MATHEMATICAL MODELS AND THEIR APPLICATION TO SALT WATER INTRUSION PROBLEMS

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ABSTRACT

Mathematical models help you to understand the relevant processes that cause salt water intrusion in coastal aquifers. A brief introduction is given to the history of applying conceptual and mathematical models for salt water intrusion issues. First, different model concepts of the phenomena of salt water intrusion in coastal aquifers are given. Marking points during recent salt water intrusion history are discussed: the Badon Ghijben-Herzberg principle, sharp interfaces models between fresh and saline groundwater, Henry's mixing model, coupled solute transport models from the middle 1980's, the Hydrocoin case up to the present state-of-the-art three-dimensional codes. General problems with 3D numerical modelling of salt water intrusion in coastal aquifers are considered: the data availability, the computer, and the numerical dispersion problems. Typical salt water intrusion problems are brought up: the outflow face at the sea, the initial density matrix and the fixed concentration boundaries of the model. Some three-dimensional cases from the low-lying Netherlands are discussed, where the impacts of human activities, sea level rise and land subsidence on groundwater flow and water management in the coastal region are quantified. Finally, some challenges for the future are suggested.

Key Words

Mathematical models; salt water intrusion; modelling of variable-density groundwater flow; sharp interface models; solute transport models; benchmarks; MOCDENS3D; 3D case-studies; The Netherlands.

RESUMEN

Los modelos matemáticos ayudan a comprender los procesos relevantes que causan la intrusión de agua salada en acuíferos costeros. Se hace una breve reseña histórica de la aplicación de los modelos conceptuales y matemáticos al estudio de la intrusión marina. Primeramente, se señalan los diferentes modelos conceptuales acerca del fenómeno de la intrusión salina. Asimismo, se reseñan los puntos de interés más importantes de la reciente historial del estudio de la intrusión: el principio de Ghijben-Herzberg, los modelos de interfaz neta entre el agua dulce y el salado, el modelo de mezcla de Henry, los modelos acoplados de transporte de solutos desde mediados de los ochenta, desde el caso Hydrocoin hasta el estado actual del arte acerca de los códigos tridimensionales. Se exponen los problemas generales de la modelación tridimensional de la intrusión marina: la disponibilidad de datos, el ordenador, y los problemas numéricos de dispersión. También son analizados los problemas típicos de la intrsuión de agua de mar: la superficie de descarga hacia el mar, la matriz de densidades iniciales y las condiciones de contorno de concentración constante en los límites del modelo. Se discuten algunos casos en 3D de la zona holandesa que está bajo el nivel del mar, en los cuales se cuantifican los impactos de la actividad humana, el aumento del nivel del mar y la subsidencia sobre el flujo del agua subterránea, y se analiza la gestión del agua en la región costera. Finalmente, se sugieren algunos retos para el futuro.

Palabras clave

Modelos matemáticos, intrusón de agua salada, modelación del flujo de agua subterránea bajo densidad variable, modelos de interfaz neta, modelos de transporte de solutos, problemas de referencia, MOCDENS3D, casos estudiados en 3D, Países Bajos.

INTRODUCTION

Up to the 1980s, the behaviour of density dependent groundwater flow has been investigated by means of analogue models (e.g. the Hele Shaw model for multiple fluid flow to study wastewater injection into a fresh-saline groundwater system) and analytical solutions. Since computers appeared on the scene, numerical models gained ground. At present, a large number of numerical models is available, capable of handling fresh and saline groundwater flow in aquifer systems. In this section, the advantages and disadvantages of the conceptual models of salt water intrusion are considered in detail.

Some good reviews of literature on fresh and saline groundwater and available computer codes and models are given in e.g. Reilly and Goodman (1985); Custodio and Bruggeman (1987) and (Bear et al., 1999). In addition, all Salt Water Intrusion Meeting-proceedings (from 1968 on) comprise a large number of case studies with different kinds of models, see e.g. SWIM-Delft'86, 1986; SWIM-Ghent'88, 1988; SWIM-Gdansk'90, 1990; SWIM-Barcelona'92, 1992; SWIM-Cagliari'94, 1994; SWIM-Malmö'96, 1996; SWIM-Ghent'98, 1998; SWIM-Miedzyzdroje'00, 2001 and SWIM-Delft'02, 2003.

Interface model versus solute transport model

The Badon Ghijben (1889)-Herzberg (1901) principle[1] describes the position of an interface between fresh and saline groundwater (figure 1). Equation 1 represents the Badon Ghijben-Herzberg principle:

$$h = \alpha H \qquad (1)$$

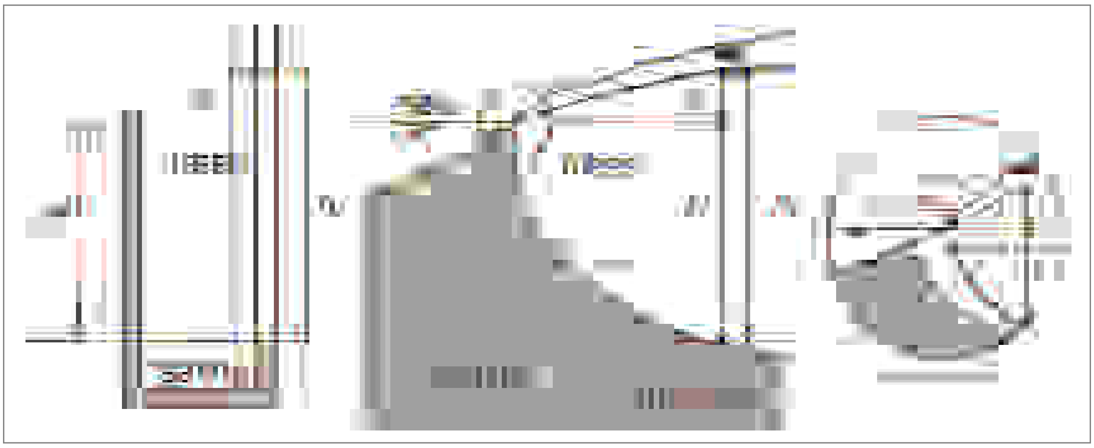

Figure 1. The Badon Ghijben-Herzberg principle: a fresh-salt interface in an unconfined coastal aquifer.

where H=depth of the fresh-salt interface below mean sea level (L), $\alpha=(\rho_s - \rho_f)/\rho_f$=relative density difference (-) and h=piezometric head of fresh water with respect to mean sea level (L). For ocean water ρ_s=1025 kg/m^3 and fresh water ρ_f=1000 kg/m^3, the relative density difference α=40. The equation is correct if there is only horizontal flow in the fresh water zone and the saline water is stagnant. Note that (Glover, 1959) obtained an analytical solution for the exact position of the interface. Though the position of the

[1] In 1889, the Dutchman Badon Ghijben, who did research for the public water supply in a dune area for the city of Amsterdam and in 1901, independently, the German Herzberg developed the equilibrium equation for this phenomenon in groundwater. Note that the American of French birth Du Commun already referred to this principle in 1828.

interface is not correct at the outflow face, the use of the equation still gives a rather good approximation of the real situation.

