Problems with large-scale modelling of salt water intrusion in 3D

G.H.P. Oude Essink and R.H. Boekelman
e-mail: g.oude.essink@ct.tudelft.nl and r.boekelman@ct.tudelft.nl
Delft University of Technology, Faculty of Civil Engineering,
Hydrology & Ecology Group, P.O. Box 5048, 2600 GA Delft, the Netherlands

Abstract

In this paper, the restrictions of three-dimensional (3D) modelling of salt water intrusion in large-scale coastal (homogeneous) aquifers are discussed. Computer codes, of which the solution of the advection-dispersion equation is based on standard finite element or finite difference techniques, cannot yet be applied to model large-scale coastal aquifers. The reason is that these codes must satisfy a condition of spatial discretization, characterized by the so-called grid Peclet number. This number imposes that the dimension of the grid block should be not greater than a few times the magnitude of the longitudinal dispersivity, as otherwise numerical dispersion will occur. In addition, stand-alone personal computers are not yet fast enough to execute models with several hundreds of thousands of grid blocks. Finally, reliable and sufficient groundwater data, required for calibration and verification, are not available in most cases. In conclusion, 3D-modelling of salt water intrusion in large-scale coastal aquifers is technically possible within some years, though the availability of data will always restrict practical applications to a certain extent.

1. Introduction

In this keynote-paper, the following topics should be discussed: intrusion of seawater, basic theories, analytical approaches, hydrodynamics, steady-unsteady state solutions, and finally, mathematical modelling. It is, however, not possible to treat all these topics within a concise paper. Therefore, only one topic, which is becoming more and more relevant, is discussed extensively: *problems with three-dimensional modelling of salt water intrusion in large-scale coastal aquifers*. Large-scale coastal aquifers are defined here as aquifer systems along the coast of several tens to a few hundreds of square kilometres. In these systems, mostly non-uniform density distributions occur.

Developments in modelling are mainly caused by the (still ongoing) breakthroughs in computation technologies and the increased possibilities of personal computers. The devices and tools, such as sophisticated graphical modules, pre- and postprocessors, are already available on the market. Now, knowledge on and experience with 3D-modelling must follow. In addition, many geo(hydro)logic events in coastal aquifers where mostly non-uniform density distributions occur should nowadays be simulated more accurately than they have been simulated up to now. For instance, the effect of different deep-well infiltration scenarios or the salinisation of fresh groundwater resources due to overpumping should not be simulated anymore with only (3D) sharp interface models or 2D solute transport models. Instead, 3D-modelling of salt water intrusion, which is based on density dependent groundwater flow and solute transport, is required.

Some people may think that around the turn of the millennium, the possibility to model, to simulate and to visualise 3D flow of groundwater and 3D transport of salt and other hydrochemical constituents is common practice. However, the near future is probably less favourable, because, in practice, 3D-modelling of salt water intrusion in large-scale coastal aquifers is restricted. In this paper, aspects of the three most important restrictions are discussed. First of all, in order to suppress *numerical dispersion*, which occurs in solutions techniques with the standard finite element method (fem) and the standard finite difference method (fdm), the dimension of the grid block must be small. This means that large-scale geometries can only be modelled with an enormous amount of grid blocks. Second, 3D-modelling of large-scale geometries is restricted by the memory allocation and the speed of the computer: this is called the *computer problem*[1]. Third, there is the *data availability problem*, as 3D-modelling requires a large amount of data sets for calibration and verification, whereas reliable data sets are, in practice, rare.

[1]Note that we are talking about the problems for geo(hydro)logists in daily practice. This means that personal computers are in question instead of (fast) workstations, supercomputers or even Cray computers.

In section 2, different types of salt water intrusion models are discussed. In section 3, the mathematical formulation of salt water intrusion is given by means of the solute transport equation. In section 4, some solution techniques are summarized. In section 5, some 3D salt water intrusion models are shortly discussed. Then, the discussion follows on the three problems: the numerical dispersion problem in section 6; the computer problem in section 7; and the data availability problem in section 8. Finally, some conclusions are drawn.

2. Types of salt water intrusion models

In the past, the behaviour of density dependent groundwater flow has been investigated by means of analogue models as well as by means of analytical models. However, since computers appeared on the scene, mathematical models[2] gained ground. At present, a large number of mathematical models is available, capable of handling fresh and saline groundwater flow in aquifer systems. The U.S. Geological Survey is the leading institute in developing 2D and 3D groundwater flow models. Important distributors of affordable computer codes are, among others, the International Ground Water Modeling Center [IGWMC: Golden, U.S.A., 1995] and the Scientific Software Group, Washington D.C., U.S.A. [1995]. Reviews of literature on fresh and saline groundwater and available computer codes and models are given in e.g. Reilly & Goodman [1985], Custodio *et al.* [1987], Strack [1989] and Maidment [1993]. Obviously, all preceding SWIM-proceedings comprise a large number of case studies with different kinds of models.

2.1 Two-dimensional versus three-dimensional models

Two-dimensional groundwater flow models, which also simulate solute transport, require quite some effort before they are completely understood. Although they can be applied in various situations, the practical application is rather limited. The most important restriction of these models is obviously that only cross-sections can be simulated. Therefore, a proper cross-section should be carefully selected.

In many cases, however, groundwater flow perpendicular to the coastline is disturbed in such a way that the schematisation and modelling of the actual situation by a cross-section cannot be allowed any more. Such situations occur for instance in polder areas where the controlled phreatic groundwater levels lead to radial flow patterns, at areas with complex geohydrologic geometries or in the vicinity of singular wells where groundwater is extracted or infiltrated. Under those circumstances, 3D-models should be applied to simulate density dependent groundwater flow. Obviously, 3D-models naturally require even more effort to be understood, implemented and utilised effectively than 2D-models. For instance, the problems that arise to visualise 3D groundwater flow and solute transport on a 2D (color) monitor should not be underestimated. Moreover, the *numerical dispersion problem* will also restrict the practical application of 3D salt water intrusion models (see section 7 for further discussion). The application of these 3D-models on a broad scale is still at an early stage of development.

