Heat and mass transport in saturated-unsaturated groundwater flow

WALTER PELKA
Institut für Wasserbau und Wasserwirtschaft,
Rheinisch Westfälische Technische Hochschule
Aachen, Mies-van-der-Rohe-Str. 1,
D-5100 Aachen, FR Germany

ABSTRACT Because of the increased demand for water in most parts of the world, and the greater intensity of water use, issues of water quality now rank with those of quantity in limiting the development of water resources. A numerical model is presented for calculating transient heat and mass transport in saturated-unsaturated groundwater flow. The present model is based on a finite element approach. While the solution of the flow field equation is generated by a generalized variational approach, the transport equations are solved by means of a weighted residual technique.

Transfert de chaleur et de masse dans l'écoulement de l'eau souterraine entre la zone saturée et la zone non saturée

RESUME Par suite d'une demande croissante d'eau dans la plupart des pays et d'une utilisation beaucoup plus intensive la qualité ainsi que la quantité disponible ont posé les problèmes les plus difficiles pour le traitement approprié des ressources en eau. On présente ici une solution numérique pour les calculs du régime transitoire de la chaleur et le transport de masse dans les zones saturées et non-saturées. Ce modèle se base sur l'application des méthodes des éléments finis. La solution de l'équation aux dérivées partielles concernant l'écoulement de l'eau souterraine est traitée à l'aide d'une approche variationnelle et généralisée, tandis que l'équation du transport de masse est résolue par la méthode de Galerkin.

NOTATION

\begin{align*}
C & \quad \text{concentration} \quad [\text{M} \cdot \text{L}^{-3}] \\
p & \quad \text{pressure} \quad [\text{M} \cdot \text{T}^{-1} \cdot \text{L}^{-1}] \\
t & \quad \text{time} \quad [\text{T}] \\
T & \quad \text{temperature} \quad [\text{K}] \\
c(T,C) & \quad \text{specific heat capacity (water)} \quad [\text{L}^2 \cdot \text{T}^{-2} \cdot \text{K}^{-1}] \\
c_B(T,C,S_r) & \quad \text{specific heat capacity (soil)} \quad [\text{L}^2 \cdot \text{T}^{-2} \cdot \text{K}^{-1}] \\
n & \quad \text{porosity} \\
S_0, p & \quad \text{specific storage coefficient} \quad [\text{M}/(\text{M} \cdot \text{T}^{-1} \cdot \text{L}^{-1})] \\
S_r & \quad \text{saturation} \\
\rho(T,C) & \quad \text{density (water)} \quad [\text{M} \cdot \text{L}^{-3}] \\
\rho_B(T,C,S_r) & \quad \text{density (soil)} \quad [\text{M} \cdot \text{L}^{-3}] \\
\end{align*}
\[ \mu(T,C) \] viscosity \([M \, L^{-1} T^{-1}]\)

\[ D_r(S_r) \] relative mechanical dispersion

\[ k_r(S_r) \] relative permeability

\[ \Lambda_r(S_r) \] relative conductivity

\[ D_{c,ij}(T) \] tensor of hydrodynamic dispersion \([L^2 T^{-1}]\)

\[ D_{d,ij}(T) \] tensor of molecular diffusion \([L^2 T^{-1}]\)

\[ D_{w,ij}(T,C,S_r) \] tensor of effective thermal dispersion \([ML T^{-3} K^{-1}]\)

\[ k_{ij} \] tensor of specific permeability \([L^2]\)

\[ \Lambda_B(ij)(T,C,S_r) \] tensor of heat conduction (soil) \([ML T^{-3} K^{-1}]\)

\[ m_i \] mass flow vector \([M \, L^{-2} T^{-1}]\)

\[ g \] gravitational acceleration \([L \, T^{-2}]\)

MOTIVATION

Because of the increased demand for water in most parts of the world, and the greater intensity of water use, issues of water quality in addition to those of quantity pose major limitations to the development of water resources. Although it appears that groundwater is buffered more against pollution than surface water, it is still subject to thermal, biological, and chemical pollution from environmental, domestic, industrial or agricultural sources. Due to the very small natural velocities, groundwater pollution usually only becomes evident a long time after contamination, and decontamination proves to be extremely difficult. To avoid or minimize deleterious effects on the environment and to optimize economic benefits, it is necessary to understand the spread of pollution in the aquifer. This knowledge, essential for developing a strategy for optimal groundwater quantity and quality management, is also an invaluable tool for tracing groundwater pollution to its source or for assessing the effectiveness of any measures to be taken against an imminent groundwater pollution at every stage of planning.
Fig. 1 shows the different steps in the development of a numerical model to calculate heat and mass (pollutant) transport in an aquifer. At each stage of development, certain requirements need to be met to ensure that the later applications of the model correspond with the original objectives. Strong feedback is a necessary feature, especially from the steps of verification and application, because experience may show that certain changes have to be made in the physical, mathematical or numerical part of the model.