Interface models are based on the assumption that the interface between fresh and saline groundwater represents the actual situation: the well-known Badon Ghijben-Herzberg principle. The straightforward interface models can be applied as an educational means to gain a clear insight into the behaviour of fresh and saline groundwater in coastal aquifer systems. As such, these interface models are still widely applied. Nice examples have been given in Bear and Dagan (1964), Dagan and Bear (1968), Schmorak and Mercado (1969), Verruijt (1971), Lee and Cheng (1974), Josselin de Jong (1977), Veer (1977a, b, c), Dam (1979), Verruijt (1980), Bear and Kapuler (1981), Dam and Sikkema (1982), Sikkema and Dam (1982), Essaid (SHARP) (1990, 1992), Schotting (1998) and Boekelman (2001). The first three articles refer to the upconing of saline groundwater under a pumping well.

Nevertheless, some restrictions on the applicability of the principle should be considered:

- 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 an interface when the maximum thickness of the brackish zone is only in the order of several meters. This condition applies only in rare situations where the freshwater lens is evolved by natural recharge, as occurs in some sand-dune areas or in (coral) islands.
- 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 Ghijben-Herzberg principle should not be applied, because the computed position of the interface deviates from the actual position as the coast is approached.

In many coastal aquifer systems, a relatively broad transition zone (or mixing zone, zone of dispersion or brackish zone between fresh, brackish and saline groundwater) is present because of various processes during geological history (e.g. regressions, transgressions), see figure 2.

In addition, the transition zone is also increasing as a result of the circulation of brackish water due to inflow of saline groundwater (mixing with fresh groundwater due to hydrodynamic dispersion), the tidal regime and human activities, such as (artificial) recharge and groundwater extraction at high and variable rates (Cooper et al., 1964). For example, this situation occurs in Dutch hydrogeologic cross-sections

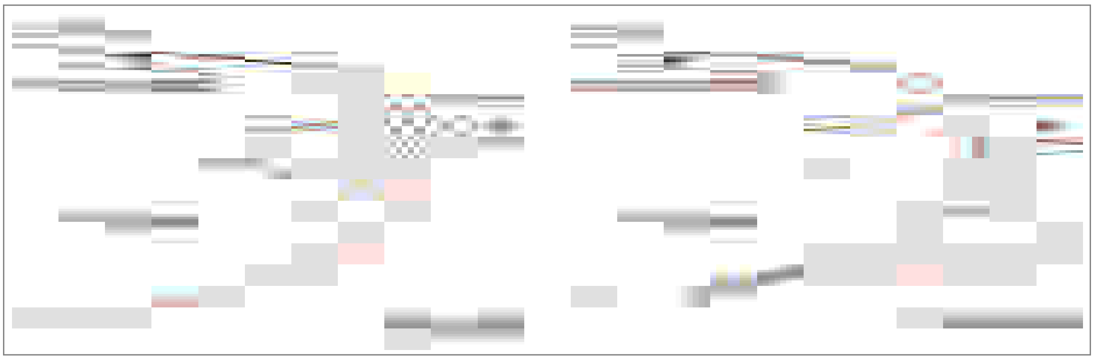

Figure 2. Salt water intrusion in a coastal aquifer: a. the interface concept: a balance between fresh water and static salt water and b. the mixing concept: circulation of salt water from the sea to the zone of diffusion and back to the sea (modified from Henry, 1964).

with Holocene and Pleistocene deposits of marine and fluviatile origin (Meinardi, 1973; Maas, 1989). Under such conditions, more sophisticated models are required than just models with expressions for interfaces: models that take into account variable densities and the transport of solutes. 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 through the equation of state. They are able to simulate, among others, salt water intrusion in coastal aquifers where mostly non-uniform density distributions occur; changes in solute concentration (e.g. near pumping wells due to upconing); and changes in storages of freshwater in sand-dune areas. As solute transport models usually apply numerical schemes, they can also be utilised to simulate aquifer systems with complex hydrogeologic geometries and inversions of fresh and saline groundwater caused by (pre)historic events. Some examples of these early solute transport models are INTERCOMP (1976) and the models of Lebbe (1983) and Voss (SUTRA, 1984). The complete mathematical description of the solute transport models can be found in Galeati et al. (1992), Diersch (1996), Person et al. (1996), Holzbecher (1998), Ingebritsen and Sanford (1998), Bear et al. (1999) and Diersch and Kolditz (2002).

Two-dimensional versus three-dimensional models

The practical application of two-dimensional groundwater flow models is rather limited when real geometries are considered. In many real situations, 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 the vicinity of singular wells where groundwater is extracted or infiltrated, in polder areas where the controlled phreatic groundwater levels lead to radial flow patterns or in areas with complex hydrogeologic geometries.

Under these circumstances, 3D models should be applied. 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 (effective velocities) and solute transport on a (2D) monitor should not be underestimated, though nowadays many sophisticated and powerful GUI's (graphical user interfaces) are available.

BENCHMARK PROBLEMS

Model testing comprises, besides comparison with the results of other models and with reality, model verification of problems for which analytical solutions exist. Unfortunately, no analytical solutions exist for density dependent groundwater flow in porous media in combination with hydrodynamic dispersion but the one Henry developed in the 1960's (Henry, 1964). As such, verification of computer codes for this groundwater flow type is rather limited. Alternative code verification comprises comparison with analytical solutions for the stable interface between fresh and saline groundwater where no hydrodynamic dispersion is taken into account (Josselin de Jong, 1977; Verruijt, 1980; Wilson and Sa da Costa, 1982 and Bakker et al., 2003), with results of other models, with well-measured laboratory experiments as the saltpool experiment (Johannsen et al., 2002), and finally, with reality.

Henry's problem

In Henry's problem (1964), saline water intrudes a hypothetical homogeneous, isotropic, confined, rectangular coastal aquifer and merges by a constant dispersion coefficient. Henry investigated the effect of dispersion on salt encroachment in coastal aquifers. The problem is based on the Biscayne aquifer of south-eastern Florida. It is (has been) common practice to apply Henry's problem as a benchmark for new computer codes that can simulate density-driven groundwater flow (Segol, 1994). New numerical techniques are often compared with the solution of Henry himself. Various researchers use Henry's problem to verify their own model. Some scientists compared their numerical solutions with Henry's final steady state solution (Lee and Cheng, 1974); other scientists compared their solutions with the unsteady state solutions of Henry's problem (Pinder and Cooper, 1970; Segol et al., 1975; Frind, 1982; Voss, 1984; Sanford and Konikow, 1985; Galeati et al., 1992).

