and the water flow. For groundwater flow a linear relation between dispersion coefficient and seepage velocity is generally adopted. If the aquifer is isotropic the dispersion coefficient may be characterized by a longitudinal and a transverse coefficient defined as

$$\begin{aligned} D_L &= \alpha_L V \\ D_T &= \alpha_T V \end{aligned} \tag{3}$$

where

- $D_L$  – longitudinal dispersion coefficient
- $D_T$  – transverse dispersion coefficient
- $\alpha_L$  – longitudinal dispersivity
- $\alpha_T$  – transverse dispersivity
- $V$  – seepage velocity

The two constants of proportionality, the longitudinal and transverse dispersivities, represent the aquifer properties.

For unsaturated flow the dispersivities are dependent on the water content in some unknown way. However, in the present model development this variation will be neglected and relations similar to Eq. (3) will be adopted.

*Immobile Water* – Several experimental displacement studies in unsaturated soils have indicated asymmetrical concentration distributions, either versus depth or as effluent curves, under conditions where the distributions should be symmetrical according to theory. This phenomenon has been explained by the existence of immobile water in dead-end or blind pores where the exchange of mass with the displacing solution rely on diffusion processes.

In order to describe the existence of immobile water Eq. (2) may be expanded as follows

$$\frac{\partial (\theta_m C_m)}{\partial t} + \frac{\partial (\theta_{im} C_{im})}{\partial t} = \frac{\partial}{\partial x_i} \left( \theta_m D_{ij} \frac{\partial C_m}{\partial x_j} \right) - \frac{\partial}{\partial x_3} (q C_m) + \text{CHEM} \quad (4)$$

$$\theta_{im} \frac{\partial C_{im}}{\partial t} = \beta (C_m - C_{im})$$

where

- $\theta_m$  – fraction of the soil containing mobile water
- $\theta_{im}$  – fraction of the soil containing immobile water
- $C_m$  – concentration in mobile phase
- $C_{im}$  – concentration in immobile phase
- $\beta$  – mass transfer coefficient

Consideration with regard to immobile water is optional in the numerical model.

*Sorption* – When a sorbing porous medium is considered the rate of absorption is included in the CHEM-term as follows

$$\text{CHEM} = - \rho \frac{\partial \bar{C}}{\partial t} \quad (5)$$

where

- $\rho$  – bulk density of the soil
- $\bar{C}$  = concentration of the chemicals adsorbed on the soil

Various expressions are proposed in the literature for the exchange rate between adsorbed and solution concentration. In the present model options are included for various equilibrium isotherms such as the Freundlich and Langmuir isotherms. Further, some selected non-equilibrium isotherms are included. These models assume a kinetic approach towards equilibrium and apply when the rate of absorption is slow compared to the rate at which the chemical move through the soil.

*Decay* – The model can describe the transport of species which undergo decay according to a first order reaction. This is included in the CHEM-term as follows

$$\text{CHEM} = - \lambda (\theta C + \rho \bar{C}) \quad (6)$$

where  $\lambda$  – decay constant

*Ion Exchange* – Ion exchanges are processes where different ions are involved in exchange processes between the solution phase and the adsorbed phase. In the model these processes are described by relations which are derived from the law of mass action

$$K_{ij} = \left( \frac{\bar{c}_i}{c_i} \right)^{V_j} \left( \frac{c_j}{\bar{c}_j} \right)^{V_i} \quad (7)$$

where

- $K_{ij}$  – selectivity coefficient for the exchangeable ions  $i$  and  $j$
- $C$  – activity of the ions in the solution phase
- $\bar{C}$  – activity of the ions in the adsorbed phase
- $V$  – valence of the ions

Application of these equilibrium equations require that the kinetics of the ion-exchange processes are much faster than the rate at which the species move through the soil. It is assumed that the processes are fully reversible and that the selectivity coefficients are constant in time. To enable quantitative predictions of the effects of ion exchange on cation concentrations in the soil water, it is further assumed that the cation-exchange capacity (CEC) of the soil is constant in time. However, the value for CEC can be specified in the model since this parameter is related to the physical and chemical characteristics of the soil material.

On the basis of the relations and assumptions discussed above, the model can predict the simultaneous transport of up to three chemical species which are interacting through ion-exchange processes.

Consideration to ion-exchange processes is of particular importance in connection with irrigation projects in arid zones. Such projects require a detailed planning to avoid the adverse effects from salt accumulation in the root zone on crop production.