**PHYSICAL MODEL**

Heat and mass transport in groundwater flow takes place by convection, mechanical dispersion, conduction and molecular diffusion, respectively. Figures 2(a), (b) and (c) show the parameters influencing the flow, temperature and concentration field, and also reflect the complex interactions and functionalities.

At this stage of planning, decisions are needed for the properties, relations and functionalities to be considered in the model. The present model is designed for a wide range of quality problems and not restricted to specific applications; all parameters and interactions indicated in Figs 2(a) - (c) need to be incorporated. This does not imply that all these options need to be exercised in every single calculation, but model flexibility is demanded to include those parameters or functionalities that are potentially important in specified cases.

**MATHEMATICAL MODEL**

Instead of dealing with the complex physical reality, a mathematical model, consisting of a system of equations which connects the parameters and variables, relevant to their physical meaning, is built by abstracting the process and introducing certain assumptions and simplifications. Obviously, the type of model depends heavily on the area of validity.

The physical process under consideration takes place in aquifers. An aquifer is a geological formation, or a group of formations, which contain water and permit the passage of significant amounts of water under ordinary field conditions. A confined aquifer is bounded both from above and below by impervious layers, whereas an unconfined aquifer consists of a saturated and an unsaturated zone, separated by the water table.

Traditionally, most of the groundwater flow and transport models cover only either the saturated (Segol et al., 1975; Stößinger, 1979) or the unsaturated (King & Norton, 1978) part of an aquifer or introduce the free surface as an artificial boundary, treating both parts separately (Lütkestratkötter, 1977; Pelka, 1980, 1981).

Groundwater flows in the saturated and unsaturated zones of an aquifer are closely coupled and this coupling is especially important in addressing problems of heat and mass transport. Many pollutants enter from the ground surface. After vertical passage to the water table they spread in the groundwater stream. Changes in groundwater temperature by injection of hot or cold water into the saturated
FIG. 2  (a) Flow and temperature field; (b) flow and concentration field; (c) concentration and temperature field.
zone interact with surface temperature and heat flow processes in
the unsaturated zone.

It becomes obvious that groundwater flow, mass transport and heat
flow in the saturated and unsaturated parts of a phreatic aquifer
must be viewed as a whole and should be described by a single
mathematical model.

The flow equation

Using assumptions for a continuous air phase at atmospheric pressure
in the unsaturated zone and negligible flow of water vapour, the
equation governing three-dimensional, time-dependent water movement
in a saturated-unsaturated porous medium can be derived from the
equation of mass conservation and the generalized Darcy's law:

$$\left( S_r S_0_p + n \frac{\partial S_r}{\partial p} \right) \frac{\partial p}{\partial t} + \frac{\partial}{\partial x_i} \left[ - \frac{\rho}{\mu} k_{ij} k_r \left( \frac{\partial P}{\partial x_j} + \rho g \frac{\partial z}{\partial x_j} \right) \right] = 0$$

The storage coefficient and the relative permeability depend on the
volumetric moisture content which can be expressed in terms of the
dependent variable p. Fluid density and dynamic viscosity are
functions of the temperature and concentration distribution.

The mass transport equation

Considering mixed saturated-unsaturated flow, the three-dimensional
spatial and temporal temperature distribution can be described by
the partial differential equation

$$\left( \rho n S_r \right) \frac{\partial C}{\partial t} + \frac{\partial}{\partial x_i} \left( \rho n_i C \right) - \frac{\partial}{\partial x_i} \left( \rho n S_r D_{C,ij} \frac{\partial C}{\partial x_j} \right) - f = 0$$