The boundary conditions of Henry's problem are shown in figure 3a. Parameters are summarised in table 1. The top and bottom boundaries are impermeable and thus no-flow boundaries. A constant fresh water flux Q enters the aquifer along the vertical at x=0. The seaside boundary at x=l is a constant saltwater head. In the solution of Henry, no mass transport over the seaside boundary occurs. Effects of tides and recharge, that make the salt water intrusion problem unsteady, are averaged and all included in the value of the hydrodynamic dispersion coefficient D_h.

Ironically, it appears that currently no method has succeeded in exactly duplicating Henry's steady state solution. Especially near the bottom of the aquifer, Henry's solution substantially differs from all numerical solution techniques. It appeared that the inaccuracies of Henry's results were a consequence of the limited computer facilities at that time. In addition, Henry probably started with a poor guess (e.g. isolines too far inland) and he did not reach a full-equilibrium solution. He may also have used a limited number of coefficients (Segol, 1994). In conclusion, Simpson and Clement (2003) found out that Henry's problem is not suitable for benchmarking variable-density groundwater flow, as the distribution of the saline water is in fact almost completely determined by forced boundaries conditions and density effects are negligible.

Hydrocoin, level 1, case 5

The Hydrocoin problem is developed to represent a rough approximation of the Gorleben salt dome in Germany, a site (which used to be) under consideration for disposal of high-level nuclear waste. It is a steady state flow and transport problem. As density variations are large (ρs=1200 kg/m^3), it is a strongly coupled problem. Geometry and boundary conditions are given in figure 4a, whereas physical parameters are summarised in table 1, see also Voss and Souza (1987), Herbert et al. (1988), Oldenburg and

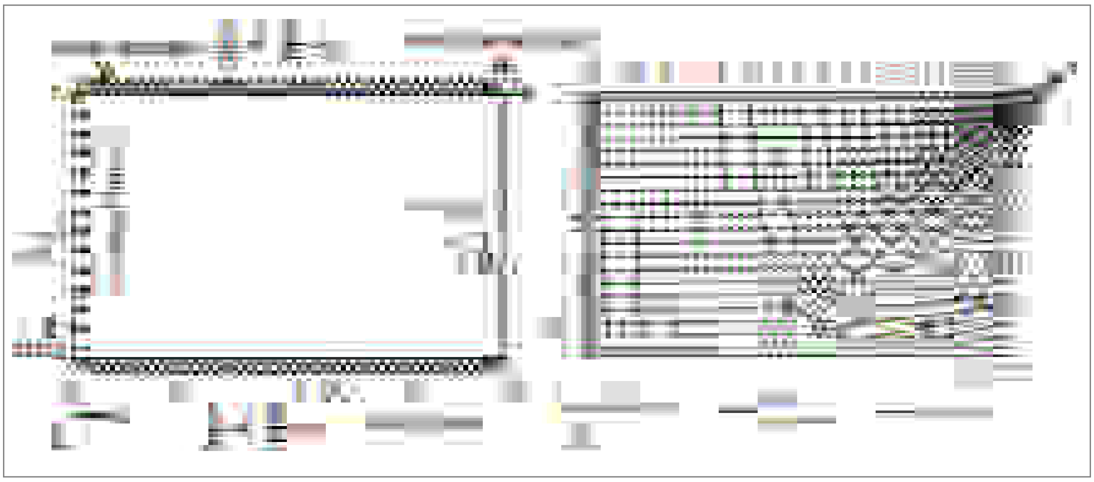

Figure 3. Henry's problem (1964): a. Saline water intrudes in a hypothetical rectangular aquifer and merges by a constant dispersion coefficient; b. Freshwater head distribution (in m), several isolines of saltwater fraction and the velocity field computed with MOCDENS3D (briefly described later) after a simulation time of 400 min.

Case	Henry	Hydrocoin	Elder	Rotating case
size modelled system [m]	2*1	900*300	600*150	300*40
hydraulic conductivity	1 cm/s	10^{-5} m/s	4.75*10^{-6} m/s	2 m/d
porosity	0.35	0.2	0.1	0.2
anisotropy [k_z/k_x]	1.0	1	1	1
long. dispersivity –$_L$ [m]	0	20	0	0
trans. dispersivity –$_T$ [m]	0	2	0	0
effective. mol. diffusion [m^2/s]	6.6*10^{-6}	0	3.565*10^{-6}	0
horizontal cell size [m]	0.05	20	3.75	1
vertical cell size [m]	0.05	4	1.875	0.5
total number active cells	800	3365 & 3420	12800	24000
number of cells	40*20	45*75 & 45*76[1]	160*80	300*80
number of particles per cell	9	16	9	16
flow time step	5 min	1/45 year	1 month	10 day
convergence head [m]	10^{-6}	10^{-5}	10^{-5}	10^{-5}
length time step arrow[2]	4 min	1 year	0.5 year	not applicable
total time	400 min	1000 year	520 year	20000 days

[1]The number of vertical cells varies to point out the effect of the bottom boundary, see the text.
[2]The lengths of the arrows correspond with the displacement of groundwater during a time step, beginning at the indicated moment in time.

Table 1. Physical parameters used in MOCDENS3D (Oude Essink, 1998) of the problems of Henry, Hydrocoin, Elder and the rotating of three immiscible fluids.

Pruess (1995), Konikow et al. (1997) and Younes et al. (1999). Fresh groundwater enters the system at the left upper boundary. It flows through the system, passing the brine region at the bottom, and flows out at the right upper boundary. In addition, density differences influence the flow field. During the 1980's and early 1990's, there was consensus that the steady flow field causes a large recirculation of brine in the bottom region (figure 4b1). This type is called the recirculation type as brine even occurs in the upward part of system between x=0 and x=300 m.

Konikow et al. (1997) found out that a constant concentration condition in the active flow field, as applied in the early numerical calculations, causes a solute flux by both advective as well as dispersive processes. However, as the original Hydrocoin benchmark imposes a no-flow boundary at the salt dome boundary, solute transport should only be dispersive and not advective. As such, the concentration condition at that boundary was not correct. Konikow et al. (1997) suggested a remedy to leave out advective transport at the constant concentration boundary. They inserted an additional row of cells and reduced the hydraulic conductivity of that additional row of cells three orders of magnitude relative to the other cells. In this situation, the advective term of salt transport is negligible (figure 4b2). This type is called the swept-forward type, as no salt is present in the upstream part of the system, viz. between x=0 and x=300 m. For the recirculation type, a substantial larger amount of brine is released in the system compared to the swept-forward type, as advective transport at the constant concentration boundary is taking place (note that a much finer vertical dicretisation also substantially reduces the brine to displace in the upstream part of the system).