### **Model Verification**

As outlined above the convection-dispersion equation is solved by numerical techniques. The accuracy of the numerical approximation can be evaluated by comparing numerical calculations with analytical solutions to the transport equation. Analytical solutions are available for some simple problems (see e.g. Bear 1979). Fig. 1 presents a comparison for the problem of one-dimensional steady-

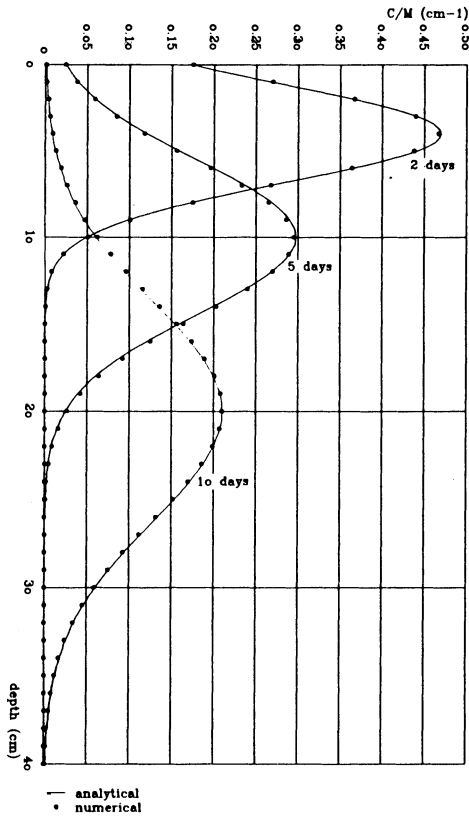


Fig. 1. Comparison between numerical and analytical solutions for an instantaneous injection of contaminant.

state flow through a homogeneous isotropic soil column where a finite mass of contaminant is released as an instantaneous slug at time zero. As seen from Fig. 1 there is essentially an exact agreement between the two solutions.

Agreements of similar accuracy are also obtained for other problems which strongly support the accuracy of the numerical procedure.

### Field Application

The model has been tested on data collected at an agricultural experimental station in Southern Denmark. The collected data include rainfall and meteorological observations and measurements of moisture content and pressure head in the unsaturated zone. Parallel to the water balance investigations (Benetzen 1978) a tracer experiment has been carried out. This involved injection of tritium and <sup>51</sup>Cr to the soil surface in the form of tritiated water and Cr-EDTA

complex. The migration of these constituents through the unsaturated zone was recorded at regular intervals. The experiment was carried out in the fall in order to diminish the influence of the evapotranspiration processes.

### **Water Flow**

Some results of the water flow calculations are demonstrated in Figs. 2 and 3. Fig. 2 shows the simulated and measured soil moisture contents at various depths under a grass covered field plot for a period of two years. The continuous lines represent the simulated moisture contents and the stars are the corresponding field measurements. As shown by the figure the simulated and observed values compare well.

Fig. 3 illustrates the corresponding variation of water flow through the profile as simulated by the model. A pronounced seasonal variation prevails which is caused by the root extraction of water during the growing season. During this period there is almost no contribution to deep percolation. Deep percolation starts in the fall after the replenishment of the water deficit in the root zone.

The time for injection of tracers is indicated in Fig. 3. As shown by the figure this time is towards the end of the growing season and hence the evapotranspiration processes are expected to cause no significant removal of tracer.

The variation in moisture content and water flow with time and distance is required for the solute transport calculations.

A more comprehensive description of the field simulation can be found in Jensen (1983).

### **Solute Transport**

The tracers are spread on the soil surface over some area around the vertical where the measurements are taken. Hence, the convection-dispersion process is considered to be one-dimensional.

Below the simulation results for the chrome-complex is shown. The concentration levels at the various depths are recorded by a radiation detector which is lowered to the recording depths through the access tube used for soil moisture measurements. The  $^{51}\text{Cr}$  of the chrome-complex is decaying radioactively and has a half life of 28 days. This value is applied in the model calculations.

The dispersion characteristics are here described by a dispersivity of 15 cm. This value is similar to the ones found in other field studies.

In Fig. 4 the model calculations are compared with measurements at five levels below the soil surface. The concentration scale represents relative values which are obtained by dividing the concentrations with the injected mass of tracer per unit area. The numbers are not dimensionless but have the unit of  $\text{cm}^{-1}$ . The continuous lines represent the calculated concentrations and the stars represent the measured ones. The measured values are adjusted for background noise.