2.2 Sharp interface model versus solute transport model

Sharp interface models are based on the assumption that a sharp interface between fresh and saline groundwater represents the actual situation. This is the well-known *Badon Ghyben-Herzberg principle*. The straightforward sharp interface models can be applied as an educational means to gain a clear insight in the behaviour of fresh and saline groundwater in coastal aquifer systems. As such, sharp interface models are still widely applied, which can be deduced from many papers, presented during the preceding Salt Water Intrusion Meetings. Nevertheless, restrictions on the applicability of the principle should be considered:

a. First, the principle only approximates the actual occurrence of fresh, brackish and saline groundwater in the subsoil. In fact, the brackish zone between fresh and saline groundwater should only be schematised by a sharp interface when the maximum thickness of the brackish zone is in the order of several metres only. This condition applies only in rare situations where the freshwater lens is evolved by natural recharge, as occurs in sand-dune areas or in (coral) islands.

[2] *"A mathematical model simulates groundwater flow indirectly by means of a governing equation ··· to represent the physical processes that occur in the system."* [Anderson & Woessner, 1992].

b. Second, the principle assumes a hydrostatic equilibrium, whereas in reality the aquifer system might considerably deviate from this equilibrium situation. In those cases, e.g. in freshwater bodies near the shoreline, the Badon Ghyben-Herzberg principle should not be applied, because the computed position of the sharp interface significantly deviates from the actual position as the coast is approached.

In many coastal aquifer systems, a relatively broad transition zone between fresh, brackish and saline groundwater is present because of various processes during geological history. In addition, the transition zone is also increasing as a result of the circulation of brackish water due to inflow of saline groundwater, the tidal regime and human activities, such as (artificial) recharge and groundwater extraction at high and variable rates. Under such conditions, more sophisticated models are required than just models with expressions for sharp interfaces: namely models which take into account variable densities. In this paper, these models are referred to as *solute transport models* or *salt water intrusion models*. They apply the advection-dispersion equation to convert solute concentration (or total dissolved solids) to density. They are able to simulate, among others, changes in solute concentration (e.g. near pumping wells due to upconing), changes in volumes of freshwater in sand-dune areas and changes in the salinity of seepage in low-lying polder areas. As solute transport models usually apply numerical schemes, they can also be utilized to simulate aquifer systems with complex geohydrologic geometries and inversions of fresh and saline groundwater.

3. Mathematical formulation of solute transport

The three-dimensional equation for solute transport in homogeneous isotropic porous media can be written as follows:

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x_i}(D_{ij}\frac{\partial C}{\partial x_j}) - \frac{\partial}{\partial x_i}(C\,V_i) + \frac{(C - C')\,W}{n_e} + \frac{\Psi}{n_e} \qquad (1)$$

where

- C = concentration of the dissolved solutes ($M\,L^{-3}$),
- t = time (T),
- D_{ij} = coefficient of hydrodynamic dispersion (see section 6) ($L^2\,T^{-1}$),
- $V_i = q_i/n_e$ = effective velocity of the groundwater in the direction of x_i ($L\,T^{-1}$),
- C' = concentration of the dissolved solutes in a source or sink ($M\,L^{-3}$),
- $W(x,y,z,t)$ = general term for sources and sinks (T^{-1}),
- n_e = effective porosity of the medium ($-$),
- Ψ = chemical reaction source or sink per unit volume ($M\,L^{-3}\,T^{-1}$). It includes equilibrium-controlled sorption or exchange and first-order irreversible rate (radioactive decay) reactions.

Equation 1 is called the *solute transport equation*, the *advection-dispersion equation* or the *transport-dispersion equation*. The first term on the right hand side represents the change in concentration of solutes due to hydrodynamic dispersion. The second term represents the effect of advective transport which is the movement of solutes attributed to transport by flowing groundwater. The third term represents the contribution and removal of solutes due to fluid sources and sinks, whereas the fourth term represents chemical reactions. With regard to the transport of a conservative solute, viz. salt, Ψ is assumed to be equal to zero.

4. Solution techniques

Various solution techniques have been developed to solve both the groundwater flow equation and the (complicated) solute transport equation. Computer codes with suitable solution techniques are already available since at least two decades. In this paper, some solution techniques will be mentioned briefly:

- Analogue method
  Analogue models have been applied to investigate the behaviour of density dependent groundwater. Analogue models are based on the fact that several physical processes are governed by equations that are similar to the equations of groundwater flow. As such, these processes are analogous with groundwater flow. If such a process can easily be realized and measured, it can be applied to study groundwater flow in a specific situation through interpretation and translation of the physical constants towards groundwater flow constants. Unfortunately, in most cases analogue models cannot be applied for simulating the movement of contaminants in groundwater. Well-known analogues are the Hele Shaw model, the membrane model, the thermal model and the electric model.

- Analytical method
  Analytical models[3] are based on (e.g. Laplace) transformations and the hodograph method (by means of conformal mapping). In addition, an effective approach was to derive analytical formulas from analogous physical processes. The similarity between groundwater flow and conduction of heat in solids appeared to be very convenient [e.g. Carslaw & Jaeger, 1959]. In this physical process, several analytical solutions are similar to those for groundwater flow in aquifers. The application of analytical models is limited as analytical solutions are only available for relatively simple problems (e.g. homogeneous aquifers, 1D or 2D, steady-state, sharp interface). Unfortunately, analytical solutions are very rarely available for problems with density dependent groundwater flow, of which the solute transport is governed by means of the advection-dispersion equation. Such a rare case is Henry's problem [1964], where saline water intrudes in a hypothetical rectangular aquifer and merges by a constant dispersion coefficient. Henry's case is a benchmark for 2D groundwater flow models that can simulate solute transport and density flow [Segol, 1994][4].

- Analytical element method
  This method is based on the theory of Strack [1989]. Analytical solutions are determined for head and discharge that satisfy the governing flow equations and specified boundary conditions within the aquifer. The most important advantage over conventional numerical methods is its lack of a fixed grid. As such, it is possible to extend the model any distance to incorporate regional features without sacrificing accuracy in the area of interest. Moreover, refinement of the discretization and zooming into a local problem can easily be accomplished.