Figure 4. Hydrocoin salt dome problem: a. *Geometry and boundary conditions of the;* b. *flow field and salt concentrations (as brine mass fraction) of the Hydrocoin problem at* t=*1000 year, computed with MOCDENS3D:* b1. *The recirculation type (grid is 45 by 75) and* b2. *The swept-forward type (grid is 45 by 76): an additional row of cells is inserted at the bottom of the geometry in order to assure that brine release is only by hydrodynamic dispersion and not also by advection, which is the case in the recirculation type.*

Elder problem

The Elder problem (Elder, 1967) is a free convection problem in a rectangular homogeneous porous medium. The system is partially heated from below. It was originally a heat flow problem (Nield, 1968, Nield and Bejan, 1992), but here it has been adapted as a (density-dependent) solute transport problem (figure 5). Parameters for the solute transport module are summarised in table 1. The Elder problem has often been used as a benchmark for code-verification, e.g. for the codes SUTRA (Voss and Souza, 1987), TOUGH2 (Oldenburg and Pruess, 1995), FEFLOW (Diersch, 1996), FAST-C(2D/3D) (Holzbecher, 1998), D^3F

Figure 5. Elder problem (1967): geometry (not at scale) and boundary conditions of the free convection problem, converted from heat transport to mass transport.

(Frolkovic and De Schepper, 2001) and Simpson and Clement (2003). The solution of the Elder problem is highly sensitive to discretisation and other numerical convergence effects.

For instance, the effect of the initial distribution of salt is demonstrated on the flow process in the domain. Figure 6 surprisingly shows that a small perturbation in initial salt concentration, as indicated in the figure, sets groundwater flow in the system in another mode. Now, flow at x=300 m is downwards instead of upwards.

Rotating immiscible interface

This benchmark problem consists of the movement of three immiscible fluids of different densities; flow is caused by density differences only (Bakker *et al.,* 2003). The benchmark problem is intended specifically for the verification of the density-dependent flow part of groundwater codes. In addition, it may be used to assess the impact of adopted approximations (such as the Dupuit approximation), and the existence and magnitude of numerical dispersion. An exact solution is available for the initial velocity distribution, and transient results will be compared.

Consider two-dimensional, confined flow in a vertical cross-section as shown in figure 7a. Parameters are summarised in table 1. All boundaries of the aquifer are impermeable. The aquifer is filled with water of three different densities; the water with three different densities will be treated as three immiscible fluids separated from each other by interfaces. Viscosity differences are ignored. The freshwater hydraulic conductivity of the aquifer is homogeneous and isotropic. The aquifer and fluids are treated as incompressible.

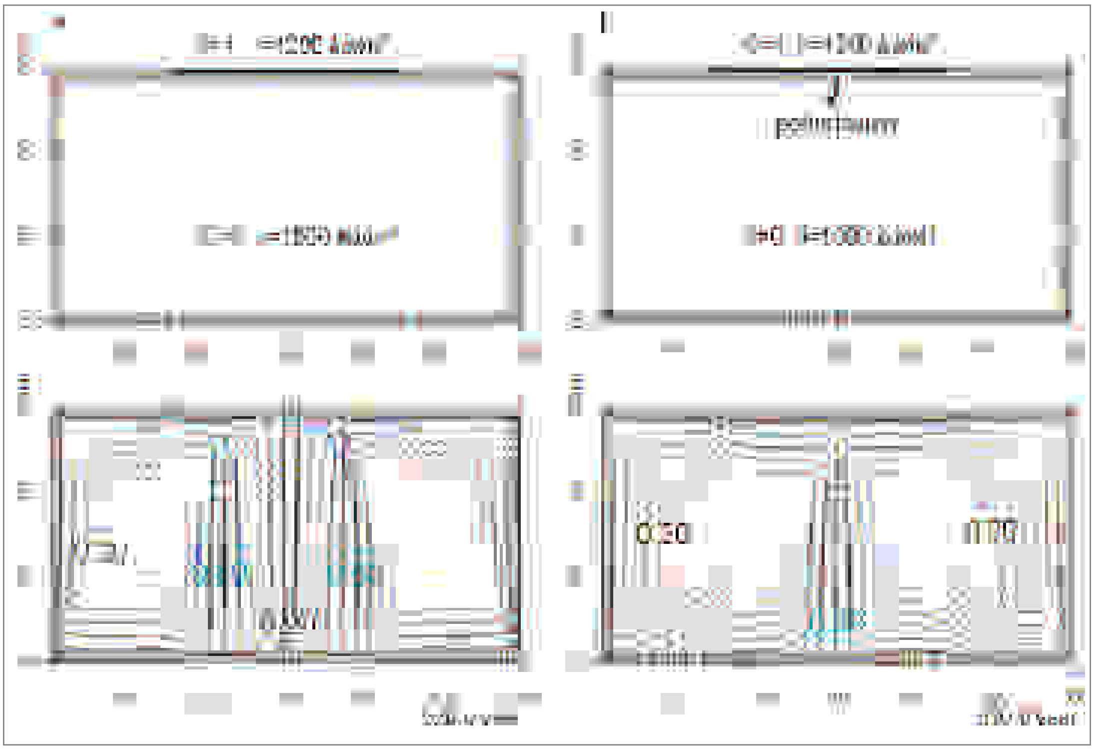

Figure 6. Effect of initial salt concentration distribution on the final flow field and salt concentration. Flow field and salt concentrations of the Elder problem are shown on t= *520.0 year, viz. after a long time of simulation, computed with MOCDENS3D. As can be seen, the convective flow fields differ from each other. The initial perturbation in case b. sets the system in a different mode.*

Initially, at time t=0, both interfaces are straight and their centers are located at x1=170 m and x2=130 m; both interfaces have a slope of 1/2. Figure 7b shows that along both the top and bottom of the aquifer the left interface moves much faster than the right interface. The brackish fluid is so much lighter than saline fluid that the tendency of brackish fluid to flow to the top is stronger than the tendency to rotate. As a result, the horizontal distance between the two interfaces will become larger at the top of the aquifer and (much) smaller at the bottom of the aquifer. During rotation, the two interfaces move so close together at the bottom of the aquifer that an interface between the fresh and the saline fluids develops, as can be seen at t=5000 days. Over time, this interface will disappear slowly (see t=20000 days).

Saltpool problem

This experiment of a 3D test case for variable-density flow in a porous medium involves a stable layering of saltwater below freshwater (Johannsen et al., 2002). An additional discharge of fresh water on the top causes a time-dependent upconing of the saltwater. Laboratory experiments support this saltpool problem. The set-up of the experiment is as follows: a cube of side length L of 0.2 m and initially filled with 0.14 m freshwater and 0.06 m saltwater on the bottom. The cube will be recharged with freshwater through a single inflow hole at one of the upper corners for a certain time and water will be discharged at the opposite corner with a variable salt-mass fraction. Two cases with different initial salt mass fractions of 1% and 10% are considered. Breakthrough curves of the experiments at the outflow hole as well as width and position of the interface have been analysed. The transversal dispersivity coefficient plays an important role in the 10 % case.

PROBLEMS WITH 3D MODELLING OF SALT WATER INTRUSION

Though 3D modelling of salt water intrusion in hydrogeologic systems is technically no problem anymore, some practical problems remain (Oude Essink and Boekelman, 1996, 1998): the data availability problem, the computer problem and the numerical dispersion problem.

