PARAMETERIZATION OF DENSITY DISTRIBUTION IN GROUNDWATER: EVALUATION IN TRIWACO-MODEL OF SCHOUWEN

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ABSTRACT

The density distribution is an important factor for groundwater flow in coastal areas. The density distribution can be derived from measured chloride concentrations. However, these measurements are usually done for water resource planning (protection or evaluation), and most are for fresh water and few for brackish and salt water. As a result, the density in the inland areas with mostly fresh water can be mapped relatively well, but the distribution in the near-shore areas and deeper aquifers cannot be derived from measurements.

Reconstruction of the distribution with historical modelling is not an option. A very long simulation period is needed in order to get results that do not depend much on the unknown initial distribution. During this period, there is a large uncertainty of important geohydrological boundary conditions.

A better option is to derive an initial distribution from measurements and geohydrological knowledge and improve the distribution in the calibration of a groundwater model. This has been tested with the existing TRIWACO-model of western Schouwen. The island of Schouwen is located in the southwestern part of the Netherlands between two former branches of the rivers Scheldt and Meuse. The North Sea surrounds the western "head" of the island on three sides. The model for the head of Schouwen has been built with the groundwater simulation package TRIWACO. A finite element flow simulator has been used with a variable density module, which accounts for the influence of the inputted density distribution. The module for automated calibration and confidence analysis has been applied to a new parameterization of the density near the coast: polygons along the coast. Two different widths have been used. The results show that the parameterization can be improved and that this will reduce the function (sum of the squares of the differences between calibration head residuals).

INTRODUCTION

The island of Schouwen is located in the Southwest of the Netherlands (see figure 1). The island lies between former estuaries of the rivers Scheldt and Meuse. The "head" of the island still borders on the North Sea. The estuary to the North of Schouwen has been closed off from the inland waters connected to the Meuse (in 1965) and the North Sea (in 1972) as a part of the Delta-works, a large plan to made after a severe flood in 1953. The island was badly hurt in this flood. The dikes broke in several places, and one large opening developed on the South side of Schouwen. The "Oosterscheldedam" the storm surge barrier in the Eastern Scheldt to the South of the island, which was one of the last "Delta-work" (completed in 1986) allows the tides still to go in.