- Finite difference method (fdm)
  This well-known method is one of the oldest and most widely used methods. It is based of the Taylor series expansions in order to determine approximations of the first and the second derivatives of the parameter in question. This method is not often used for solving the advection-dispersion equation because numerical dispersion can easily develop in the finite difference scheme[5]. For more information, see Konikow & Bredehoeft [1978]; and Kinzelbach [1987a].

- Finite element method (fem)
  This numerical method (already applied in the early 1950's to problems of solid mechanics) is a very well-known method to solve the governing partial differential equations. An advantage of this method is that it is easier to change a finite element grid than a finite difference grid, because the nodes can be added very easily in the finite element grid without redesigning the entire grid. As such, a fem is preferred to a fdm, if the exact representation of the boundaries is important. It goes beyond the scope of this paper to describe this method, however, relevant information can be found in Zienkiewicz [1971]; Pinder & Gray [1977]; Kinzelbach [1987a] and Bear & Verruijt [1987].

- Method of characteristics
  This method can be applied in salt water intrusion problems to solve the (hyperbolic) advection-

[3] Also the vortex theory has an analytic character. It solves groundwater flow in combination with a sharp interface.

[4] It appears that currently no method has succeeded in reproducing Henry's steady state solution. Henry solved the equations with the Galerkin technique by using Fourier series. The inaccuracies of Henry's results are probably a consequence of the limited computer facilities at the time [Segol, 1994].

[5] There appear to be (five point) finite difference schemes which also take into account the second order approximation. As such, numerical dispersion and oscillations do not occur.

dispersion equation for groundwater flow. By decoupling the advective and the dispersive component of the equation, and solving them sequentially, numerical dispersion can be suppressed to a large extent. Moving points are introduced in this method, namely particles, that can be traced through the flow field within the stationary coordinates of the finite difference grid. This process is called *particle tracking*. For more information, see Garder, Peaceman & Pozzi [1964]; Konikow & Bredehoeft [1978]; and Kinzelbach [1987a, 1987b].

- Random walk method
  The random walk method also uses the particle tracking method. Each particle represents a fixed mass of pollutant. Both the advective and the dispersive transport are represented by particle movements. The first step in the procedure is to follow particles along the direction of the flow field while the second step consists of adding a random movement by means of statistical properties in order to take into account the dispersive transport. Only the superposition of the particle paths and the counting of mass reveals the concentrations in each grid cell of the overlain grid. The random walk method can be used to simulate groundwater contaminant transport at great Peclet numbers (see section 6.1). An advantage of this method is that particles are only introduced where contaminants are present. For more information, see Kinzelbach [1987a, 1987b]; and Uffink [1990].

It appears that most of the salt water intrusion models are based on the fem or the fdm. At present, however, the method of characteristics and the random walk method come to the front. These methods can more easily simulate the flow of groundwater in combination with the (complicated) transport of solutes without (numerical) dispersion problems (this problem will be discussed in section 6).

5. Three-dimensional salt water intrusion models

There are already quite a few 3D computer codes available which can cope with salt water intrusion in coastal aquifers. Here, a selection of some codes is given:

- HST3D [Kipp, 1986] is a 3D finite difference code that can simulate heat and solute transport. Ossenkoppele [1993] showed that modelling the sand-dune area of Amsterdam Waterworks along the Dutch coast (dimensions: 12,000 · 20,000 m^2 by 160 m) with HST3D appeared to be rather complicated. Large dispersivities (e.g. α_L=200 m) had to be applied as otherwise the solute transport equation does not converge to a solution. As a consequence of simulations with great dispersivities, excessive hydrodynamic dispersion created extensive and unrealistic brackish zones which do not agree with the actual situation.

- SWICHA [Huyakorn *et al.*, 1987; Lester, 1991] is a 3D finite element code. It can simulate variable density fluid flow and solute transport processes in saturated porous media. The applications range from simple one-dimensional to complex three-dimensional, coupled flow and solute transport. The groundwater flow and solute equations are solved by the Galerkin technique. An implicit Picard iterative scheme is applied to treat the nonlinearity of the problems. For a transient solution of the seawater intrusion problem, the Crank-Nicholson time step scheme is applied to handle the temporal discretization. Spatial discretization is performed using rectangular or triangular elements. The solute transport equation may not converge to a solution, if a so-called *critical Peclet number* is exceeded in a grid block. In order to solve this problem, SWICHA offers a trick at the user's option: numerical dispersion (the so-called *artificial dispersion*) is added to the solute transport equation matrix. Then, spatial oscillations are suppressed and the critical Peclet number is no longer exceeded in that grid block. Subsequently, the solution will converge. It appears that convergence difficulties especially occur when small dispersivities are used, unless: (1) a lot of artificial dispersion is added to the matrix (then, the overall dispersion is great again), or (2) the grid is refined to avoid local numerical oscillations which come with the Galerkin technique.

- METROPOL [Sauter *et al.*, 1993] (**ME**thod for the **TR**ansport **O**f **POL**lutants) simulates 3D groundwater flow with varying density and simultaneous transport of contaminants. It is based on the finite element method. METROPOL is developed by the Dutch National Institute of Public

Health and Environmental Protection RIVM. It has been applied to simulate safety assessments of the geological disposal of radionuclear waste in (high-brine) salt formations.

- MVAEM [Strack, 1995] is the analytical element model MLAEM which has recently been extended with a variable density module. MVAEM is now able to calculate the 3D-water pressure distribution, on condition that the 3D-density distribution within an aquifer is given. De Lange [1996] has applied the analytical element method to develop the NAtional GRoundwater Model (NAGROM) for density dependent aquifer systems in the Netherlands. Note that, at present, MVAEM has some drawbacks. First, it is not (yet) possible to simulate hydrodynamic dispersion and anisotropy. Second, it is still a steady-state model for the simulation of density-dependent groundwater flow. The displacement of the points with densities through the known velocity distributions is not solved yet. As such, salt water intrusion as a function of time can not be simulated. Third, it appears that the so-called multiquadric-biharmonic interpolator, which is used to provide the initial 3D-density distribution within an aquifer (by means of two parameters (Δ and h_{scale})) and to control the smoothness and the spatial behaviour of the distribution, may not be robust enough to produce reliable 3D-density distribution under all circumstances [van Gerven & de Lange, 1994].