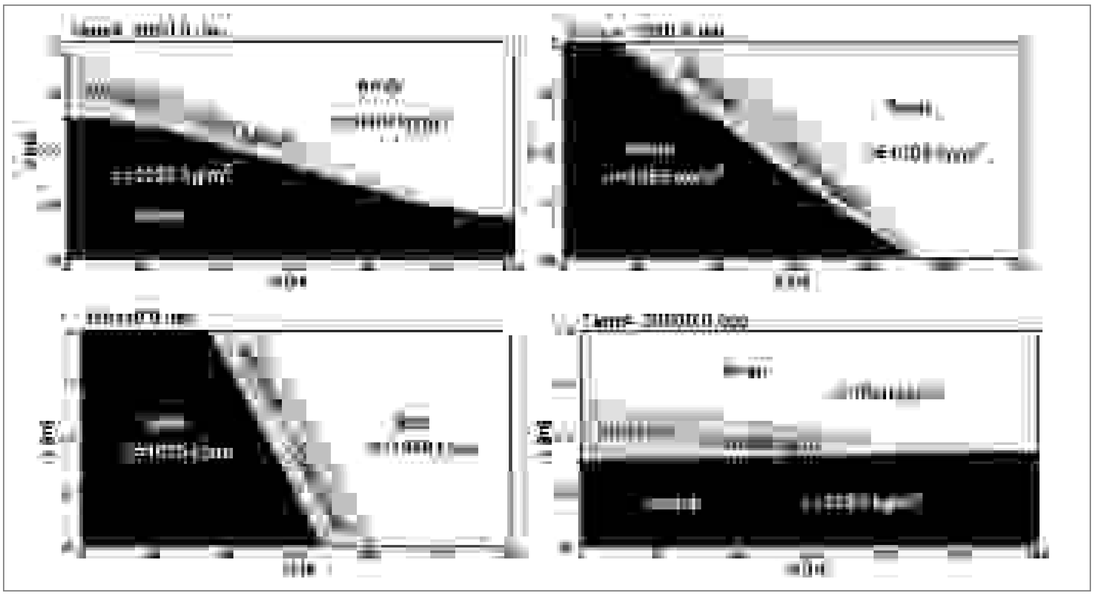

Figure 7. Rotating immiscible interface problem: the development of the position of three fluids, calculated with MOCDENS3D.

The data availability problem

A numerical model of salt water intrusion in a coastal hydrogeologic system must be calibrated and verified with available hydrogeological data in order to prove its predictive capability, accuracy and reliability. Regrettably, in many cases reliable and sufficient data are very scarce. As such, 3D modelling is (and will probably always be) restricted seriously. Some common problems are:

- Upscaling of data from 1D (a point source such as a groundwater level from a observation well) and 2D (from a line source as borehole information) to 3D: in fact, the collection of data is one- or two-dimensional. This information must be extrapolated or interpolated to a 3D distribution of subsoil parameters. This upscaling obviously faces difficulties; especially inter- and extrapolation of concentration measurements to a 3D density field is difficult.
- Long time series of hydrochemical constituents: the calibration of a transient groundwater flow model with salinities changing over time is still rather laborious. As the flow of groundwater and subsequently the transport of hydrochemical constituents are slow processes, it takes many years before salinisation can actually be detected. As such, relative long time series of monitored salinities (of some tens of years or even more) are necessary to accurately calibrate transient 3D salt water intrusion in large-scale coastal hydrogeologic systems. Unfortunately, these time series are available only occasionally. As a consequence, the calibration of this transient process will be less reliable and less good.

In conclusion, it has to be accepted that the availability of data will lag behind the developments in computer possibilities, and thus, will restrict practical applications to a certain extent.

The computer problem

Until some years ago, 3D modelling of salt water intrusion in large-scale coastal hydrogeologic systems was also difficult due to 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). This situation has changed pretty fast. Nowadays, the memory in a computer can be increased with several hundreds Mb of EM RAM at low costs. In addition, powerful standard personal computers significantly reduce the execution time, though this obviously depends on the disk-speed of the computer, the size of the model, the efficiency of the compiler and the type of the output device.

The numerical dispersion problem

Numerical approximations of the derivatives of the non-linear solute transport equation may introduce truncation errors and oscillation errors (see figure 8). The truncation error has the appearance of an additional dispersion-like term, 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.

There is a close relation between numerical accuracy (numerical dispersion) and stability (oscillation) (Peaceman, 1977; Pinder and Gray, 1977). In fact, numerical dispersion acts to stabilize the solution of the solute transport equation. Numerical dispersion spreads a sharp front, e.g. an interface between fresh and saline groundwater, by generating a solution that applies a greater dispersion than the true hydrodynamic dispersion. To suppress numerical dispersion, the numerical discretisation scheme (spatial as well as temporal) should be adapted. However, this scheme may lead to over and undershooting, and subsequently, oscillation may be amplified. Therefore, the numerical discretisation scheme should be chosen carefully in order to control both numerical accuracy and stability.

Eigenvalue analyses of the advection-dispersion equation and Taylor series expansions are performed to demonstrate the numerical accuracy of a solution and the importance of the element dimension (Peaceman, 1977; Frind and Pinder, 1983; Bear and Verruijt, 1987). Approximations of the first-order derivatives generate errors in the order of magnitude of the second-order derivatives.

Figure 8. Schematisation of numerical dispersion and oscillation.

For the analysis of the truncation error, the so-called grid Peclet number Pe_{grid} is defined:

$$Pe_{grid} = \left| \frac{V\Delta x}{D_h} \right| \qquad (1)$$

where Pe_{grid}=grid Peclet number (-), V=effective velocity of groundwater (LT^{-1}), Δx=dimension of the element (L) and D_h=hydrodynamic dispersion (L^2T^{-1}). Grid Peclet numbers (and Courant numbers[2]) have been mentioned in various quantitative descriptions. Whether or not the numerical dispersion is suppressed, depends on the discretisation technique applied (Jensen and Finlayson, 1978; Voss and Souza, 1987). In summary, it appears that in order to obtain real and distinct eigenvalues, the spatial discretisation should meet the grid Peclet number condition (Daus et al., 1985): Pe_{grid}<= 2 for finite difference algorithms; Pe_{grid}<= 2 for finite element algorithms, linear basic and Pe_{grid}<= 4 for finite element algorithms, quadratic basic.

This grid Peclet number condition imposes that the dimension of the element should be not greater than a few times the magnitude of the longitudinal dispersivity that represents hydrodynamic dispersion. Computer codes, of which the solution of the advection-dispersion equation is based on standard finite element or finite difference techniques, must satisfy this condition of spatial discretisation. Both widely used techniques 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).

For example, if the (longitudinal) dispersivity is small (Gelhar et al., 1992), e.g. in the order of decimeters for Holocene and Pleistocene deposits of marine and fluviatile origin, the dimensions of the elements must be in the order of meters. When the dimension of a 3D hydrogeologic system in question is in the order to tens of kilometers by tens of meters depth, many hundreds of millions of elements are needed to model large-scale coastal hydrogeologic systems properly. This amount is (very) difficult to achieve in 2003 for effective transient modelling of variable-density groundwater flow.

