SENSITIVITY ANALYSES OF A PUMPING TEST IN A FRESH-SALT WATER AQUIFER
1. CONCENTRATION CHANGES

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ABSTRACT

A density dependent groundwater flow model, MOCDENS3D (Oude Essink, 1998) is used to simulate the upconing of a fresh-salt water interface. The conceptual model is based on geological and hydrogeological information as found in the central part of the Belgian Coastal Plain. The modelled area is 1600 m^2 and the deposits are 40 m thick. This area is divided into 80 columns and 80 rows each with a length and width of 0.5 m. There are 20 layers with varying thickness. The upconing was simulated without any stability problems or significant numerical dispersion, although it required substantial computer memory and computing time. These results were then used for sensitivity analyses. Considering the variation of salt water concentration in the vicinity of the fresh-salt water interface the most sensitive parameter is the vertical conductivity, followed by the horizontal conductivity and in decreasing order of sensitivity: the porosity, the specific elastic storage and the longitudinal dispersivity. The transverse dispersivity has such a small sensitivity that it becomes an unidentifiable parameter.

INTRODUCTION

The present paper is the first part of a preliminary study for the interpretation of a pumping test in density dependent groundwater flow. With an inverse model the optimal parameter values are determined using the fresh water heads and concentration observations. Besides the optimal values a joint confidence region of the parameters can be calculated. In a regional simulation observations can be provided by a piezometric network delivering the necessary head and concentration measurements. On a smaller scale one can try to determine the hydraulic and transport parameters through a pumping test. Determining transport parameters has been increasingly the subject of recent scientific research. Column experiments have been used to determine dispersivity values from breakthrough curves. As the distance dependency of the parameter became clear, field tests were developed to determine these values on a larger scale. Tracer tests all have the same basic principle; injecting a tracer and monitoring its course with several observation wells and pumping the tracer back to the surface either from the injection well or a well further away. From the observation wells the data are interpreted as breakthrough curves (e.g. Pickens and Grisak, 1981; Silliman and Simpson, 1987). Mostly though, research efforts have been concentrated on theoretical developments of calculating a macroscopic dispersivity from a microdispersivity value (e.g. Gelhar and Rajaram, 1995). The interpretation of pumping tests has lately received some attention with the development of new inverse numerical interpretation methods (Lebbe, 1999; Hvilshøj et al. 1999), although the majority of interpretations is still carried out with simplified analytical models. The objective of this publication is to simulate a pumping test in an area where a natural tracer, salt water, occurs. The evolution of the salt concentration is monitored around the rising salt-fresh water transition zone in the vicinity of the pumping well. The sensitivities of these concentrations with respect to the hydraulic and transport parameters are determined.

PRINCIPLES OF MOCDENS3D

MOCDENS3D (Oude Essink, 1998) is a finite-difference model that is capable of simulating three-dimensional density dependent groundwater flow. It is an adaptation of MOC3D (Konikow et al., 1996), a finite-difference model that simulates three-dimensional solute transport in flowing groundwater using the Method Of Characteristics. It considers solute transport as changes in concentration caused by advective transport, hydrodynamic dispersion, mixing or dilution from fluid sources and very simple chemical reactions such as sorption and decay. This requires the simultaneous solution of the partial differential equations for groundwater flow and transport, the advection-dispersion equation. The advective transport is solved using a particle tracking method and the dispersion using finite-difference methods. This reduces the risk for numerical dispersion so that small dispersivities can be used in larger grid cells. The adaptation of MOC3D for density differences was accomplished by two actions. First the hydraulic heads used in MODFLOW were changed into fresh water heads. Next a buoyancy term was added to the vertical velocity expression of MODFLOW (Lebbe, 1981; Lebbe, 1983). More information on MOC3D and MOCDENS3D can be found in the cited articles. Since it is a finite-difference model it divides the model area in a number of columns (east to west), a number of rows (north to south) and a number of layers (bottom to top). Because an adjustment has been made for density dependent flow the columns and rows should all have the same dimensions and each layer has a constant thickness. The two partial differential equations are solved consecutively. The simulation time is divided into a number of stress periods. This stress period is further divided into a number of solute time steps. During a stress period information about discharge rates, infiltration, river heads, etc. remain unaltered, but because the density distribution changes as a consequence of the moving particles and dispersive transport the velocity field is updated after each solute time step. MOCDENS3D automatically calculates three stability criteria, when one of these stability criteria is violated, the solute time steps are still further divided into particle moves. The stability criteria are related to dispersivity values (also called Neumann number), recharge/discharge values and the Courant number (Konikow and Bredehoeft, 1978; Konikow et al., 1996).