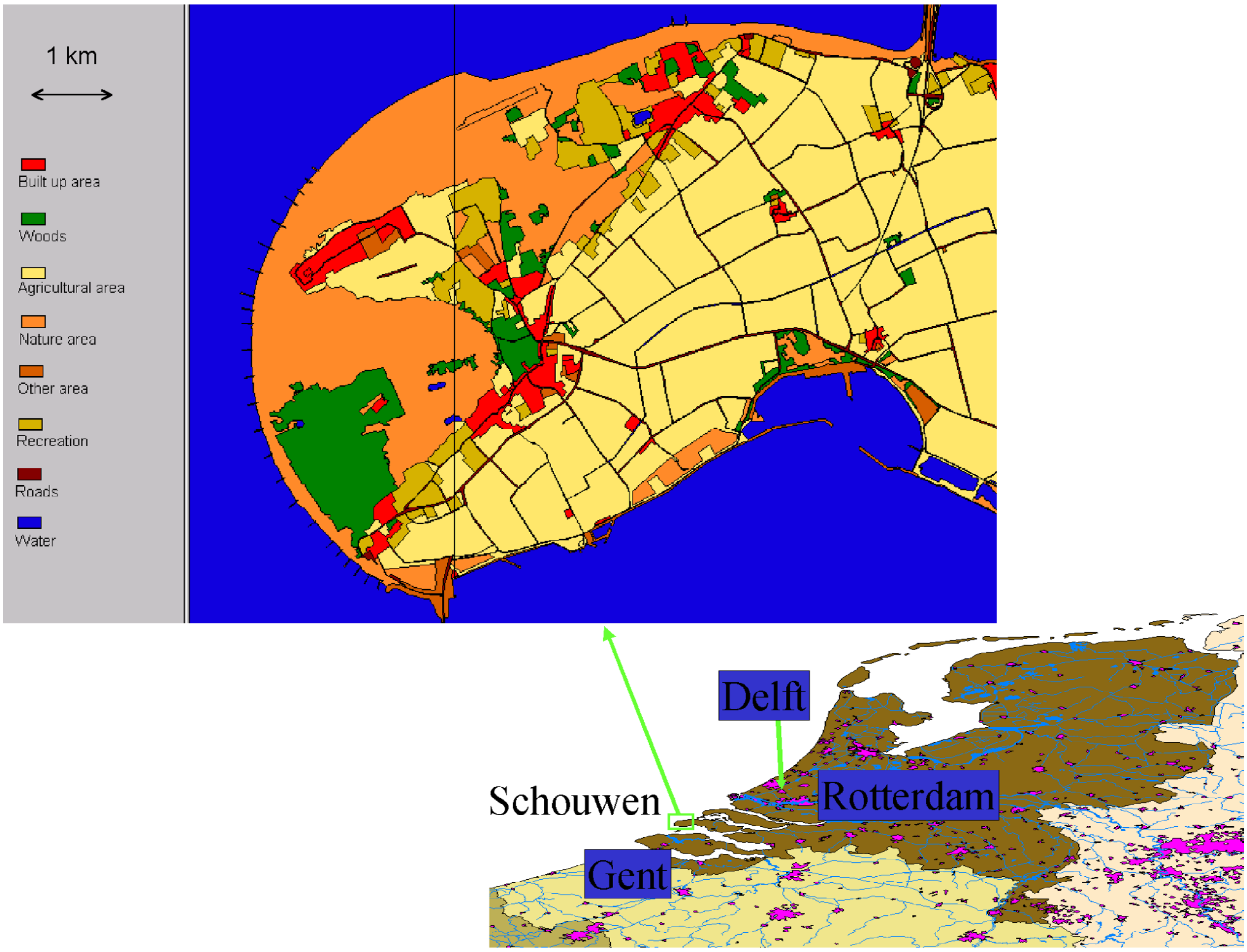


Figure 1 *Island of Schouwen*

The head of the island consists for a large part of dunes with lower lying polders behind them. Recreation is important in the area, there are nature preserves and groundwater is abstracted for the local drinking water supply. In the depression in the 1930 large areas were planted with fir trees, like in several places in the Netherlands. The depression was over before the trees could produce timber and economic production has never been feasible. In more recent years people became aware of relatively high the transpiration of the trees. There may have been other changes that have influenced the hydrology on the island of Schouwen. As a result the precious ecology of the wet dune valleys has been damaged and the drinking water supply threatened with salinization of the extraction wells. The groundwater conditions are not optimal for agricultural purposes either.

In order to improve the geohydrology, projects have been started to improve the water management on the island of Schouwen. An example is the replacement of the fir trees with deciduous trees and a partial removal of the woods altogether. A groundwater model has been set up to guide these projects. The model accounts for the density differences due to the salt to make accurate enough predictions. The density distribution can be derived from measured chloride concentrations. However, measurements are only available from inland piezometers. As a result, the density underneath the inland can be mapped relatively well, but the distribution in the near-shore cannot be derived from the measurements. This is a typical situation, as piezometers are usually installed for fresh water resource planning (protection or evaluation), and most filters are located in fresh water and few in brackish and salt water.