Some salt water intrusion computer codes

Here follows a summary of various computer codes which can simulate density dependent groundwater flow and solute transport in order to model salt water intrusion. The interest is focused on the grid Peclet number condition.

[2] The Courant condition, Co=(V Δt)\Δx, is physically interpreted as the ratio of the advective transport distance during one time step to the spatial discretisation.

SUTRA is a well-documented two-dimensional finite element code (Voss, 1984). This code has become thé widely accepted 2D variable-density groundwater flow model throughout the world (Voss and Souza, 1987; Souza and Voss, 1987). It can simulate density dependent groundwater flow with (thermal) energy transport or chemically reactive (single-species) solute transport. The 3D beta-version is available now. The grid Peclet number condition is applied here: Pe_{grid}<= 4. Narrow transition zones require a careful choice of spatial and temporal discretisation.

HST3D is a 3D finite difference code that can simulate heat and solute transport (Kipp, 1986). Modelling a large-scale coastal hydrogeologic system with a non-uniform density distribution with HST3D appears to be rather complicated when small longitudinal dispersivities should be applied. For heat transport applications, this code seems to be much more appropriate; for instance, it often used for modelling geothermal systems in the Netherlands.

SWICHA is a 3D finite element code (Huyakorn et al., 1987; Lester, 1991). It can simulate variable-density fluid flow and solute transport processes in saturated porous media. The applications range from simple 1D to complex 3D, coupled flow and solute transport. The solute transport equation may not converge to a solution if a so-called critical Peclet number is exceeded in an element. To solve this problem, SWICHA offers a trick at the user's option: artificial dispersion is added to the solute transport equation matrix. Spatial oscillations are then suppressed and the critical Peclet number is no longer exceeded in that element.

METROPOL (MEthod for the TRansport Of POLlutants) simulates 3D groundwater flow with varying density and simultaneous transport of contaminants (Sauter *et al.,* 1993). 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 radio nuclear waste in (high-brine) salt formations.

SWIFT (Sandia Waste-Isolation Flow and Transport model) is a 3D code to simulate groundwater flow, heat (energy), brine and radio nuclide transport in porous and fractured media (Ward, 1991; Ward and Benegar, 1998). It is stated that though grid Peclet numbers greater than 4 may cause problems (e.g. oscillations), a value of 10 or more is sometimes acceptable.

FAST-C(2D/3D) (Holzbecher, 1998) can be applied to model density driven flow in porous media using the streamfunction formulation. Density variations are caused by temperature or salinity gradients. Steady state as well as transient modelling of confined aquifers are possible.

FEFLOW is a 3D computer code, which employs the finite element method (Diersch, 1996). The governing partial differential equations describe groundwater flow, where differences in density affect the fluid flow. Fluid density effects are caused by contaminant mass as well as temperature differences simultaneously, inducing thermohaline flow.

D^3F (Distributed Density Driven Flow) is one of the newest, sophisticated, computer codes to simulate density-driven groundwater flow (Fein et al., 1998). It is based on the volume element method. Permeabilities, porosities, values for boundary and initial conditions can be defined as constants as well as simple spatial user-defined functions. In addition, a stochastic permeability distribution technique is available to consider small-scale heterogeneities. Fluid density and viscosity are functions of salt concentration and temperature. The code can run on serial as well as massively parallel computers.

MOCDENS3D (Oude Essink, 1998, 2001) is MOC3D (Konikow et al., 1996), but adapted for density differences. Buoyancy terms are introduced in the vertical effective velocities to take into account density effects. The adapted MODFLOW module solves the equation of density dependent groundwater flow. Solute transport is modelled by the method of characteristics (MOC) module in MOCDENS3D. The particle tracking method is used to solve advective solute transport and the finite difference method is used for hydrodynamic dispersive transport. As such, the movement of fresh, brackish and saline groundwater in porous media can be modelled in 3D. Numerical dispersion and oscillation is limited as the method of characteristics is applied.

SEAWAT (Guo and Bennett, 1998; Guo and Langevin, 2002) is a combination of MODFLOW and MT3DMS (Zheng and Wang, 1999). It is designed to simulate 3D variable-density ground water flow and solute transport. The program was developed by modifying MODFLOW subroutines to solve a variable-density form of the ground water flow equation and by combining MODFLOW and MT3DMS into a single program.

EXAMPLES OF THREE-DIMENSIONAL CASES IN THE NETHERLANDS

Recently, the code MOCDENS3D has been used to model the effect of sea level rise and land subsidence in four 3D regional groundwater systems in the Netherlands (Oude Essink, 2001, 2003a, b; Oude Essink and Schaars, 2003). Two-dimensional variable-density modelling has been performed in Oude Essink (1996). The effects of sea level rise has been overestimated in 2D profiles, due to an incorrect schematisation of the representative (polder) areas. In addition, there are often not enough densities measurements to model salt water intrusion in these Dutch coastal aquifer systems in a very accurate way.

Figure 9 shows the positions of the different case studies and table 2 for the applied specific parameters on geometry, subsoil and model parameters. In all the four case studies, the interest was focussed on the impact of sea level rise on the salinity distribution in the regional groundwater flow system and on seepage and salt load quantities at the top system as a function of time. In addition, the model for the Rijnland case also considered land subsidence and changes in recharge and groundwater extraction rates. It appears that salinisation of the Dutch coastal aquifers is a non-stationary process. Three physi-