MODELLING CONCEPT

Geology and hydrogeology

In the presented paper the upconing of the fresh-salt water interface is treated as a completely synthetic problem. However, it was done in part to plan a real field pumping test in the central part of the Belgian Coastal Plain. The geology and the position of the fresh-salt water interface were derived from a number of drillings and Long Normal (LN) resistivity measurements. The phreatic aquifer of the Belgian coastal plain is made up of Quaternary deposits, it is bounded below by a heavy Tertiary clay that can be considered as an impermeable lower boundary in the model. In the top part the Quaternary sediments are mostly sand deposits with changing clay content. There are some clay sequences intercalated with peat layers. In the area where the pumping test will occur the following simplified sequence of layers can be observed from top to bottom. A sandy layer that is part of an Old Inner Dune deposit forms the top, a clay-peat layer is present underneath and is followed by a thick sand deposit that may have some clay lenses in it. This sequence has a total thickness of about 40 m and is divided into 20 layers in the numerical model. The transmissivity values are initially derived from observations made by Devos (1984) close to the cited area and are given in table 1.

Table 1. Horizontal and vertical conductivity values of the numerical layers

Layer	Horizontal conductivity (m/day)	Vertical conductivity (m/day)
1	2.0	3.0
2	0.007	0.4
3	7.0	3.5
4	7.0	3.5
5	8.8	4.4
6-20	8.0	4.0

Fresh-salt water distribution

Once completely filled with salt water, the Quaternary deposits have been freshening through recharge on the nearby dunes developed during the Subatlantic period (Mostaert, 1985). This freshening lead to the present fresh-salt water distribution. Long Normal (LN) resistivity measurements revealed the current distribution (fig. 1). Fresh water is present in the upper part (high resistivity) and somewhat saltier water is present in the clay-peat sequence (lower resitivity). In the thick sand deposit fresh water is present up to a depth of about 34 m, from then on the resistivity drops sharply to a minimum around the Quaternary-Tertiary boundary (40 m). The actual fresh and salt water content of the deposits was derived using the Archie-equation (1942):

$$\rho_b = F * \rho_w$$

ρ_b is the bulk resistivity, ρ_w is the resistivity of the pore water and F is the formation factor. To know the pore water resitivity a value for F has to be found. From analyses in some 13 wells with a filter in the lower sand deposit of the central coastal plain a value for the groundwater resistivity was derived and consequently a formation factor of 4 was deduced. Using this formation factor the resistivity values of the drilling (fig.1) on the pumping test site were transformed to concentration values. These values are correct for the sand deposit, but not for the clay-peat layer. In this synthetic problem it was, therefore, assumed that this section contained the same concentration as the sand above and below the clay-peat layer. The concentration distribution in the twenty model layers is given in table 2.

Table 2: Concentration distribution in the layers of the numerical model

Layer	concentration	Layer	concentration
1	500	11	1400
2	500	12	1500
3	500	13	1600
4	1200	14	2000
5	1200	15	2800
6	1200	16	4500
7	1200	17	6500
8	1200	18	8800
9	1200	19	11400
10	1200	20	12700