- SWIFT [Ward, 1991] (**S**andia **W**aste-**I**solation **F**low and **T**ransport model) is a 3D-model to simulate groundwater flow, heat (energy), brine and radionuclide transport in porous and fractured media [Maidment, 1993]. The equations for flow, heat and brine are coupled by fluid density, viscosity and porosity. The equations are solved by the finite difference method.

6. The numerical dispersion problem

Numerical approximations of the derivatives of the nonlinear solute transport equation may introduce *truncation errors* and *oscillation errors* (see figure 1). As such, these errors limit the techniques that solve the partial differential equation. The truncation error has the appearance of an additional dispersion-like term, the so-called *numerical dispersion*, which may dominate the numerical accuracy of the solution. *Oscillations* may occur in the solution of the solute transport equation as a result of over and undershooting of the solute concentration values. If the oscillation reaches unacceptable values, the solution may even become unstable.

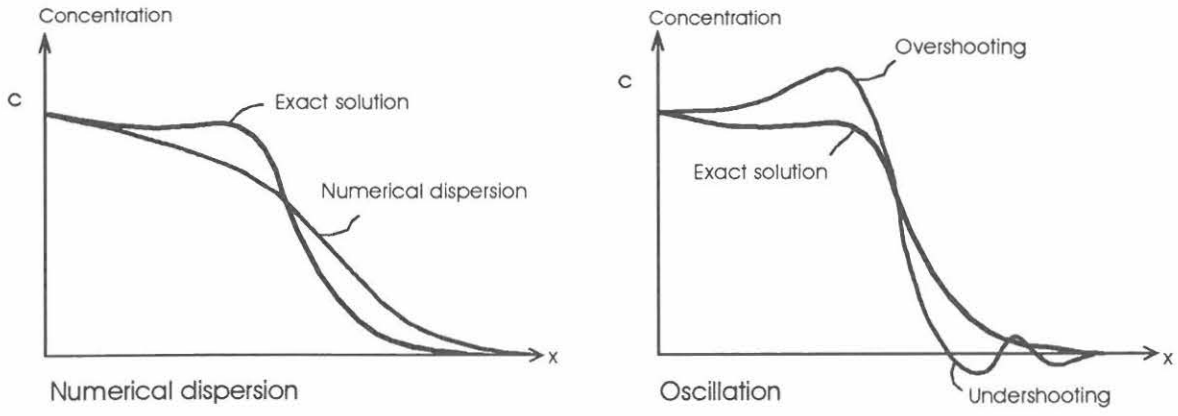

Figure 1: Schematisation of numerical dispersion and oscillation.

There is a close relation between numerical accuracy (numerical dispersion) and stability (oscillation) [Peaceman, 1977; Pinder & Gray, 1977]. In fact, numerical dispersion acts to stabilize the solution of the solute transport equation. Numerical dispersion spreads the sharp front by generating a solution which applies a greater dispersion than the hydrodynamic dispersion. In order to suppress the numerical dispersion, the numerical scheme (spatial as well as temporal) can be adapted. Meanwhile, this scheme may lead to over and undershooting, and subsequently, oscillation may be amplified. For these reasons,

the discretization scheme should be chosen carefully in order to control both numerical accuracy and stability. In this paper, the interest is focussed on the spatial discretization which is largely responsible for the numerical dispersion.

6.1 Analysis of the truncation error

In order to quantify numerical accuracy, an *eigenvalue analysis* of the advection-dispersion equation should be performed[6]. Such an analysis will demonstrate the importance of the dimension of the grid block [see e.g. Frind & Pinder, 1983]. Which of the terms of the advection-dispersion equation is more dominant depends on the relative size of the advective and dispersive fluxes at the level of the discretization element [Kinzelbach, 1987a]. The grid Peclet number can be applied to assess the most dominant process. For small grid Peclet numbers ($Pe_{grid} < 1$) the dispersive fluxes (viz. the parabolic nature of the advection-dispersion equation) prevails, whereas for great grid Peclet numbers ($Pe_{grid} > 2$) the advective fluxes (the hyperbolic nature) dominates. In field problems, advective transport of solute mostly dominates over dispersive transport. Numerical solving (by means of standard fem and fdm) of an equation with a hyperbolic nature is more difficult than solving an equation with a parabolic nature.

A one-dimensional schematisation of the standard advection-dispersion equation is often applied to demonstrate, in case of the finite difference method[7], in a simple way the principle of assessing truncation errors [e.g. Bear & Verruijt, 1987]. Approximations of the first-order derivatives generate errors in the order of magnitude of the second-order derivatives. This is shown by using Taylor series expansions [e.g. Lantz, 1971; INTERCOMP, 1976; Bear & Verruijt, 1987]. The truncation errors depend on the chosen numerical approximation scheme (e.g. backward, central or forward difference in space and time). For the analysis of the truncation error, the so-called *grid Peclet number* Pe_{grid} is defined:

$$Pe_{grid} = \left| \frac{V \Delta x}{D_h} \right| \tag{2}$$

where

- Pe_{grid} = grid Peclet number $(-)$,
- V = effective velocity of groundwater $(L\,T^{-1})$,
- Δx = dimension of the grid block (L),
- D_h = hydrodynamic dispersion $(L^2\,T^{-1})$.

Grid Peclet numbers (and Courant numbers[8]) have been mentioned in various quantitative descriptions. Whether or not the numerical dispersion is suppressed, depends on the discretization technique applied [e.g. Jensen & Finlayson, 1978; Voss & Souza, 1987]. In summary, it appears that in order to obtain real and distinct eigenvalues, the spatial discretization should meet the condition [Daus *et al.*, 1985]:

$Pe_{grid} \leq 2$	Finite difference algorithm, central in space	
$Pe_{grid} \leq 2$	Finite element algorithm, linear basic functions	
$Pe_{grid} \leq 4$	Finite element algorithm, quadratic basic functions	(3)

The solution of the advection-dispersion equation is faced with difficulties, since models based on the standard fem and fdm may yield unreliable results if the spatial discretization conditions are not met. Both widely used methods have in common that they produce poor results at great (grid) Peclet numbers. As such, it is peculiar that this well-known fact does not have a broader attention in numerical modelling practices of groundwater contaminant transport [Uffink, 1990].