At the two upper depth levels some larger deviations are present immediately

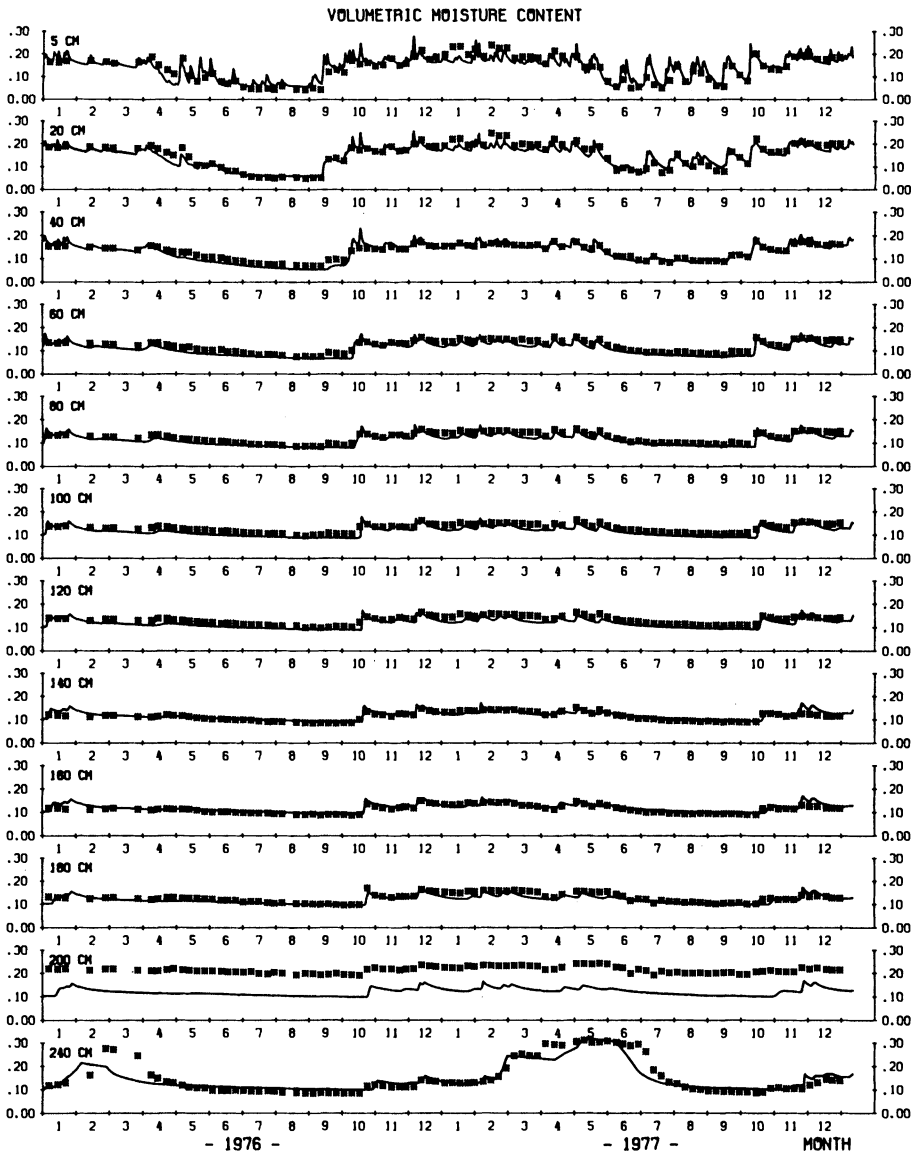


Fig. 2. Calculated and measured variation in moisture content with depth and time.  
— calculated  
\* measured (Bennetzen 1978)