Moreover, the distance from the coast is not well known where the groundwater in the various aquifers extending below the see bottom has the same density as the seawater. One way to determine this distance is to determine the equilibrium density (and salt) distribution in a coupled flow and transport simulation. One problem for such a simulation is that the aquifer and aquitard properties are less known near the shore. But in this case more important is this fact that the distribution may be far from an equilibrium situation due to the many geohydrological changes in the past century. For this paper we decided not to try this path, but in stead try to determine whether we can find a reasonable parameterization in which the density values can be optimised with automatic calibration tools.

TRIWACO

The groundwater simulation package TRIWACO (www.triwaco.com) has been set up originally in 1984 and has been improved and expanded since (Royal Haskoning, 2002). It offers a large variety in top systems (boundary condition at the top of the aquifer system) that allow the user to define recharge relations accounting for e.g. precipitation, surface run-off, irrigation and drainage. Next to the top system, rivers or canals can be explicitly put in as line segments that are assigned a width, water level, infiltration and drainage resistance. TRIWACO allows up to 99 aquifers and both quasi 3D and fully 3D simulations can be carried out with the restriction that the one principal direction of the (anisotropic) permeability tensor must be vertical. The package has options for a sharp salt-fresh interface as well as variable density flow. The package contains a module for automatic parameter optimization and model reliability. Recently interfaces for the public domain groundwater flow simulator Modflow96 and the transport codes M/RT3D(ms) have been added. While the first version was designed for a DOS platform, it is a true 32-bits Windows package now (Iwaco, 1999). At the same time it has evolved from a set of separate programs into a modelling system. The system promotes modelling efficiency because of the emphasis on conceptual modelling, the data and scenario management, the strong graphical capabilities and the open structure with e.g. easy exchange with a GIS like ArcInfo/ArcView.