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[6] In addition, a stability analysis should determine the stability condition [e.g. Peaceman, 1977].

[7] The analysis of (truncation and oscillation) errors caused by numerical dispersion and oscillation by means of central finite difference approximations for the fdm is similar for the fem [Pinder & Gray, 1977; Kinzelbach, 1987a].

[8] The Courant condition Co, $\frac{V \Delta t}{\Delta x}$, is physically interpreted as the ratio of the advective transport distance during one time step to the spatial discretization.

6.2 The dispersion coefficient

Hydrodynamic dispersion D_h is defined as the combined effect of two processes, mechanical dispersion and molecular diffusion:

$$D_h = D_m + D_d \tag{4}$$

where

- D_m $(L^2\,T^{-1})$ = mechanical (or convective) dispersion coefficient. This process is caused by velocity variations at the microscopic scale. The spreading depends on both fluid flow and the characteristics of the pore system through which the flow takes place,
- D_d $(L^2\,T^{-1})$ = molecular diffusion coefficient. This process is caused by the random movement of molecules in a fluid and depends on concentration gradients, the properties of the fluid and the soil.

Under normal groundwater flow conditions, molecular diffusion is of marginal importance with respect to mechanical dispersion. The subdivision of the hydrodynamic dispersion into mechanical dispersion and molecular diffusion is artificial. The mechanical dispersion coefficient, which is a second-rank symmetrical tensor, can be defined for an isotropic aquifer in terms of two constants:

$$\begin{aligned} D_L &= \alpha_L\,|V| \\ D_T &= \alpha_T\,|V| \end{aligned} \tag{5}$$

where

- α_L = longitudinal dispersivity of the aquifer (L),
- α_T = transversal dispersivity of the aquifer (L).

The exact determination of the hydrodynamic dispersion is very difficult, if not impossible, as it depends on many features (e.g. scale effect, fingering, transient effects [Anderson & Woessner, 1992]). In fact, the more one knows about the hydraulic conductivity and porosity distribution, and subsequently, the exact velocity distribution, the more the hydrodynamic dispersion value will converge to the value of molecular diffusion. As such, one should model the heterogeneous and anisotropic medium as accurately as possible. However, as it is not possible to determine the exact hydraulic conductivity distribution as well as the velocity distribution, the exact value of the dispersion coefficient can not be given. For this reason, the mechanical dispersion, which is inserted in the model, may (somewhat) be increased to take into account these uncertainties in the subsoil parameters. The less one knows, the higher the model dispersivities must be.

Gelhar *et al.* [1992] reviewed 59 different field sites in order to classify the dispersivity data into three reliability classes. The representative scale of the cases ranges from 10^{-1} to 10^{5} m. They found that for these cases, the longitudinal dispersivity ranges from 10^{-2} to 10^{4} m. In conclusion, the variation in dispersivity reflects the influence of different degrees of aquifer heterogeneity at different field sites. They concluded that in general, longitudinal dispersivities in the lower part of the indicated range are more likely to be realistic for field applications. Therefore, the so-called *scale-dependency* of dispersivities ($\alpha_L = 0.1\,L$, where L is the traveled distance of the contaminant), determined from field data, should be reviewed critically. Furthermore, they indicated that there is a need for long-term, very large-scale experiments extending to several kilometres.

In contrast with some field sites in especially the U.S.A. (see, e.g., the cases in Gelhar *et al.*, 1992), the best estimates of the longitudinal dispersivities in Dutch and Belgian large-scale aquifer systems with Holocene and Pleistocene deposits of marine and fluviatile origin appear to yield rather small values. This observation is based on various case studies, such as Lebbe [1983], Kooiman *et al.* [1986], Stuyfzand [1991]; Walraevens *et al.* [1993]; and Oude Essink [1993]. For instance, computations have indicated that if a great hydrodynamic dispersion (that means great dispersivities) is simulated during long simulation times, unrealistic solutions are generated [Oude Essink, 1996]. In figure 2, the effect of the longitudinal dispersivity α_L is evaluated by comparing the results of simulations with four different