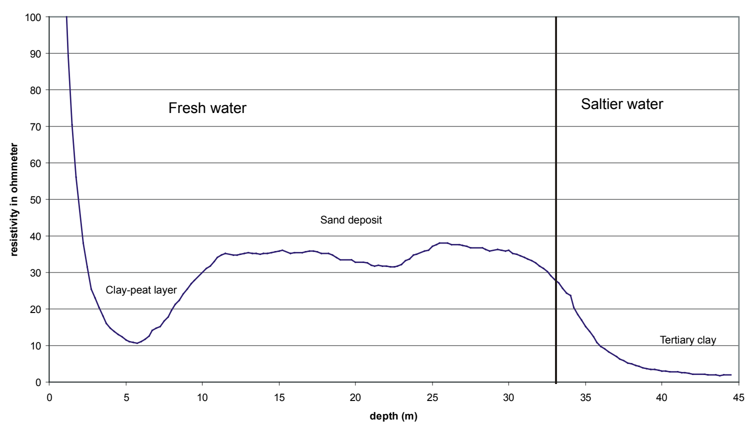

Figure 1 LN resistivity profile of a well in the central part of the Belgian Coastal Plain with indication of the fresh-salt water transition zone

Discretisation, boundary conditions and model input

The considered pumping test is situated in the centre of a squared area with a side of 40 metre. Due to the symmetric nature of the treated flow problem only the lower right quarter of the considered area was modelled (fig. 2). The considered finite-difference grid consists of 80 columns, 80 rows and 20 layers. All finite-difference cells have the same squared base with a side of 0.5 meter. The layers have varying thickness (table 3). The pumping well is situated in layers 6 to 10 equalling a filter screen of 10 m. It has a total discharge rate of 4

m^3/h and the simulation time is 11718 minutes or about 8 days.

Table 3: thickness of the layers of the numerical model

layer	Thickness (m)
1	3
2	2
3	5
4	6
5	4
6-10	2
11-20	1

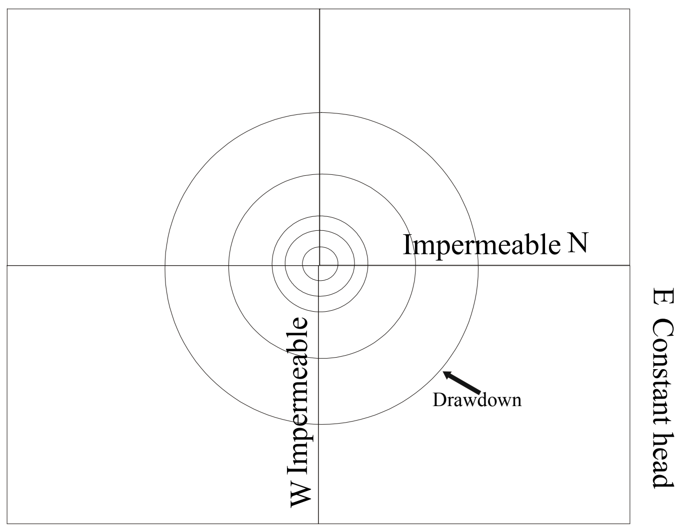

Figure 2 Indication of modelling concept

The southern and eastern boundaries are constant head boundaries, the northern and western boundaries are impermeable (fig. 2). To make sure no unwanted vertical flow initiates at the constant head boundaries it is necessary to take the density differences in account when calculating the value for the constant heads in the different layers. This is done with the formula:

$$h_{fl+1} = h_{fl} + \frac{C_l + C_{l+1}}{2 * C_{\max}} * \frac{t_l + t_{l+1}}{2} * \frac{(d_s - d_f)}{d_f}$$

Where h_{fl} is the fresh water head of layer l, C_l is the concentration of layer l, t_l is thickness of layer l, d_s is the density of salt water (1.025 kg/l), d_f is the density of fresh water (1.0 kg/l) and C_{max} is the maximum concentration of the salt water in the problem (25000 mg/l TDS).