The finite element flow simulator has been used with a variable density module, which accounts for the influences of the inputted density distribution. The tools for automated calibration have been used to analyse and improve the parameterization of the density distribution in the model.

MODEL "HEAD OF SCHOUWEN"

The model has been built with the groundwater simulation package TRIWACO. The model area is 124 km^2. A zone of about 2km width into the sea has been included in the model. A finite element mesh has been created that is strongly refined in the area of interest. The node distance is 500 m in the sea, 150 m near the coast and land inward it decreases via 75, 25 and 10 to 5 meters at some dune lakes to be restored. This resulted in 7895 nodes and 15657 triangular elements (see figure 2). The model has five aquifers that follow the important geohydrological strata (see figure 3).

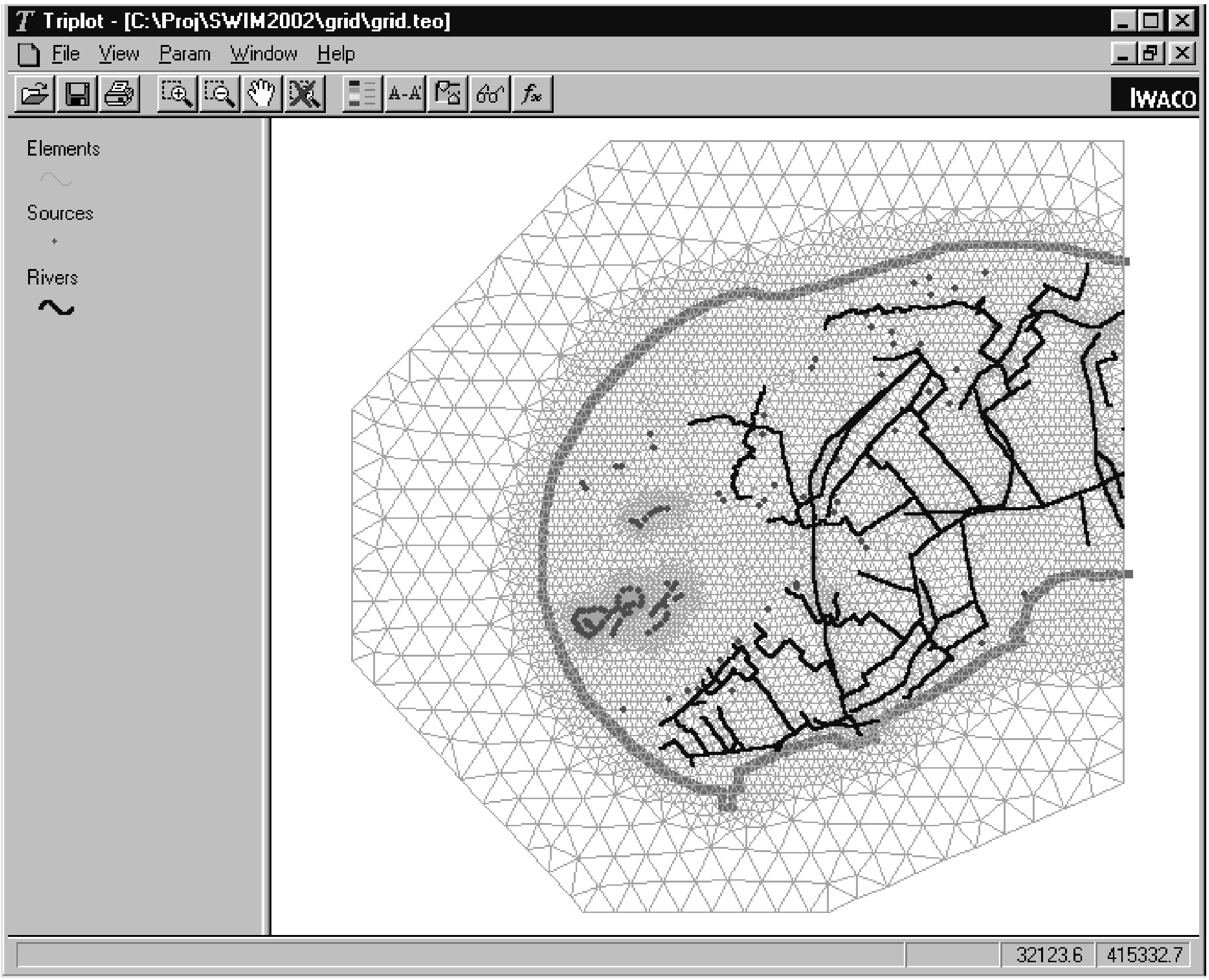


Figure 2 *Plan view of model*

DENSITY DISTRIBUTION

Following the TRIWACO philosophy the density distribution is defined independently of the nodes of grid. Thus is can easily be applied to a new grid if the first one is not satisfactorily, or to test the influence of the node distances, etc. (so that a model can be re-used with a new finite element mesh or finite difference grid with the same basic data). The density has been defined with a separate map for each aquifer and is assumed to be constant over the vertical of the aquifer. The maps contain point values from measurements on island, and polygons in the sea where the density has been set to 1025 (see figure 4).

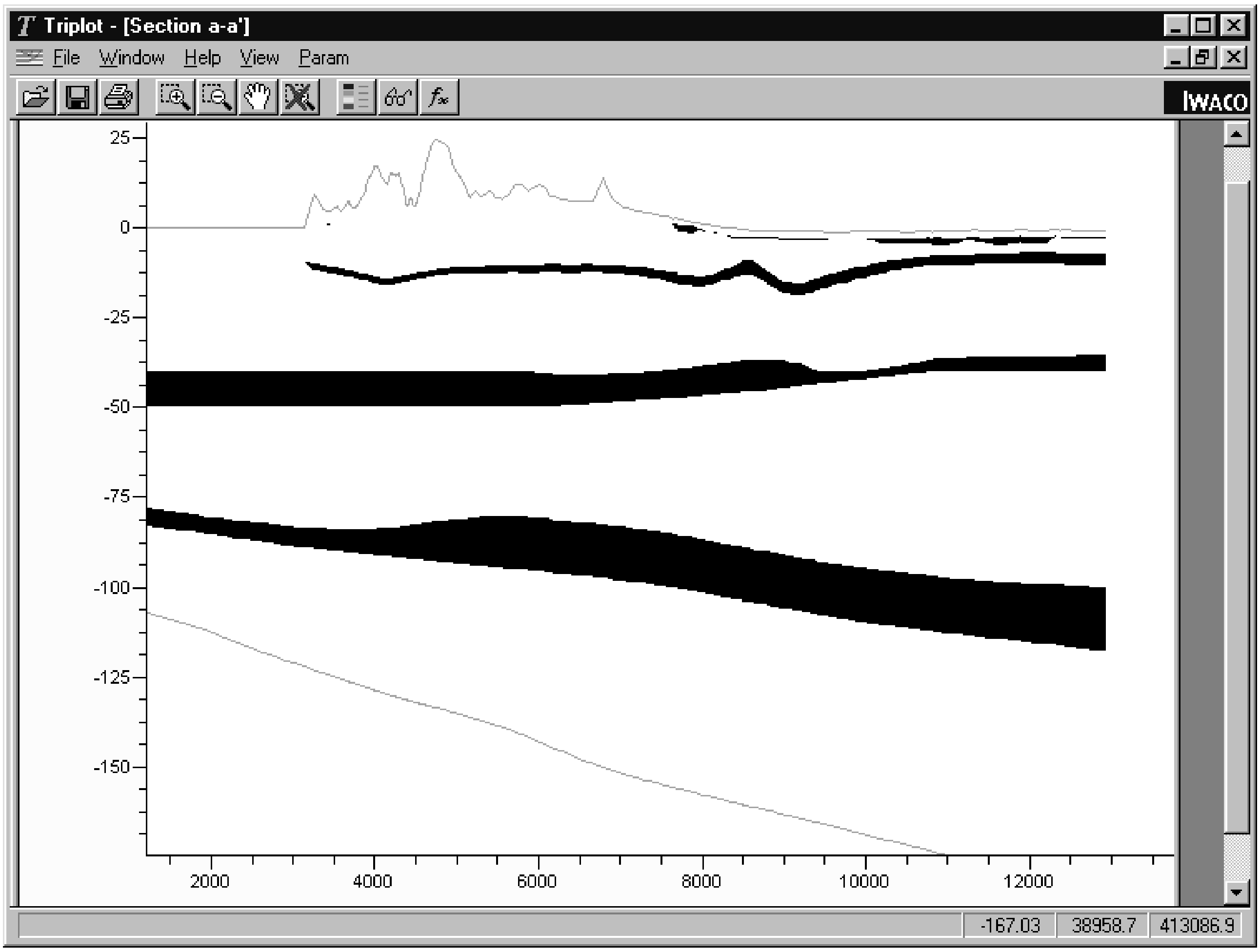
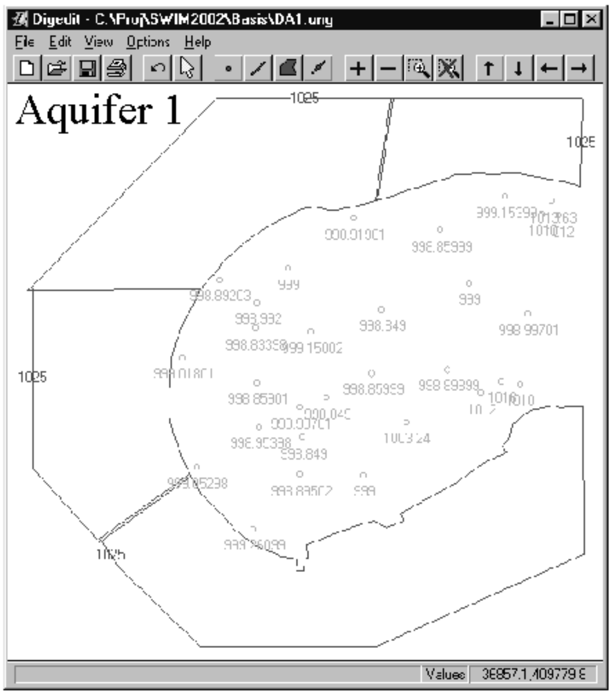