The first term describes the mass of solute stored in a balance
volume due to the changes of concentration with time. The second
term of the differential equation characterizes the transport by
convection and the third term represents the diffusive/dispersive
portion of the transport. The tensor of effective hydromechanical
dispersion combines the velocity dependent tensor of mechanical
dispersion and the molecular diffusion tensor

$$D_{C,ij} = D_{m,ij} D_r (S_r) + D_{d,ij} (T, S_r)$$

The heat transport equation

The heat transport equation proves to be similar to the mass
transport equation, but while the solute transport is assumed to take
place only in the pores of the matrix, heat conduction occurs in
the solid matrix as well

$$\left( \rho c_B \right) \frac{\partial T}{\partial t} + \frac{\partial}{\partial x_i} \left( \rho c_B \right) - \frac{\partial}{\partial x_i} \left( D_w, ij \frac{\partial T}{\partial x_j} \right) = 0$$
The first term describes the heat stored in a balance volume due to the temperature changes with time. The second term of the differential equation characterizes the heat transport by convection, and the third term represents the conductive/dispersive portion of the transport. The tensor of effective thermal dispersion $D_{w,ij}$ combines the velocity dependent tensor of mechanical dispersion and the effective heat conduction. Bulk density, bulk heat capacity and the effective heat conduction are functions of the volumetric moisture content:

$$D_{w,ij} = nS_r cD_m,ij D_r(S_r) + \Delta B,ij \Delta B,ij \Delta r(S_r)$$

The system of the three differential equations (1), (2), and (4) is a mathematical model which describes groundwater flow, heat and mass transport in saturated, unsaturated and mixed saturated-unsaturated zones of an aquifer.

**NUMERICAL MODEL**

Only a few analytical solutions have been found for diffusion-convection problems. All these solutions share the problem of including many simplifications necessary to obtain a solution. The soil and fluid parameters are assumed to be homogeneous, isotropic and constant in the area under consideration. The geometry of the area, the boundary conditions, and the velocity distribution must be simple, and hence, analytical solutions are not suitable for most practical problems.

One of the most powerful tools for solving diffusion-convection problems numerically is the finite element method. The final set of equations is coupled and highly nonlinear, requiring considerable care in generating the numerical solution. A linearization and decoupling is necessary in computation with a stable and a rapidly converging iterative algorithm. Due to the strong nonlinearities concerning the unsaturated zone, it is opportune to iterate within every time step instead of using time-coupled iterative schemes (Pelka, 1983a, b).

It is important to note that an accurate solution of the transport equations for saturated-unsaturated flow requires a rigorous description of velocity, especially in a continuous, mass conserving flow field (Pinder & Gray, 1977). This can be achieved either by employing a first order continuous basis function finite element scheme or by solving a three equation formulation. The present model is based on a generalized variational approach (Meissner, 1973) with independent basis functions defined for pressure and velocity to generate the essentially continuous flow field.

The conduction-convection and diffusion-convection equations, although now linearized, are not self-adjoint, due to the convective term and hence a variational principle does not exist. A solution is achieved by a weighted residual technique based on the Galerkin approach.

**PROGRAM, CODE**

The numerical model was programmed and coded in FORTRAN 77 (ANSI X3.9-
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1978) and implemented on CDC CYBER 175 and PRIME 250 equipment. Due to the complexity of the numerical solution it is absolutely necessary to start with a hierarchical decomposition of the problem and to conserve a corresponding structure in the program.

VERIFICATION

The results of the numerical model were in close agreement with solutions obtained by analytical methods. However, as an analytical solution is relevant to only a narrow range of conditions, numerous such solutions are needed to assess the performance of the numerical model for a wide scope of flow and transport problems. Moreover, it should be noted, that only a part of the mathematical-numerical model, numeric solution and code, can be checked in this way. Since the closed solution starts from the same, in many cases simplified, differential equation, a test of the mathematical-numerical model as a whole is not achieved.

In order to validate the physical, mathematical and numerical components of the overall model, the present model was tested against results of field experiments (Balke & Brenner, 1980; Balke, 1982). Figure 3 shows excellent agreement between observed and computed data for the temperature profile of an aquifer for two contrasting seasonal conditions.

APPLICATION

The mathematical model described here with its generalized structure and in avoiding simplifying and restricting assumptions associated with computation, offers potential application for a wide range of
flow, mass transport and heat transport problems. The flow region may be completely saturated or unsaturated as well as mixed saturated-unsaturated.

Salt water intrusion into coastal aquifers, invasion of brackish or polluted groundwater from adjacent aquifers, infiltration from sanitary landfills or polluted surface waters, artificial groundwater recharge, influences of hot or cold water injections from heat pumps or air conditioning, groundwater pollution caused by domestic or industrial accidents and infiltrating fertilizers or pesticides are only a part of an incomplete list of possible applications of the model.

REFERENCES


