5. MMOC2 - A NUMERICAL MODEL FOR WATER FLOW AND TRANSPORT IN VARIABLY SATURATED POROUS MEDIA

For the numerical simulation of flow and transport through a vertical cross-section of a heterogeneous soil, the combined flow and transport model described by Yeh et al. (1993) (henceforth referred to as "MMOC2") is used and modified for the purposes of this study. This chapter summarizes the main features of MMOC2 and the conceptual changes from the description in Yeh et al. (1993). For the details of MMOC2 the reader is referred to the original publication.

The numerical flow model solves the governing equation for two-dimensional flow in porous media, and handles saturated as well as unsaturated or partially saturated flow (Neuman, 1973):

$$\frac{\partial}{\partial x_i}\left(K_{ij}(h,\mathbf{x})\frac{\partial}{\partial x_j}(h+x_2)\right) = \left(C(h,\mathbf{x})+\beta_s S_s(\mathbf{x})\right)\frac{\partial h}{\partial t} - q_s \qquad \textbf{(5-1)}$$

where i,j = 1,2. x_1 and x_2 are the horizontal and vertical spatial coordinates, respectively, with x_2 pointing upward (see notation in previous chapters). $K_{ij}(h)$ is the hydraulic conductivity tensor, which reduces to an isotropic, spatially variable, single parameter $K(h,\mathbf{x})$ for all purposes of this study i.e., only locally isotropic phenomena are investigated. $K(h,\mathbf{x})$ is a function of the soil matric potential only under unsaturated conditions (see chapter 4) and it equals the saturated hydraulic conductivity $K_s(\mathbf{x})$ under saturated conditions. β_s is an index for saturation and is 0 under unsaturated conditions ($h < 0$) and 1 for saturated conditions $h \geq 0$. $C(h,\mathbf{x})$ is the soil water capacity function and $S_s(\mathbf{x})$ is the specific storage capacity of the saturated soil. The numerical solution of the flow equation - transient or steady-state ($\partial h/\partial t=0$) - is achieved through the Galerkin finite-element technique (FE) using triangular or rectangular elements. For this study, only rectangular elements are used, over which bilinear shape-functions are

defined. The nonlinear equations can be solved either by the Picard or by the Newton-Raphson technique. For the purpose of this study the Newton-Raphson method is chosen since it gives satisfactory results at high computational efficiency. The Picard scheme is not used in any applications of this study. The resulting linear matrix equation is solved through an incomplete LU-decomposition of the coefficient matrix as a preconditioner to the conjugate gradient method. Automatic time stepping is implemented for a more efficient handling of transient infiltration processes.

After the matric potential is found by solving (5-1), MMOC2 also solves Darcy's equation (4-2) by a Galerkin finite element method using the same bilinear shape functions as for the solution of the flow equation (5-1). The FE solution of Darcy's equation guarantees a continuous flux field $q(\mathbf{x})$ throughout the domain, which is advantageous when solving the transport equation.

Transport of solutes through porous media is governed by the advection-dispersion equation:

$$\frac{\partial}{\partial x_i}\left(D_{ij}\frac{\partial c}{\partial x_j}\right) - q_i\frac{\partial c}{\partial x_i} - \lambda R c = \theta R\frac{\partial c}{\partial t} \qquad \textbf{(5-2)}$$

for i,j=1,2. D_{ij} is the local dispersion tensor computed as a function of the local flux $q(\mathbf{x}) = (q_i(\mathbf{x})\, q_j(\mathbf{x}))^{1/2}$:

$$D_{ij} = (\alpha_L - \alpha_T)\frac{q_i q_j}{q} + \alpha_T q \delta_{ij} + D_0 \qquad \textbf{(5-3)}$$

α_L is the longitudinal dispersivity and α_T is the transverse dispersivity. δ_{ij}=1 for i=j, δ_{ij}=0 otherwise, is the Kronecker delta. D_0 is the apparent molecular diffusion. λ is a non-selective, first-order decay rate constant. R is the retardation coefficient and is related to the equilibrium sorption coefficient K_d by:

$$R = (1 + \rho_b K_d) \qquad \textbf{(5-4)}$$

The modified version of MMOC2 used for this study solves equation (5-2) by applying a one-step reverse particle tracking method to solve the advective part of (5-2) and a Galerkin finite element method to solve the dispersive transport (Neuman, 1984). The transport model described by Yeh et al. (1993) includes terms for kinetic adsorption and desorption processes, which have been omitted from this model version, since such processes have not been investigated in this study. Notice that in (5-4) a non-selective decay term has been added to the transport equation, not originally contained in the model by Yeh et. al (1993). The decay and the sorption partitioning terms are part of the advective transport formulation solved numerically by the particle tracking method described in Yeh et al. (1993).

This version of MMOC2 also changes an option affecting the particle tracking near boundaries: Unlike described by Yeh et al. (1993) the backward particle tracking algorithm assumes that particles at no-flow boundaries are *not* reflected back into the domain, since the applications in this study never use a no-flow boundary specifically to simulate a symmetry boundary. Only under the symmetry-assumption is a reflection of particles at no-flow boundaries justified. Finally, for reasons of both accuracy and efficiency, the time-step in the transport simulation is selected such that the displacement $\Delta\mathbf{X} = |\mathbf{v}\Delta t|$ of each particle per time-step is at the most the distance between two nodes $\Delta\mathbf{x}$, i.e. the Courant number $\Delta\mathbf{X}/\Delta\mathbf{x}$ is always smaller than 1.

The model has been tested for a wide range of boundary and initial conditions by Yeh et al. (1993). Local dispersion in all applications of this study is presumed to be on the order of 1/10 to 1/100 of the element-length. Such a small dispersion is sufficiently well reproduced by simply relying on numerical dispersion and setting the input dispersion coefficient to zero. Calculation of the dispersive terms in equation (5-2) is computationally very expensive. Solving the advective transport equation only, and using numerical dispersion *in lieu* of solving the dispersion equation in (5-2), saves a considerable amount of computation time in Monte

Carlo simulations. However, the exact amount of numerical dispersion varies both with velocity and from location to location and cannot be exactly quantified. While local dispersion plays an important role in spreading an initially small contamination plume, the macrodispersion or overall spreading of the contamination plume in most of this study's applications is several orders of magnitudes larger than the spreading due to numerical dispersion or otherwise specified local dispersion. The spreading of a plume in heterogeneous media is predominantly controlled by the heterogeneities in the soil. Hence, while the existence of local dispersion is important, its exact amount is relatively insignificant if it has an upper bound that is comparable to the actual local dispersion desired. Figure 5.1 shows an application of MMOC2 to a hypothetical contamination problem in a heterogeneous soil. The finite elements are squares with a side-length of 10 cm. The first simulation omitted the computation of the dispersive portion in equation (5-2). In the other simulations shown, the local dispersivities were assumed to be isotropic. Simulations with dispersivities of 0.001 cm, 0.01 cm, 0.1 cm, and 1 cm were implemented, and it is obvious that only local dispersivities of 0.1 cm or 1/100 of the element-length and larger disperse the plume stronger than numerical dispersion alone. From several such experiments it is found that the empirical, numerical dispersivity in simulations of transport through heterogeneous soils is on the order of 1/10 to 1/100 of the element size. In most applications in this study the element size varies between 10 cm and 30 cm. Hence, the numerical dispersion is equivalent to a local dispersivity on the order of 1 mm to 1 cm, which is realistic for many soils. This justifies the use of particle tracking alone to solve (5-2).