Figure 3 *Cross sectional view of model*



Sea:
Polygons with 1025
Island:
Kriging of point values

Aquifer	Points
1	30
2	34 + 2
3	34 + 12
4	19 + 18
5	31 + 21

Figure 4 *Density map*

The allocation assigns the polygon values to the points inside and uses kriging of point values for the values outside the polygons. This results in the density contours of figure 5.

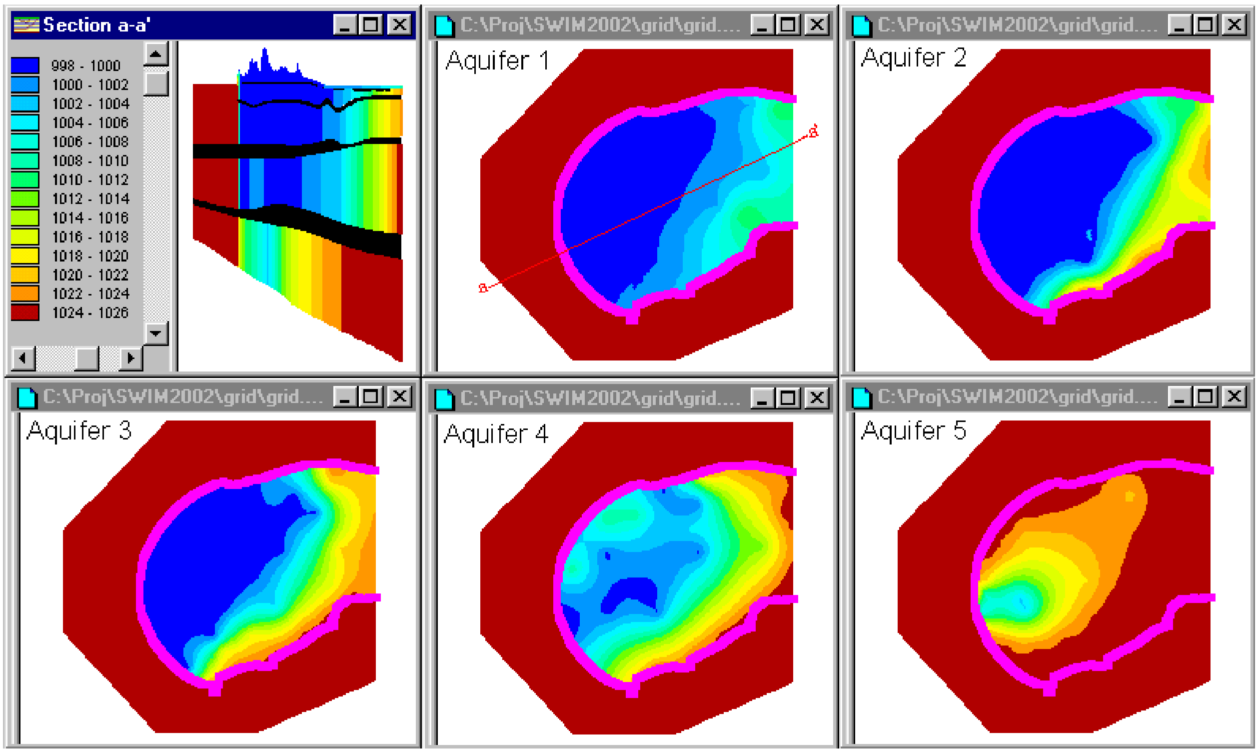


***Figure 5** Density contours*

PARAMETRIZATIONS

The existing parameterization of the density did not allow for calibration of the density in the transition zone from fresh to salt. We can think of various options to allow for this:

1. Replace the “sea”-polygon with ficticious density points;
2. Insert constant value polygons between the island and the “sea”-polygon;
3. Create a zone with discontinuous interpolation between the island and the “sea”-polygon.

Ad 1. This option has the advantage that the extent of the groundwater as salt as the sea does not need to be fixed beforehand. Disadvantage is very many points are needed for the shallow aquifers to get a reasonable transition because the rate of change near the shore is much greater than inland and off-shore (plus the under- and overshoot that the interpolation may give). The ficticious points would give too many degrees of freedom for the automatic parameter optimization.

Ad 2. This option puts in a transition zone between the (fresh) inland groundwater water (of which the density is reasonably well known) and the salt offshore groundwater (which can be assumed to have seawater density). The transition zone is split in a number of parts along the coast but has a single value from the coast into the sea.

Ad 3. This option is refinement of the previous option that asks for more degrees of freedom, but does more justice to the real distribution. Question is whether the variation of the density gives better results for the area of interest than the constant “representative” value of the previous option.

We decided that option 2 would be a good starting point. The width of the polygons probably is a very sensitive one, so we take that into account (see figure 6).

