Analytical relations between model input statistics and output reliability for verification of a numerical groundwater model

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Abstract Analytical relations between input parameters, output variables and statistics for confidence are derived in order to verify automatic parameter optimization and model reliability packages to be used with a groundwater flow simulation package. The relations are based on the analytical solution for a semi-confined circular island with an extraction well in the centre. Piezometric heads are considered as well as the capture zone of the well. The relations have been used to test the calibration and confidence module TrCalCon of the groundwater flow simulation package TRIWACO. The module allows both linear-variance and Monte-Carlo confidence calculations. The latter show that the nonlinearity of the test problem causes significantly wider confidence intervals in the model results than the output of the former, and is tested with the analytical calculations.

Key words analytic solution; automatic parameter optimization; confidence analysis; numerical model

INTRODUCTION

Although verification of model codes always has been important, the testing of simulation programs has attracted renewed attention due to the ISO-9000 certification procedures that have started in many places. The consulting services of IWACO have been certified and in the procedure, tests have been set up for TRIWACO. This is a package for the simulation of groundwater flow which was originally setup in 1984 and has been improved and expanded since. It offers a large variety in top systems (i.e. the 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 three-dimensional (3-D) and fully 3-D 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. 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 now a true 32-bit Windows package (IWACO, 1999).

**Currently at:* IWACO Consultants for water and environment, PO Box 8520, 3009 AM Rotterdam, The Netherlands.

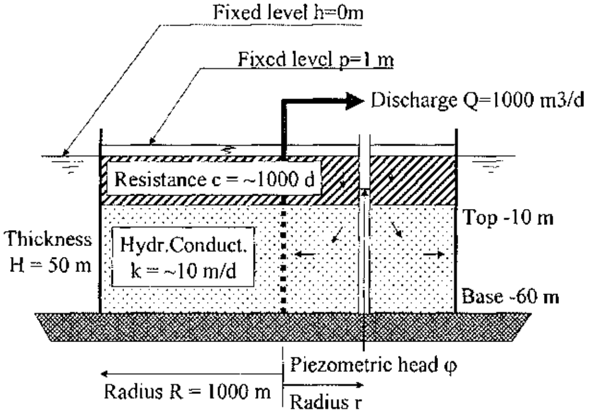

Fig. 1 Circular island with semi-confined aquifer and central extraction.

The tests had to be expanded when a module for automatic parameter optimization and model reliability assessment were added: TrCalCon (TRIWACO Calibration and Confidence). One of the tests has been based on the analytical solution for a semi-confined flow in a circular island with a central well (Fig. 1).

The advantages of this flow problem are that an analytical solution is available, and that aquitard resistance as well as hydraulic conductivity of the aquifer play a role in both the head distribution and the capture zone radius. Thus the covariance matrix of resistance and hydraulic conductivity obtained from the parameter optimization can be used to determine variances for the head and capture zone.

ANALYTIC DERIVATIONS

The piezometric head for the flow problem sketched in Fig. 1 can be derived from the general solution containing the modified Bessel functions of the first and second kind and order zero with the ratio of the radius r and the length λ as the argument (Strack, 1989). This length is equal to the square root of the product of the hydraulic conductivity k and thickness H of the aquifer and the resistance of the confining layer c: $\lambda = \sqrt{kHc}$. The resistance c relates the vertical flux through the confining layer to the difference between the piezometric head φ in the aquifer and p the constant polder level above the confining layer: $q_{vertical} = (\varphi - p)/c$. The coefficient of the modified Bessel function of the second kind K_0 is determined by the discharge of the central well and is equal to the coefficient in the well-formula of de Glee (Kruseman *et al.*, 1989). The boundary head h at the perimeter of the island with radius R determines the coefficient of the modified Bessel function of the first kind I_0. This results in the following equation for the piezometric head φ:

$$\varphi = \frac{\left[h - p + \frac{Q}{2\pi kH} \mathrm{K}_0(R/\lambda)\right]}{\mathrm{I}_0(R/\lambda)} \mathrm{I}_0(r/\lambda) - \frac{Q}{2\pi kH} \mathrm{K}_0(r/\lambda) + p \qquad (1)$$

The corresponding specific discharge q_r can be derived by applying Darcy's law $q_r = -k\dfrac{d\varphi}{dr}$ to equation (1) to get:

$$q_r = -\frac{k(h-p) + \dfrac{Q}{2\pi H}\mathrm{K}_0(\tfrac{R}{\lambda})}{\lambda \mathrm{I}_0(\tfrac{R}{\lambda})}\mathrm{I}_1(\tfrac{r}{\lambda}) - \frac{Q}{2\pi H\lambda}\mathrm{K}_1(\tfrac{r}{\lambda}) \tag{2}$$

The specific discharge is equal to zero at the perimeter of the capture zone. However, the author was unable to derive an analytical expression for this radius either by hand or using the symbolic mathematical package Maple V release 5. Instead a numerical approximation of the radius and its derivatives was developed.