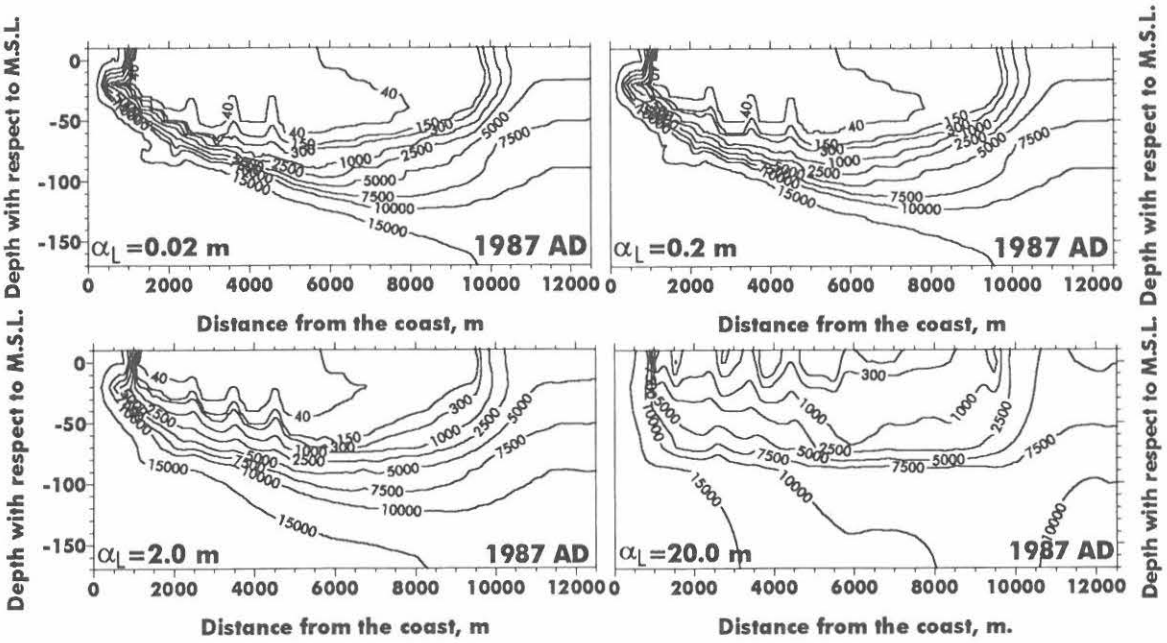

Figure 2: Chloride distributions (in $mg\ Cl^-/l$) in 1987 in a cross-section of the sand-dune area of Amsterdam Waterworks, the Netherlands, calculated with MOC [Konikow & Bredehoeft, 1978] (adapted for density differences to model vertical cross-sections [Oude Essink, 1996]) for four different longitudinal dispersivities: α_L=0.02 m, α_L=0.2 m, α_L=2.0 m and α_L=20.0 m. A thick freshwater lens is only simulated for small dispersivities.

values of α_L: 0.02 m, 0.2 m, 2.0 m and 20.0 m. The chloride distributions of the cross-section are given after a simulation time of 134 years: from 1854 till the end of 1987. The cross-section is situated in a sand-dune area along the Dutch coast where a freshwater lens has been formed. The calculated chloride distribution matches the observed distribution best if small longitudinal dispersivities are applied, namely α_L=0.02 m and α_L=0.2 m. By contrast, the case with α_L=2.0 m shows a freshwater lens that is too thin, whereas the case with α_L=20.0 m does not simulate a freshwater lens any more: the aquifer system only consists of a large brackish zone. This situation does not occur in reality.

6.3 The dimension of the grid block

If mechanical dispersion dominates over molecular diffusion, the hydrodynamic dispersion D_h in equation 2 can be expressed as $D_h=\alpha_L\,|V|$, and thus, equation 3 becomes:

$$\begin{aligned} \Delta x &\leq 2\,\alpha_L \quad && \text{Finite difference algorithm, central in space} \\ \Delta x &\leq 2\,\alpha_L \quad && \text{Finite element algorithm, linear basic functions} \\ \Delta x &\leq 4\,\alpha_L \quad && \text{Finite element algorithm, quadratic basic functions} \end{aligned} \tag{6}$$

Note that there are acceptable solutions obtained with values up to $\Delta x < 10\,\alpha_L$[9]. As such, this restriction is not very compulsory. Under those circumstances, the solution can still be satisfactory though in some places over and undershooting (viz. oscillation) may occur.

From the formulations in equation 6 can be deduced that the application to model salt water intrusion in large-scale coastal aquifers is restricted for 3D computer codes which are based on the standard fdm and fem (see figure 3). Because, as a matter of fact, the restriction means that the dimension of the grid block may not be larger than four times the magnitude of the longitudinal dispersivity. Unfortunately, the longitudinal dispersivity is for many aquifer systems in the order of (at maximum) metres, and thus the dimension of the grid block should also be in the order of (tens) of metres. Consequently, a very large number of grid blocks is necessary to model large-scale areas of various square kilometres. For the

[9]Sudicky [1989] even obtained highly accurate solutions for grid Peclet numbers in excess of 30 for the finite element method, based on a Laplace transformation of the temporal derivatives.

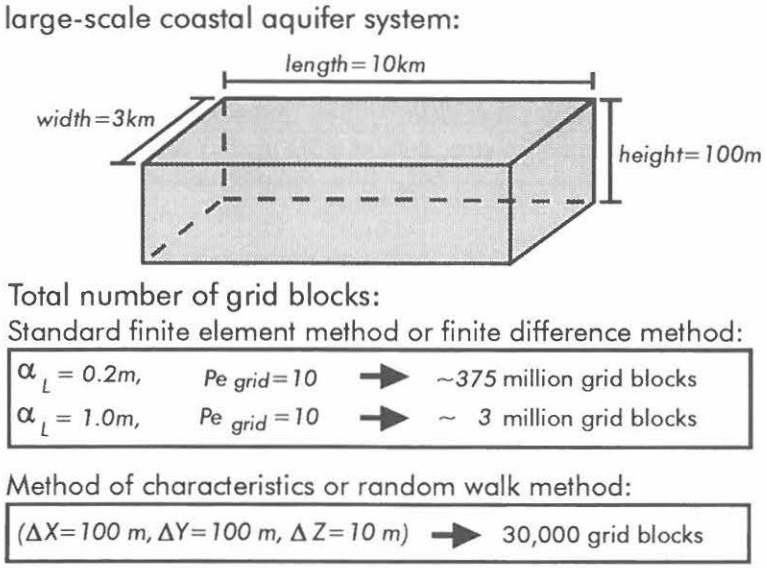

Figure 3: Effect of the longitudinal dispersivity α_L on the total number of grid blocks which are required to simulate a large-scale coastal aquifer by means of a model based on the standard finite element or finite difference method and a model based on the method of characteristics or the random walk method (viz. no effect of α_L !).

time being, the allowed number of grid blocks is restricted by computer memory capacity and execution time. In conclusion, when standard fdm and fem are applied, 3D-modelling of salt water intrusion of coastal aquifer systems is, for the time being, only possible on the scale of small geometries, such as small islands.