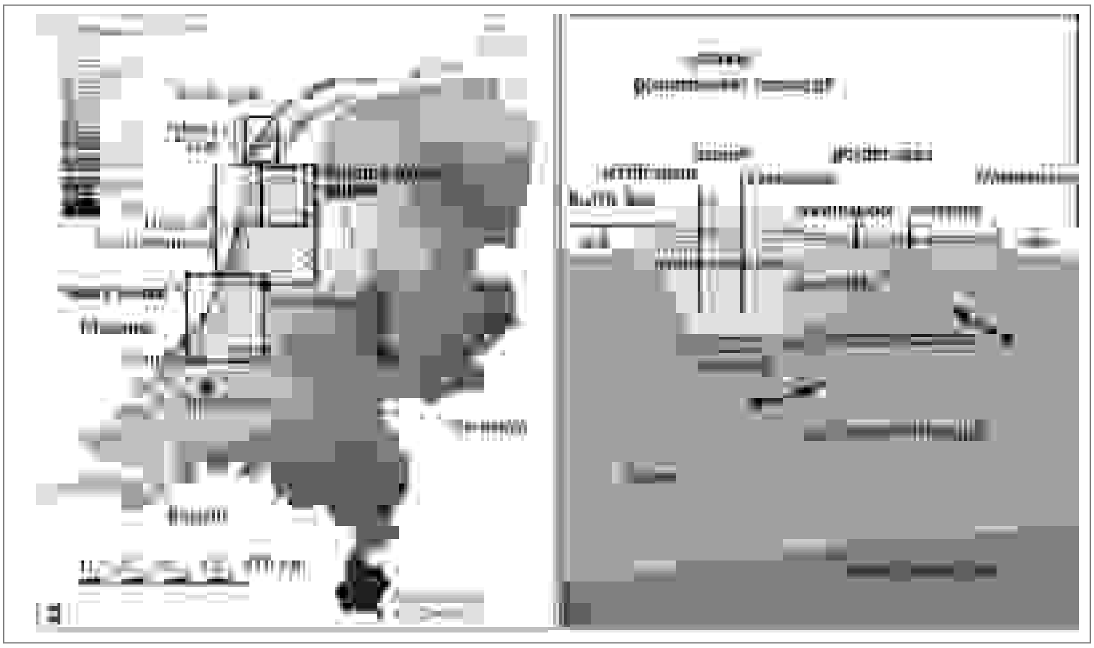

Figure 9: a. Ground surface at The Netherlands and positions of four 3D groundwater flow models in the coastal zone; b: a schematisation of the hydrogeological situation in The Netherlands.

cal processes threaten the Dutch aquifers: autonomous development, land subsidence and sea level rise. For some specific regions close to the shoreline, the increase in seepage (e.g. see Rijnland case, figure 10) and salt load (e.g., see Texel case, figure 11) can be severe during the coming tens (to hundreds) of years.

DIFFICULT ISSUES IN 3D MODELLING OF VARIABLE-DENSITY FLOW

Here, some difficult issues related to 3D modelling of variable-density flow in a regional system are addressed, based on the numerical modelling of the above-mentioned Dutch case studies:

- Initial density matrix:
  In a variable-density flow system, the initial density that should be implemented in the numerical model can highly determine the velocities and thus the transport of fresh, brackish and saline groundwater. An accurate 3D-density matrix can be critical for the accuracy of the model. Under certain hydrogeological conditions, the initial density distribution for a numerical model can be derived by just simulating the groundwater flow system under consideration for many (tens of) years until a steady-state situation from a density point of view is achieved. For instance, the initial (undisturbed) density distribution of a freshwater lens in a dune area can be derived by implementing natural fresh groundwater recharge in a completely saline aquifer system and simulate the system long enough. The obtained steady-state density distribution will probably be the original distribution without human activities as groundwater extractions.

Case	North-Holland	Texel	Wieringer-meerpolder	Rijnland
total land surface [km^2]	2150	130	200	1100
L_x*L_y modelled area [km]	65*51	20*29	23*27	52*60
depth system [m –N.A.P]	290	302	385	190
aquifer hydr.cond. [m/d]	5-70	5-30	15-40	12-70
aquitard hydr.cond. [m/d]	0.12-0.001	0.01-1	0.012-0.056	$2.5*10^{-4}$-0.8
porosity	0.35	0.3	0.25	0.25
anisotropy [k_z/k_x]	0.4	0.4	0.25	0.1
long. dispersivity αL [m]**	2	2	2	1
# head & conc. observations	not applicable*	111	95	1632
characteristics head calibration	not applicable*	**$\Delta\varphi$= 0.24 m**	**$\Delta\varphi$= 0.34 m**	**$\Delta\varphi$= 0.60 m**
		σ= 0.77 m	**σ= 0.21 m**	**σ= 0.77 m**
horizontal cell size [m]	1250*1250	250*250	200*200	250*250
vertical cell size [m]	10	1.5 to 20	2 to 70	5 to 10
total # active cells	~40.000	~216.000	~312.000	~1.200.000
# cells	41*52*29	80*116*23	116*136*22	209*241*24
# particles per cell	27	8	8	8
total time [yr]	1000	500	200	500

*calibration with heads, seepage & salt load in polders in a qualitative way; **molecular diffusion=10^{-9} m^2/s; transversal dispersivity α_T=1/10*longitudinal dispersivity α_L; convergence head criterion= $10^{-5}/10^{-4}$ m; flow time step to recalculate the groundwater flow equation is **Δt=1 year.**

Table 2. Geometry, subsoil and model parameters of the four 3D Dutch aquifers.

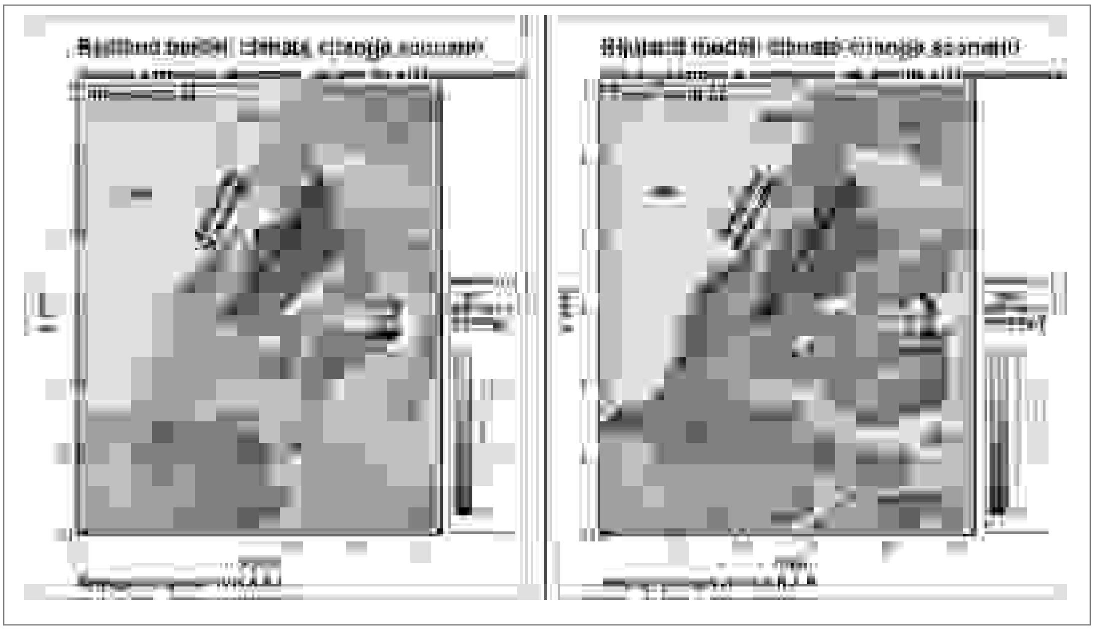

Figure 10: Seepage changes in the topsystem of the water board of Rijnland as a result of autonomous developments, sea level rise (0.9 m per century), land subsidence (up to 1.0 m per century for peat areas), an increase of natural groundwater recharge in the sand-dune area and a reduction of groundwater extractions from the sand-dune areas of 5.8 million m^3 per year (from Oude Essink and Schaars, 2003).