A transient simulation is considered, so the initial values for the concentration and the heads are important. The initial concentration values are equivalent to the fresh-salt water distribution cited above (table 2), it is constant within one layer. Since the simulation is transient a value for the specific elastic storage of every layer and the storage coefficient near the water table or specific yield for the upper layer is also needed. Values for the transport parameters such as the longitudinal and horizontal and vertical transverse dispersivity should be given as well. These are given in table 4. As one can see a rather small value for the dispersivity is assumed, this is in accordance to what Lebbe (1996) derived with a two-dimensional inverse model for the western coastal plain.

Table 4: hydraulic parameters and transport parameters

layer	Specific elastic storage (m^{-1})
1	0.02 (specific yield)
2	0.00004
3	0.00009
4	0.00011
5	0.00007
6-20	0.00010

Solute transport:

Parameter	Value for all layers
Longitudinal dispersivity	0.1 m
Transverse horizontal dispersivity	0.01 m
Transverse vertical dispersivity	0.01 m
Porosity	0.38

Apart from all the physical parameters there are also a number of model parameters that have to be chosen. First of all, the number of particles allocated to each cell. For a three-dimensional problem the choice is between 1, 8 and 27 particles. Twenty-seven particles require an enormous amount of computer memory and time with the current discretisation. Between 1 particle and 8 particles per cell a substantial difference exists in the calculated upconing curve of the fresh-salt water interface (fig. 3). Therefore, 8 particles were used in the simulation. CELDIS is another model parameter that may be adjusted. There was not any difference in the model response when changing the value from 0.7 to either 0.5 or 0.9. A value of 0.7 means that a particle can move a maximum distance in one solute time step that equals 70% of the cell length. Finally, one can wonder if it was really necessary to take the cell dimensions as small as 0.5 metre. But when changing the dimension to 1.0 metre with 20 columns and 20 rows, the calculated upconing curve showed less detail than in the case when cell dimensions were equal to 0.5 metre.

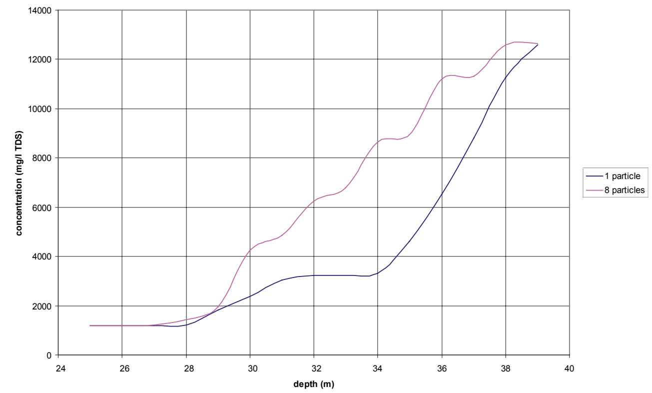

Figure 3 Difference in upconing curve for 1 particle and 8 particles per cell after three days of pumping

SIMULATION

The results of a simple forward run with the parameter values as they are listed in the tables 1, 2 and 4 are the upconing of the fresh-salt water transition zone in time. As can be seen in fig. 4 the upconing starts slowly in the flexing point of the initial transition zone. It is also in this flexing point that the interface moves a maximum distance in 8 days of about 4 m. In the higher concentration zone and the lower concentration zone the interface moves less far.

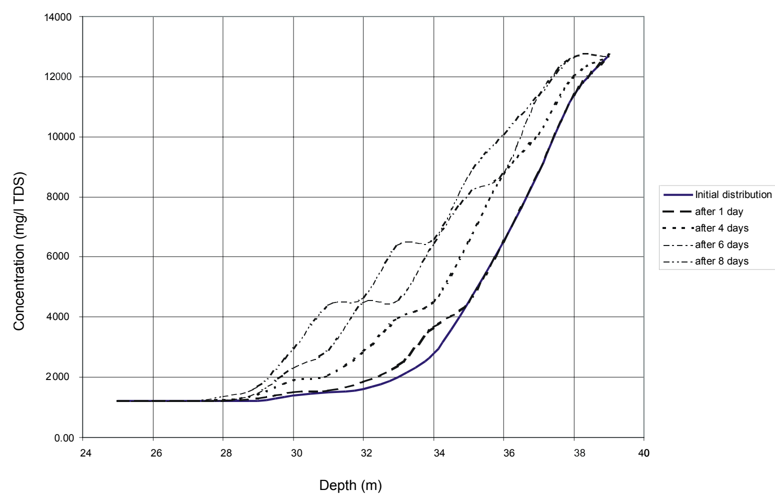

Figure 4 Result of the forward run. Upconing of the transition zone at different moments in time