6.4 Remedy for the numerical dispersion problem

To avoid the numerical dispersion problems associated with standard finite element and finite difference solutions of the advection-dispersion equations, particle tracking solutions should be used, such as the method of characteristics (particle tracking for advection with a finite difference solution of the dispersion part) or the random walk method (to reproduce a Gaussian distribution of particles to simulate dispersion). As such, we think that an interconnected model of the well-known MODFLOW [McDonald & Harbaugh, 1984] and MT3D [Zheng, 1990] can avoid the numerical dispersion problem (see figure 3). MODFLOW is the most widely used groundwater flow model in the world. A recently (1994) released model is the modular 3D transport model called MT3D that is completely compatible with MODFLOW. MT3D applies the method of characteristics, the modified method of characteristics or a hybrid of these two methods. It is developed to simulate solute transport[10] without the complications of heat and density effects. However, the combined model can be made suitable for simulating density dependent groundwater flow by adapting the original model of MODFLOW with an additional term to the vertical Darcian specific discharge in the groundwater flow equation, the so-called *buoyancy* or *vertical density gradient velocity*. This adaption has already been executed with success for the 2D-model MOC [Lebbe, 1983; Oude Essink, 1996]. Schaars [1996] already adapted MODFLOW for density differences by converting, with the help of the MATLAB (a package that is able to manipulate and present matrices), the standard subsoil parameters to density dependent subsoil parameters (based on an article of Maas & Emke [1989]). At present, that model still steady-state, thus salt water intrusion as a function of time cannot yet be simulated.

In addition, research is taken place to develop more effective solution techniques based on the finite element method with the purpose to reduce numerical dispersion [Sudicky, 1989; Esch, van, personal communication, 1996].

[10]Note that MT3D is not free of errors: it appears that the error in the solute mass balance is not yet of minor importance.

7. The computer problem

Until some years ago, 3D-modelling of salt water intrusion in large-scale coastal aquifers was not really possible due to shortcomings in computer possibilities[11]. Two major reasons restricting the application are the memory problem (limited memory to store data of a 3D-model) and the speed problem (limited computer speed to execute a (transient) 3D-model). It is common knowledge that this situation is changing very fast.

7.1 The memory problem

A computer system with sufficient *random access memory* (RAM) is required to store data and arrays during the execution of the model. Until a few years ago, most FORTRAN compilers accessed only 640 Kb of RAM, which is the standard memory limit of DOS. As such, the possibility to store large amounts of data was limited. So, the arrays which represent the parameters and the number of grid blocks should not be dimensioned too large. The problem of insufficient memory has recently been solved. Since the late 1980's, much more memory is available on the personal computer: the so-called *Extended Memory RAM* (EM RAM). Executables of computer codes can address this EM RAM beyond the usual 640 Kb RAM-limit of DOS through sophisticated compilers (e.g. the Lahey Fortran compiler F77L-EM/32 in combination with the Lahey/Ergo/Phar-Lab 386 Operating System). As such, even stand-alone personal computers can accommodate a much larger number of grid blocks than under 640 Kb of conventional RAM.

Table 1 gives the number of elements or grid blocks of some computer codes. For instance, originally, the number of grid cells in MOC[12] [Konikow & Bredehoeft, 1978] was 400 (20 by 20 grid cells) which required about 302 Kb of RAM. As the maximum number of grid cells under 640 Kb of RAM was only 900 grid cells (591 Kb of RAM), the application of MOC for large-scale geometries was rather limited. Even more data must be stored for 3D-models. For instance, Navoy [1991] applied 52,470 grid blocks to model an area of 60 km · 45 km with MODFLOW (5 layers, 106 columns and 99 rows). The sand-dune area of Amsterdam Waterworks in the Netherlands, which has a geometry of 19,000 m · 12,000 m by 160 m, has been schematised by 40,000 grid blocks using MODFLOW [Schaars, 1996], and by 11,408 grid blocks using HST3D and METROPOL [Ossenkoppele, 1993]. In order to model a large-scale geometry with the dimensions 10,000 m · 20,000 m by 150 m with MODFLOW (adapted and interconnected with MT3D, see subsection 6.4), 300,000 grid blocks with a dimension[13] of 100 m · 100 m · 10 m are required. As such, the memory to store data must increase significantly: up to several tens of Mb of RAM. Nowadays, the EM RAM in a computer can be increased without high costs. For instance, 4 Mb of EM RAM costs only ± 130 US$ (summer 1996[14]). Standard computer systems contain several (tens of) Mb of EM RAM, so the memory problem has been disposed for 2D and some 3D problems. Anyway, now (1996), the application on a broad scale of 3D-models for extensive and complex geometries is still in an early stage.

7.2 The speed problem

The length of time necessary to execute the computations with the computer program for a given set of input data of a geohydrologic problem is the so-called *execution time*. This execution time depends on four factors:

a. the speed of the computer

   Table 2 illustrates how some types of computer systems perform. The difference in MHz does not matter much. As can be seen, the new computer systems with faster processors (disk-speed) open the application of 3D-modelling of large-scale geometries.

b. the size of the model

   The number of grid blocks and type of the governing equations being solved determines the size

[11] Three-dimensional modelling of oil and gas reservoir behaviour by the petroleum industry is already taking place for many years: apparently, the benefit of predicting reliable oil and gas reservoir has been higher.

[12] Nowadays, MOC is also called USGS 2-D TRANSPORT.

[13] Note that at areas where changes in the future salinity distribution are limited, the grid may be more coarse, which will reduce the number of grid blocks.

[14] In September 1995, 4 Mb of EM RAM cost ± 260 US$, whereas in spring 1990, it cost ± 2500 US$!

Table 1: The number of elements or grid blocks of executable computer codes depends on the free Extended Memory RAM (EM RAM) of the computer [source: Scientific Software Group, 1995]. Note that, e.g., in an 8 Mb EM RAM computer, only some 7 Mb is free for memory allocation.

Computer code	Extended Memory RAM (Mb)	Number of (2D) elements or (3D) grid blocks
MOC (2D), adapted*	†0.3	‡400
for density differences	†0.6	900
by Oude Essink [1996]	3.5	10000
	6.7	20000
	16.4	50000
MOCDENSE (2D)♡	2.5	2500
SUTRA (2D)•	4	1300
	8	2175
	16	6525
HST3D (3D)	4	2500
	8	7000
	16	14000
MODFLOW (3D)	◇4	60000

*: MOC (USGS 2-D TRANSPORT) is adapted to simulate salt water intrusion in vertical cross-sections [Oude Essink, 1996].
†: under 640 Kb of conventional RAM, the standard memory limit of DOS.
‡: in the case with 400 grid cells, the number of particles per grid cell is 8, whereas for the other cases the number of particles is 9.
♡: MOCDENSE [Sanford & Konikow, 1985] is an adapted version of MOC, developed for vertical cross-sections (it is based on pressures).
•: the main reason for this small number of grid cells relative to MOC is that SUTRA [Voss, 1984] has to allocate arrays for additional subsoil characteristics.
◇: it is also possible to apply a virtual memory system, which uses disk storage to supplement the computer's memory. Note, however, that then the computer speed will drop significantly.