Unfortunately, many coastal aquifer systems are at present not in dynamic equilibrium, for instance due to long-term sea level fluctuations (Meisler et al., 1984) or large-scale human activities with long-term effects on the groundwater system (e.g. the reclamation of low-lying areas in the Dutch coastal zone during the seventeenth century). For these specific cases, the best estimate of the 'initial' density distribution is the present measured one. In general, data of the density distribution is often scarce, and 3D modelling of variable-density groundwater flow in coastal aquifers is often based on insufficient data of good quality.

- Outflow face
  Velocities of fresh groundwater at the outflow face from the inland sand-dune area towards the sea can by enormous. Analytical formulae estimated the length of these faces to (tens of) meters (Glover, 1959; Veer, 1977a). From a numerical point of view, modelling of these zones is difficult and restricts the application of regional models for long-term transient simulations of fresh, brackish and saline groundwater.
- Concentration boundaries
  It is difficult to determine the concentration boundaries of regional transient variable-density groundwater flow models when long-term simulations are considered. Obviously, the verbs concentration boundaries imply that the concentration stay fixed, though incoming concentrations will probably vary. Therefore, these boundaries should be positioned far away from the area of interest, especially because these concentrations effect density and thus variable-density groundwater flow in the system.

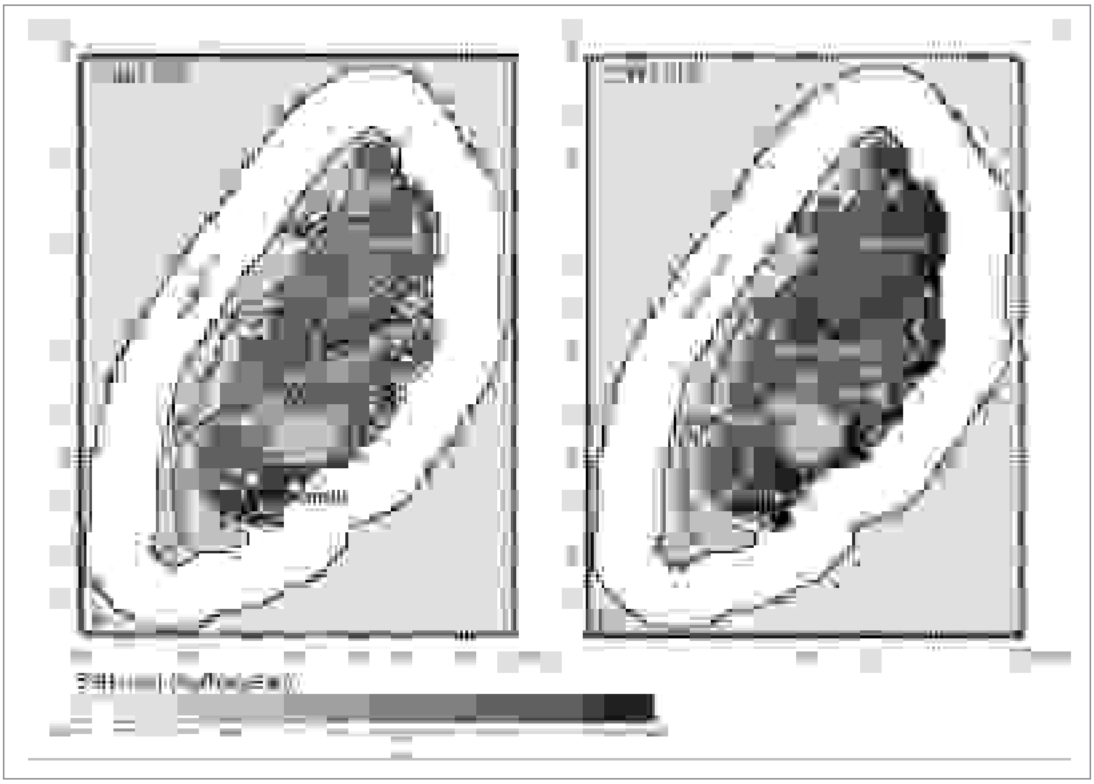

Figure 11: Salt load (in kg/ha/year) in the top layer at -0.75 m N.A.P. for the years 2000 and 2200 AD. Sea level rise is 0.75 meter per century (from Oude Essink, 2003a).

NEW CHALLENGES FOR THE FUTURE

- The 3D-density matrix highly determines the accuracy of the velocity field. Under normal circumstances, accurate 3D density distributions are not available. It is therefore essential for this type of groundwater flow modelling to increase (expensive) quality measurements of concentrations and/or electric conductivities.
- Processes such as sea level rise and increased human activities (e.g. increasing groundwater extractions, changes in land use) intensify the external stresses in many coastal aquifers. In addition, the interaction between the land surface and the sea through groundwater and solute fluxes jeopardise water resources in the coastal zone (ecological marine environment). Research on the combined effects of these processes is of interest to water (management) authorities.
- Optimalisation of a number of compensating techniques to prevent upconing and salt water intrusion in coastal aquifers could lead to a sustainable groundwater management. Examples are strategies of groundwater extraction schemes and technical measurements as creating physical barriers (e.g. EC-project CRYSTECHSALIN).
- The calibration of variable-density flow models is traditionally based on stagnant (freshwater) heads and chloride concentration records. Extending the calibration of these models could be possible when transient data of concentration and freshwater head, isotopes as well as geochemical information of pore waters are applied. In low-

lying polder areas in the Netherlands, seepage values, salt load values, and ecological information of vegetation also improve the quality of calibration.In addition, in deep hydrogeologic systems, even thermal hydrogeological information should be taken into account. If necessary, thermohaline mathematical models should be used to cope with double-diffusive convection processes in hypersaline geothermal systems.

- Combining 3D transient variable-density groundwater flow models of coastal aquifers with multi-species reactive solute transport modules which take into account kinetic geochemical interactions, would be the challenge for the coming five years. Parallel computing will probably be necessary to account for all relevant hydrogeological and hydrogeochemical processes in the subsoil.

CONCLUSIONS

Modelling of variable-density groundwater flow in coastal zone where the density distribution is non-uniform has obviously been improved during the last decades. The increase in computer capacity was one of the major reasons, though research on the mathematical equations did speed up the progress. Models that simulated the interface between fresh and saline groundwater were very useful to roughly simulate the existence of variable-density groundwater. The movement of the interface through time due to external processes such as changes in extraction rates could be modelled. Solute transport models, however, replaced the interfaces models, because these mixing models could more easily comprehend the concept of the transition zone in the subsoil. The interface models still have their educational means. Several benchmark problems were posed to validate the variable-density flow computer codes. The so-called saltpool benchmark seems to have good prospects, though the saltlake benchmark (not mentioned here, see Wooding et al., 1997a, b) is also favourable. Nowadays, models that cope with 3D transient variable-density groundwater flow and coupled multi-component reactive solute transport will be the state-of-the-art for at least the coming five years. Calibration techniques will be improved, whereas an increase in data collection is still essential to get reliable predictive models.

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