SENSITIVITY ANALYSES

Definition

When the response of the model changes drastically when changing the value of a parameter with a certain factor, the parameter is called sensitive. When the model response remains unaltered, or as good as the same, the parameter is said to be insensitive. For MOCDENS3D, the process of changing the parameter value and recalculating the model response was automated. There are 7 parameters of interest, namely, the horizontal conductivity, the vertical conductivity, the specific elastic storage, the longitudinal dispersivity, the horizontal transverse and vertical transverse dispersivity and the porosity. In this test all parameters were studied. Thus, the model was run 8 times. Once with the initial parameter estimate and next 7 times where each time one parameter estimate was adjusted and the others remained fixed. The calculated concentration results were followed in a number of observation wells. The total computation time of these sensitivity analyses requires 55 hours on a PC pentium II (64 Mb RAM and 266 MHz, program compiled with Fortran Lahey compiler 32 bits).

The results of the successive calculations were written in a file, which was thereafter used to calculate the sensitivities. The definition of sensitivities as they are used in inverse models can have different forms (Lebbe, 1999). In this case the sensitivities were taken as the difference between the residuals without any parameter adjustment and the residuals with a parameter adjustment divided by the common logarithm of the sensitivity factor.

$$\frac{\partial F}{\partial P} = \frac{r - r^*}{\log_{10} SENFAC}$$

r is the residual without any parameter adjustment, r^* is the residual with a parameter adjustment, SENFAC is the sensitivity factor and was taken as $10^{0.3}$. This sensitivity factor is the value with which the parameters are adjusted during the sensitivity analysis. The residual (r) is the common logarithmic difference between the calculated concentration at a given time and place and the observed concentration at the same time and place.

$$r = \log_{10} C_{cal} - \log_{10} C_{obs}$$

C_{cal} is the calculated concentration and C_{obs} is the observed concentration.

The sensitivities are represented in three-dimensional figures (fig. 6). The three axes are the depth, the time and the sensitivity value. The larger the absolute value of the sensitivities, the more sensitive the model output is to changes in this parameter. When the parameter is sensitive enough, observations of the model output should help in identifying this parameter in an inverse model.

Results and interpretation

The sensitivities were only calculated with respect to the concentration and not with respect to the hydraulic head. Observations were generated from a depth of 21 m to 40 m. The diagrams of the different parameters are all similar in form. They have a peak value where the fresh-salt water transition zone moves. They also have rising sensitivities with time. The longer the pumping goes on and hence the further the transition zone moves the more sensitive the concentrations around the transition zone are for determining the parameter. In maximum absolute values the most sensitive parameter is the vertical conductivity, followed by the horizontal conductivity and the specific elastic storage. For the transport parameters the porosity is about equally sensitive as the specific elastic storage. The others are less sensitive. The longitudinal dispersivity is about five times less sensitive than the least sensitive hydraulic parameter. The transverse dispersivities are probably unidentifiable in an inverse model of this test. It should be noted in the diagrams that of the considered depth interval, only a small depth interval contributes to the sensitivity of the parameter. This is because of the calculated narrow transition zone. A larger transition zone would lead to a greater depth interval with noticeable sensitivity values. In the planned pumping test two observation wells will be installed. One at 2.5 metres from the pumping well and the second at 6 metres from the pumping well. When comparing the sensitivities in the two wells it can be noted that the sensitivity of the parameter drops substantially at greater distance from the pumping well (fig. 5 presents just the horizontal conductivity). Another way of comparing sensitivities is to calculate the average sum of the squared sensitivities of each parameter (table 5). From these calculations some interesting conclusions can be drawn. Whereas in the diagrams the peak values are compared to draw up a ranking for sensitivities of the parameters, this method considers all sensitivities over the entire depth interval. In this way the porosity becomes the third most sensitive parameter, and the sensitivity of the specific elastic storage becomes far less important. This emphasises the very narrow sensitivity peak of the specific elastic storage in the diagram and the broader sensitivity peak of the porosity. Another interesting feature of this table 5 is that at a greater distance from the pumping well not all sensitivities change the same way. The sensitivity of the vertical conductivity is divided by ten, whereas the sensitivity of the horizontal is divided by four and the sensitivity of the porosity is divided by only three. The sensitivity of the specific elastic storage remains equal.