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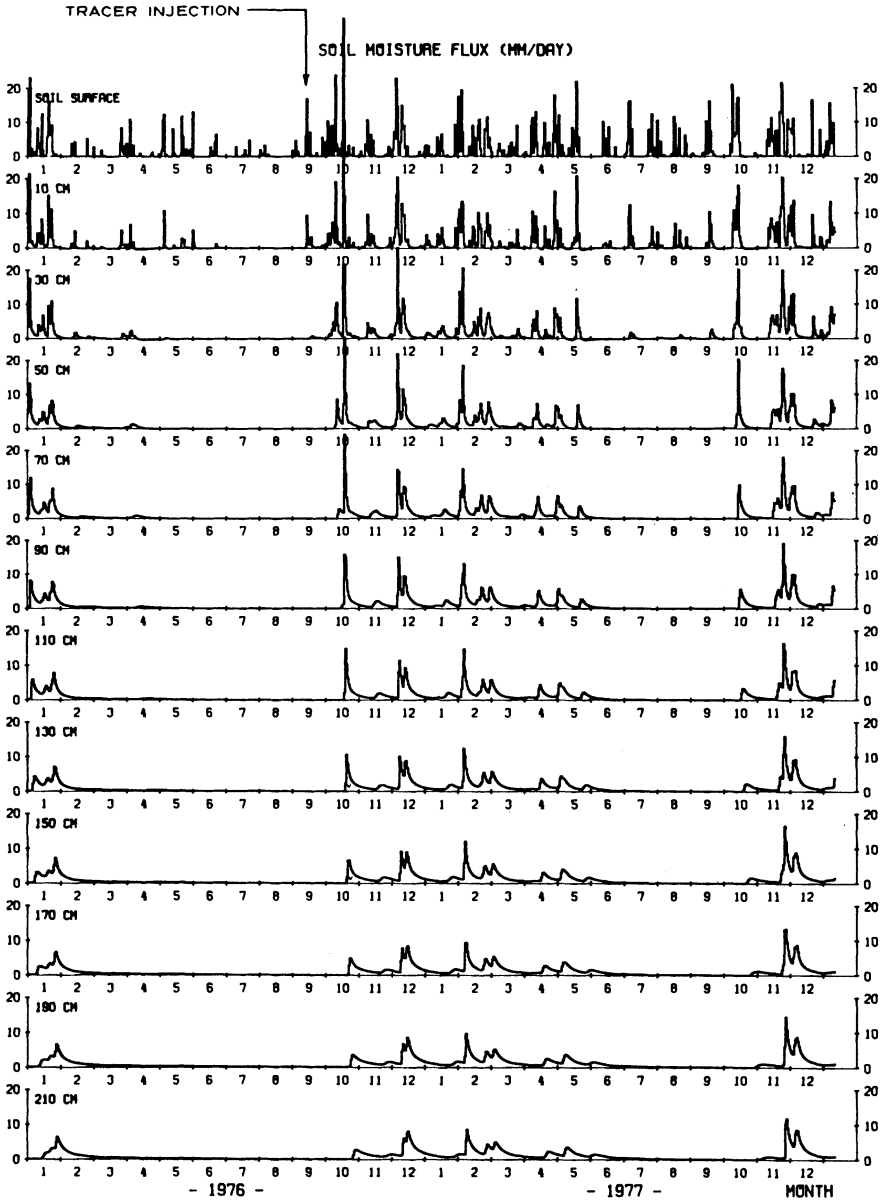


Fig. 3. Calculated variation in water flow with depth and time.