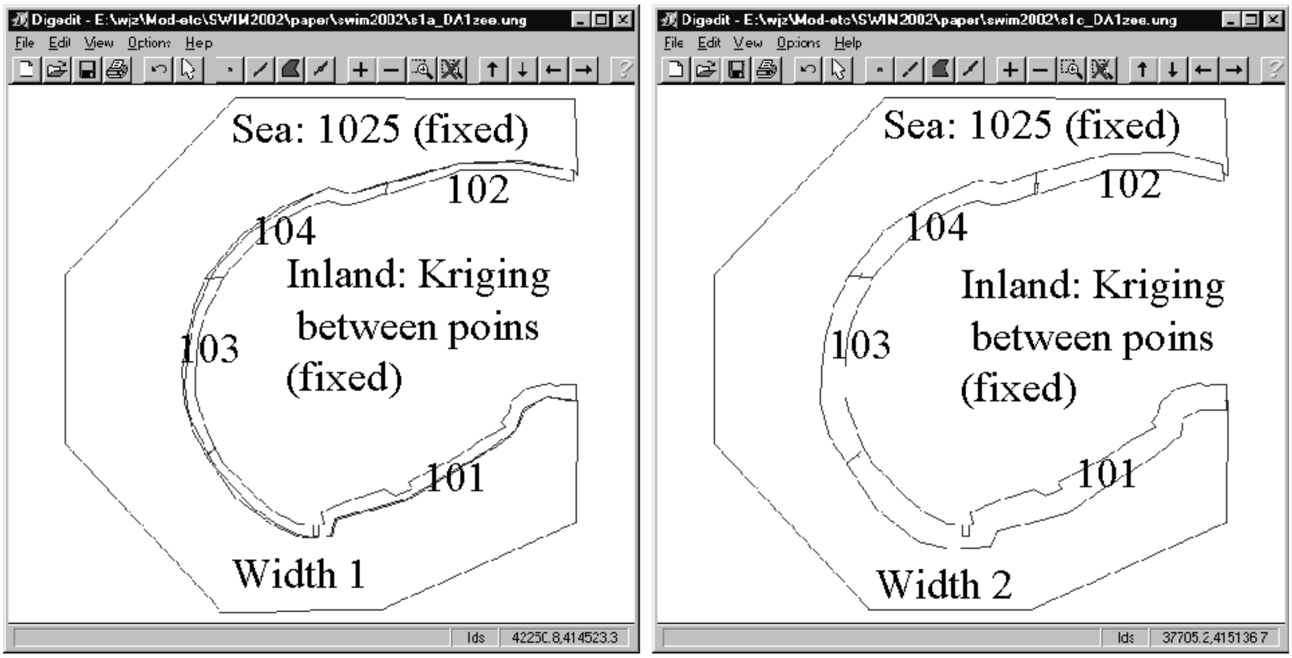


Figure 6 *Degrees of freedom for density parameterization*

PARAMETER SENSITIVITIES

The parameter sensitivities have been determined using TrCalCon, the **TRI**WACO module for **Cal**ibration and **Con**fidence (Zaadnoordijk, 2001). The parameter analysis consisted of a number of steps:

1. Sensitivity run with 16 calibration parameter items for both widths of the transition zone (4 zones in 4 model aquifers) in which the sensitivities and covariance matrix of these items is determined for the initial parameter item values;
2. Confidence calculations in which the parameter item co-variances of step 1 are translated into head and leakage variances using linear variance analysis;
3. Optimization runs in which the optimal values are determined for the most sensitive parameter items.

The calculated sensitivities from the first step are given in table 1.

ID	101		102		103		104		Σ 101 to 104	
Aquifer	Width 1	Width 2	Width 1	Width 2	Width 1	Width 2	Width 1	Width 2	Width 1	Width 2
1	19,5	19,7	0,1	0,1	2,3	2,8	0,5	0,7	22	23
2	143,5	554,9	13,8	31,0	2069,0	2937,0	145,8	224,5	2372	3747
3	1439,0	4693,0	335,9	810,9	4959,0	8259,0	973,0	2285,0	7707	16048
4	1371,0	2365,0	124,8	401,2	272,2	902,8	256,6	785,8	2025	4455
Σ 1 to 4	2973	7633	475	1243	7302	12102	1376	3296		

Table 1 *Calculated sensitivities*

The summed values at the bottom of the table show that the density polygons in the third aquifer are the most sensitive and polygon 103 is the most sensitive when looking at all aquifers. This holds for both widths of the polygons at the coast. Looking at the individual combinations there is some variation in the order of the sensitivities.

Whereas these sensitivities are abstract and only have meaning in a relative sense, the variances do have a physical meaning. The values are inversely proportional as a larger sensitivity means that a parameter item can be determined more accurately based on the calibration variables (head measurements in this case) and the resulting variance is smaller. Table 2 gives the minimum and maximum variances for the parameter items in the sensitivity runs.

Variance	Width 1	width 2
Maximum	179	114
	DA1/102	DA1/102
Minimum	0,0020	0,0023
	DA3/103	DA3/103

***Table 2** Extremes of the variances from the sensitivity calculations*

The minimum variance is very small, indicating that the value of polygon 103 in the third aquifer has a large influence on the head at the piezometers and can be calibrated using the measured values. The maximum variance is very large so that it is no use trying to improve the value of polygon 102 in aquifer 1 with automatic parameter optimization based on only these head values.

Before we select parameter items to optimise it is good to see how much the uncertainty in the densities contributes to the uncertainty in the model results that we are interested in.

Linear variance analysis allows the calculation of head and flux variances from parameter variances (see a textbook on statistics like Papoulis, 1984, or Zaadnoordijk, 2001). This has been implemented in TrCalCon (this TRIWACO-module also allows for non-linear variance analysis using the Monte Carlo method). The standard deviation (square root of the variance) of the head in the first aquifer as a result of the 16 density item variances is shown in figure 7.