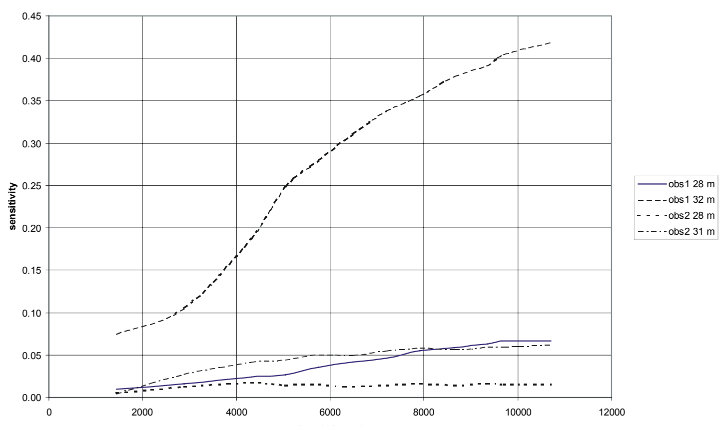

Figure 5 Difference in sensitivity of the concentration for the first (obs1 at 28 m and 32 m depth) and second observation well (obs2 at 28 and 31 m depth)

Table 5: Sum of squared sensitivities for the first and second observation well for all parameters.

Parameter	Hcont	Vcont	Ss	ALONG	ATRANH	ATRANV	POR
First well	7.553533	17.24325	0.337885	0.087825	3.11E-07	0.000529	9.234284
Second well	1.83583	1.721721	0.350018	0.020744	3.74E-06	7.82E-05	3.630486