Table 2: Execution time of different computer systems (processors) with different MHz on a benchmark problem [Anderson & Woessner, 1992].

Computer system	Execution time	Speed (relative to PC)
PC	$49^m\ 43^s$	1
XT	$26^m\ 13^s$	1.9
286 (AT)	$7^m\ 7^s$	7.0
386 16 MHz	$5^m\ 8^s$	9.7
386 25 MHz	$5^m\ 2^s$	9.9
486 25 MHz	$1^m\ 40^s$	29.8
486 33 MHz	$1^m\ 16^s$	39.3
486 50 MHz†	$\pm\ 1^m$	49.7
Pentium 120 MHz†	$\pm\ 16^s$	186.4

†: based on the author's own experience.

of the model. The larger the number of grid blocks, the longer the execution time will be.

c. the efficiency of the compiler

To execute the model, an executable file of the computer code must be produced by an appropriate compiler. A compiler reads the source code and generates machine language statements for the computer hardware. Some compilers go through commands and information more efficiently than others. For example, the Lahey Fortran compiler (e.g. F77L-EM/32) is capable of a very rapid compilation of FORTRAN-codes. This compiler could already address the Extended Memory

RAM at least since the end of the 1980's.

d. the type of the output device

Some models ask for keyboard input during the execution or frequently write to the screen printer or even an output file. These actions increase the execution time (massive output files of several Mb's may increase the execution time substantially). The output devices can be reduced by setting the printing options to minimal output.

8. The data availability problem

Obviously, a numerical model, which is applied to simulate groundwater flow and solute transport in a coastal aquifer, must be calibrated and verified with available groundwater data in order to prove its predictive capability, accuracy and reliability. Examples of groundwater data are subsoil parameters (e.g. the hydraulic conductivity, the exact position of aquitards; the effective porosity; the anisotropy, and the hydrodynamic dispersion), groundwater extraction rates, and salinity and piezometric level distributions as a function of space and time. Regrettably, in many cases reliable and sufficient data are scarce. The availability of enough reliable data is obviously even more pinching for 3D-models than for 2D-models. As such, the application of 3D computer codes is restricted seriously.

8.1 Upscaling of data from 1D and 2D to 3D

In fact, the collection of data is one- or two-dimensional. Geohydrologic information is mostly obtained from a point source (e.g. groundwater level from a observation well) or from a line source (geohydrologic information from a geohydrologic column). This information must be extrapolated or interpolated to a 3D distribution of subsoil parameters. This upscaling obviously faces some difficulties.

8.2 Long time series of hydrochemical constituents

Another problem is that the calibration of groundwater flow models with salinities changing over time and space is still rather laborious. As the flow of groundwater and subsequently the transport of hydrochemical constituents are slow processes, it takes quite some years before a salinisation can be detected. As such, relative long time series of monitored salinities (of some tens of years or even more) are necessary in order to accurately calibrate 3D salt water intrusion in large-scale coastal aquifers. Unfortunately, these time series are available only occasionally and reliable measurements are scarce in many cases. As a consequence, the calibration will be less reliable. One has to collect many data during many years before a good calibration can be achieved.

8.3 Remedy for the data availability problem

The collection and the analysis of reliable groundwater data should be intensified, varying from subsoil parameters to records of solute concentrations and piezometric levels as functions of time and space. The present salinisation process should be monitored as a function of time to detect long-term changes. The geometry and geohydrologic parameters of the coastal aquifer systems should be determined and described, particularly for those aquifer systems which are vulnerable and sensitive to natural and man-induced processes.

To solve the data availability problem to a certain extent, so-called *Geohydrologic Information Systems* can be very useful. In these systems, all relevant geohydrologic data can be stored. By analysing these systems, areas with a lack of data can be detected immediately. In 1990, research institutes, governmental organizations and drinking water companies in the Netherlands started the development of a so-called REgional Geohydrologic Information System (REGIS). In REGIS, a database is available to supply all types of relevant geohydrologic information, such as geo-electric data, groundwater levels (observation well data), chemical data, geohydrologic columns, topographic information, pumping and borehole test data, locations of contaminants, etc. Now, the system is operational and has already proven to be profitable.

Conclusions

Though 3D-modelling of salt water intrusion in large-scale coastal aquifers is technically possible, a number of practical problems arise.

First of all, to suppress truncation and oscillation errors in the solution of the advection-dispersion equation, models based on the standard fem or fdm should satisfy the condition that the spatial discretization (that is the dimension of the grid block) should not be greater than a few times the magnitude of the (longitudinal) dispersivity that represents hydrodynamic dispersion. When the dimension of the aquifer system in question is large and the (longitudinal) dispersivity is small (e.g. in the order of decimetres for Holocene and Pleistocene deposits of marine and fluviatile origin), the dimensions of the grid blocks must be in the order of (tens of) metres. This condition of spatial discretization considerably restricts the practical application of 3D computer codes with dispersive solute transport, such as HST3D, SWICHA and METROPOL, to simulate 3D salt water intrusion in large-scale coastal (homogeneous) aquifers. However, an interconnected model of MODFLOW (adapted for simulating density dependent groundwater flow) and the transport model MT3D will probably avoid the numerical dispersion problem.

Second, the required number of grid blocks to model large-scale coastal (homogeneous) aquifers is enormous, e.g. of several hundreds of thousands of grid blocks. Nowadays, the (personal or mini) computer which is applied to execute a model with this number of grid blocks is still not fast enough, but it will be within a few years. The memory allocation is no problem any more, as computers with some tens of Mb of Extended Memory RAM are already available on a large scale.

Third, the large number of groundwater data, required for calibration and verification, are not yet available in most cases. As such, data collection should be intensified. However, we have to accept that the collection of data will always lag behind the developments in computer possibilities.

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