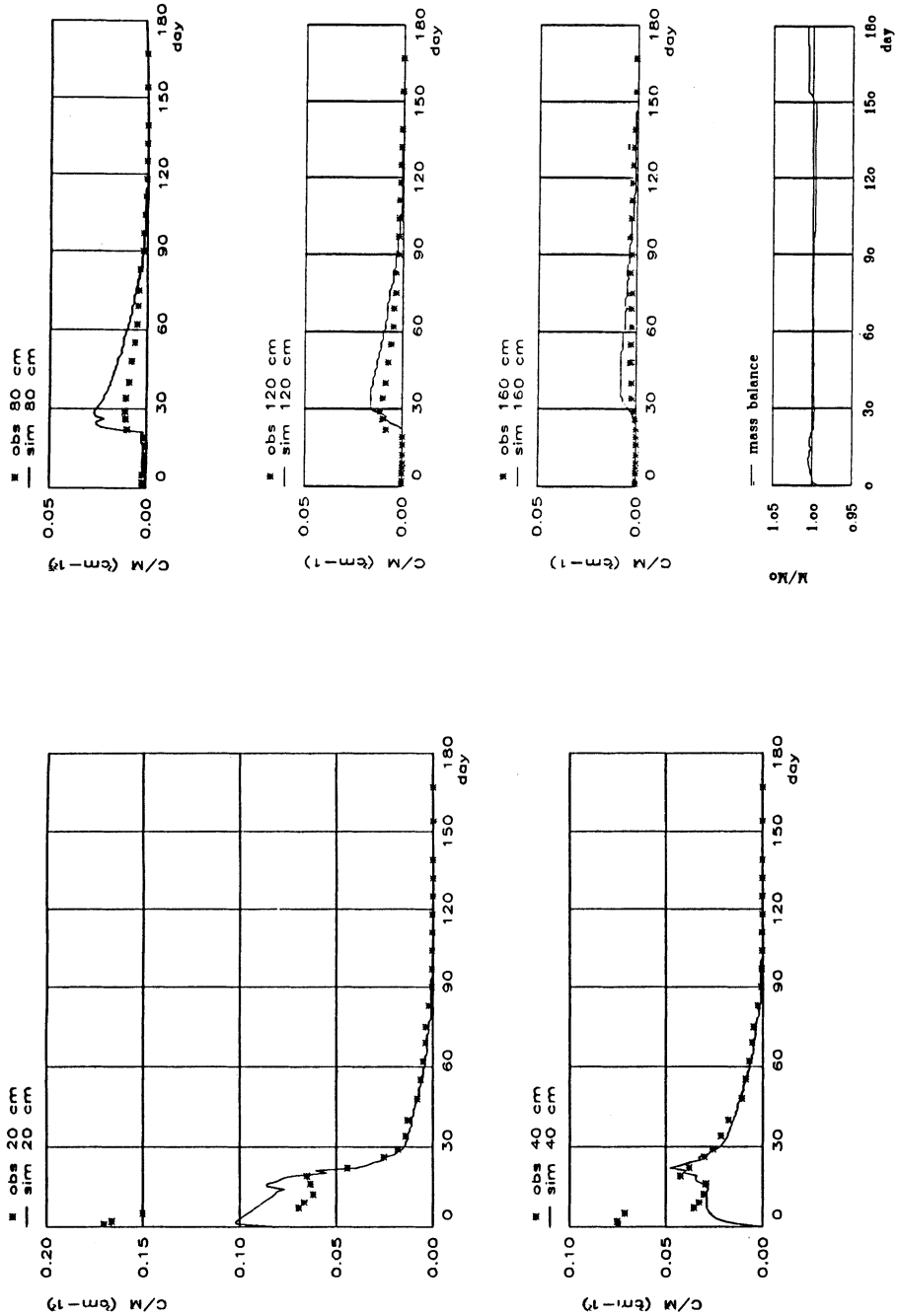


Fig. 4. Calculated and measured variation in concentration with depth and time. — calculated \* measured

after the injection. It is believed that the explanation for the high observations the first days after the injection is seepage along the access tube. On the other hand the recession period is described very accurately.

At larger depth the model description in general is less accurate. At 80 cm below the surface the arrival of the tracer front is in agreement with measurements; however, the concentrations are too high. At the depths of 120 and 160 cm the arrivals of the front deviate somewhat from measurements. However, the deviation is not one-sided. The simulated concentrations are also here a little too high.

At the bottom of the figure the mass balance error of the model calculations is depicted. Being less than 1% it is by all means satisfactory.

## **Conclusions**

A numerical model for solute transport under unsaturated conditions is described. The model is based on the differential equation for soil water flow and the convection-dispersion equation, which both are solved by numerical techniques.

The model has been compared with analytical solutions to the convection-dispersion equation. An almost exact agreement is found between the numerical and analytical solutions. In terms of conservation of mass in the calculations the numerical approximation has proven to be very accurate.

In the field application some deviations are observed between model predictions and measurements. The model provides a satisfactory description of the conditions in the upper layers, although it does not simulate the high values right after the injection. For the lower depths larger deviations are observed.

When evaluating the model applicability on the basis of the field tracer experiment discussed here, the following should be observed: solute transport simulation is a "second level" modelling, since it relies on the water flow description. Although calculated and measured moisture content compares well in the present field application, deviations are inevitable and these will consequently affect the subsequent solute transport calculations. Hence, solute transport simulations can be expected to be less accurate than water flow simulations. For the present field tracer experiment also some experimental problems are reported. These will also contribute to the discrepancies between simulation and experiments.

The present field application provides a reasonable validation of the model; however, it is not possible on this alone to make any firm confirmation of the general applicability of the model. For this the measurements are too uncertain.

The present model development relies on the traditional convection-dispersion equation. This equation may prove to be inappropriate for field simulation as

recently pointed out in the literature. For a more thorough discussion of these problems reference is made to Refsgaard et al. (1984). Much more field testing will be required to identify the appropriate approach.

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