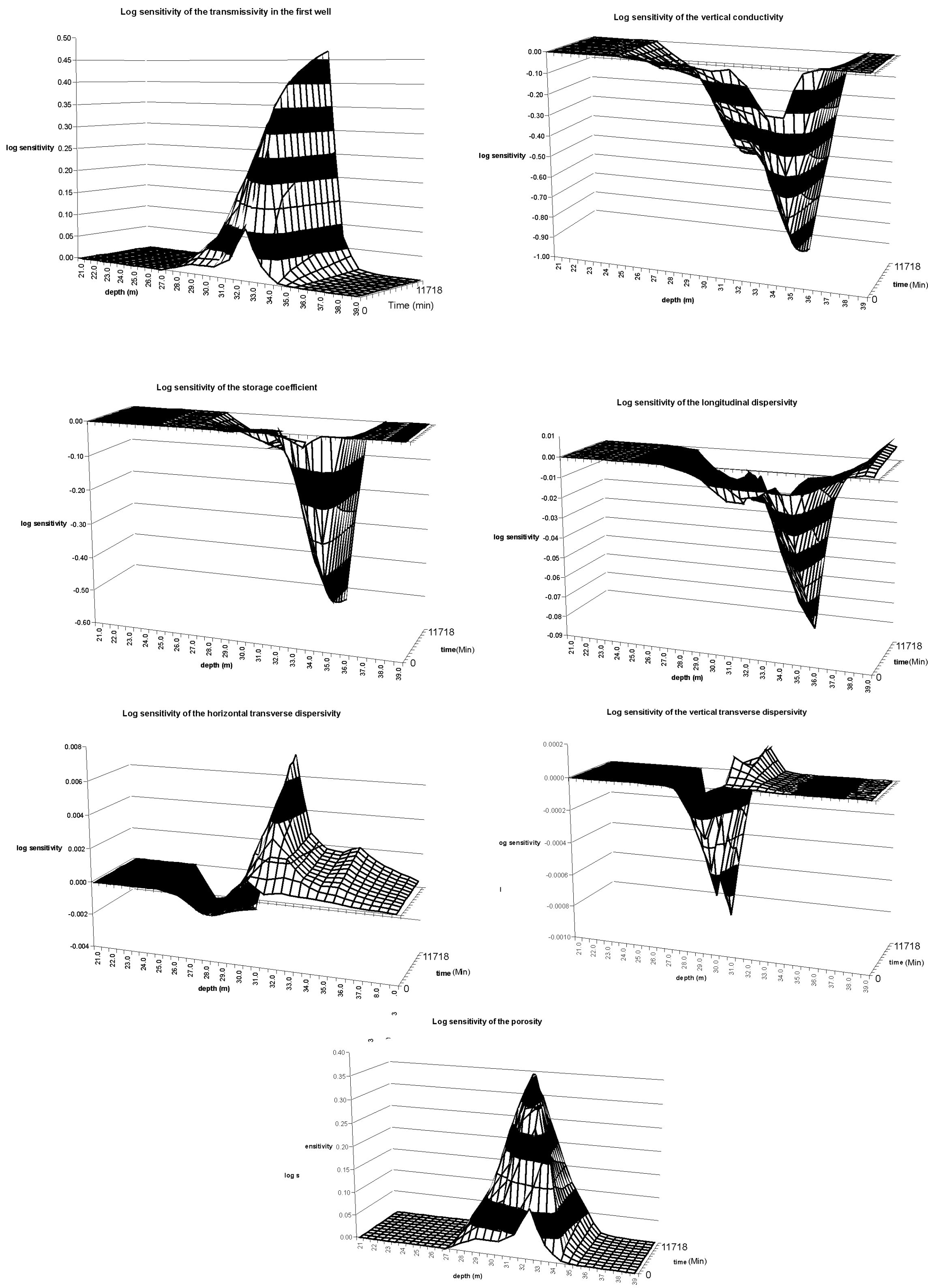

Figure 6 Sensitivity diagrams for the first observation well for all parameters

CONCLUSION

The simulation of the upconing of a fresh-salt transition zone with MOCDENS3D in a synthetic problem was studied. Although artificial, the discretisation and model concept is based on the actual field situation in the central part of the Belgian Coastal Plain. As such, the modelling served to design a real pumping test. The MOCDENS3D-code was adjusted for carrying out consecutive sensitivity analyses. Seven analyses were considered: the vertical conductivity, the horizontal conductivity, the specific elastic storage, the longitudinal dispersivity, the transverse horizontal dispersivity, the transverse vertical dispersivity and the porosity. A sensitivity factor of $10^{0.3}$ was used. The results of the sensitivity analyses are depicted in different ways. In the three-dimensional diagrams of the closest observation wells the same shape was noted for all parameters. The parameters have a maximum sensitivity in the vicinity of the fresh-salt water transition zone and the sensitivity increases with time. In absolute value the most sensitive parameter is the vertical conductivity, followed by the horizontal conductivity and the specific elastic storage. Of the transport parameters the transverse dispersivities have a very small sensitivity and are probably unidentifiable from the observation of the pumping test. The sensitivity of the longitudinal dispersivity is rather small due to the initial sharp transition zone and a rather small estimated value for it. The porosity is the most sensitive transport parameter. When comparing the results for the sensitivities of the first and second observation wells for the horizontal conductivity a decrease can be seen in the second well's sensitivities. Finally, when taking the sum of the squared sensitivity values over the entire depth range some interesting information appears. When taken over the entire depth range the porosity has a greater sensitivity for the concentration than the specific elastic storage and the drop in sensitivity in the second observation well is not equal for all parameters.

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