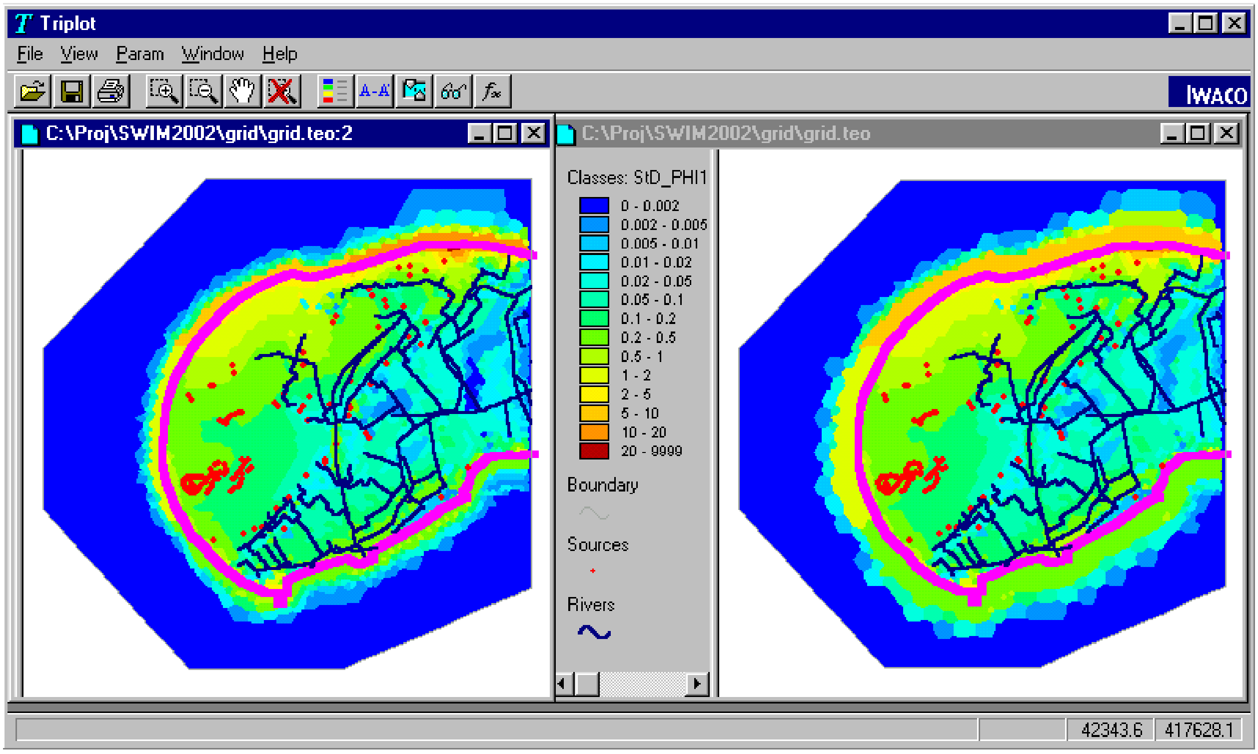


***Figure 7** Standard deviation of head in aquifer 1 as a result of the density item variances*

The values between 0.2 and 0.5 m in the area of interest indicate that the values of the density in the polygons along the coast have a significant influence on the heads in this area. Thus it is worthwhile to continue the exercise.

The next step has been to optimise the most sensitive items. We selected polygon 103 both in aquifer 2 and 3. In the optimization the objective function decreased from 849 to 824 (for the smaller width) and 823 (for width 2). The optimised values with the 95% confidence interval are given in table 3.

Aquifer	Width 1	Width 2
2	912 (717 – 1160)	979 (781 – 1229)
3	915 (793 – 1057)	916 (800 – 1049)

Table 3 *Optimized values for density in polygon 103 (with 95% confidence interval)*

The optimised values clearly show that the optimization compensates for errors in other parameters or the set-up of the model. So these results cannot be used directly. On the other hand, the differences between Width 1 and 2 suggest that a wider transition (or even fresh water) zone into the sea could be an improvement of the model. Thus the steps that we described above are only initial steps toward a better density transition at the coast in the head of Schouwen-model.

CONCLUDING REMARKS

Definition of the density distribution at the coast generally is difficult.

Reconstruction of the distribution with historical modelling is not an option. A very long simulation period is needed in order to get results that do not depend much on the unknown initial distribution. During this period, there is a large uncertainty of important geohydrological boundary conditions.

A better option is to derive an initial distribution from measurements and geohydrological knowledge and improve the distribution in the calibration of a groundwater model. In order to do this effectively, automatic parameter optimization should be used. Moreover, it should be possible to effectively test hypotheses, such as an equilibrium density distribution at the coast. This means that a good parameterization of the density is needed that gives proper degrees of freedom for the automatic calibration and that allows various hypotheses to be implemented. Additionally the parameterization can offer insight where the distribution is changing (where salt water is intruding and where the groundwater is freshening).

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