Equation (1) can be used to generate n "measurements" of the piezometric head φ_i ($i = 1\ldots n$) that can be used in an inverse procedure. When the measurements are given a random offset, automatic parameter optimization will result in non-zero head residuals and a non-zero covariance matrix for the optimized parameters. The hydraulic conductivity k and the resistance c are selected for the optimization, which minimises the sum S of the squares of the head residuals:

$$S = \sum_{i=1}^{n} w_i(\varphi(r_i) - \varphi_i)^2 \tag{3}$$

where $\varphi(r_i)$ is the value calculated with equation (1) at the radius r_i of measurement φ_i, that is weighed with weight w_i, and n is the total number of measurements.

The values and variances that are determined by the minimum of S (equation (3)) can be translated into variances of dependent quantities by means of linear variance analysis (Papoulis, 1984):

$$\mathrm{var}(V(a,b)) = \mathrm{var}(a)\left(\frac{\partial V}{\partial a}\right)^2 + \mathrm{var}(b)\left(\frac{\partial V}{\partial b}\right)^2 + 2\mathrm{cov}(a,b)\frac{\partial V}{\partial a}\frac{\partial V}{\partial b} \tag{4}$$

The derivatives of the head (equation (1)) with respect to the logs of the resistance and hydraulic conductivity have been derived with Maple V release 5. The expressions are quite involved although the derivations are straightforward (see Appendix).

Analytical values for the variance and covariance can be derived from the sensitivity matrix or "Jacobian" and the residual heads after the parameter optimization (Lebbe, 1999):

$$\mathbf{C} = \frac{S}{n-m}(\mathbf{J}^T\mathbf{W}\mathbf{J})^{-1} \tag{5}$$

where $\mathbf{C}$ is the covariance matrix that contains the variances of the optimized parameters on the main diagonal, and the covariances as off-diagonal elements. The sum S is given by equation (3), m is the number of optimized parameters, $\mathbf{W}$ is a diagonal matrix with the weights of equation (3) as diagonal elements and $\mathbf{J}$ is the Jacobian matrix with elements:

$$J_{ij} = \frac{\partial \varphi_i}{\partial P_j} \quad (i = 1\ldots n;\ \ j = 1\ldots m) \tag{6}$$

where P_j stands for one of the optimized parameters.

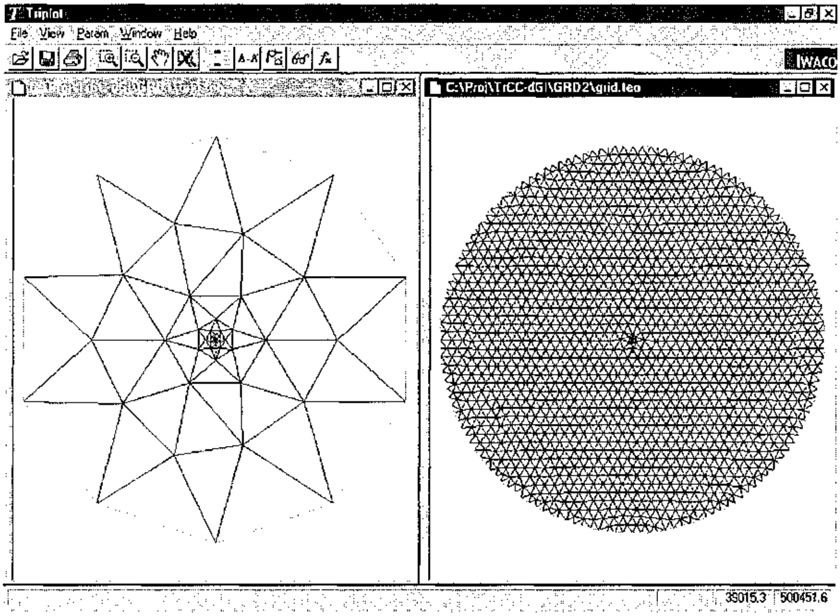

Fig. 2 Two finite element meshes for the test calculations.

CALCULATIONS

The parameter values in Fig. 1 have been used to generate 15 head measurements. Random offsets with a standard deviation of 0.25 m have been added to the exact values. The resulting "measurements" were the input for the automatic log-parameter optimization of the hydraulic conductivity *k* and the resistance *c*. The optimizations were carried out for two finite element meshes (Fig. 2). The coarse mesh has 57 nodes and 102 triangular elements. The 10 boundary nodes lie at a distance of 1000 m from the well, as do the 144 boundary nodes of the fine mesh, which give a much better representation of the circular boundary of the island. The fine mesh has 1546 nodes and 2946 elements (most node distances are 50 m).

RESULTS

The optimized parameter values and the covariance matrices are given in Table 1. The resulting variances for the head at a point halfway between the well and the boundary are given in Table 2. The analytic values compare well with the LVA results from the

Table 1 Optimized parameter values and covariance matrices.

	Theoretical:			TriCalb coarse grid:			TriCalb fine grid:		
	Value	Var.	Cov.	Value	Var.	Cov.	Value	Var.	Cov.
$^{10}\log k$	1.027	0.026	0.0016	0.936	0.029	0.0027	1.006	0.026	0.0012
$^{10}\log c$	2.949	0.015	0.0016	2.948	0.015	0.0027	2.953	0.014	0.0012

Table 2 Results for head at 500 m east of well.

	Head in m	Var(head) in m^2 Equations (4), (5) and (6)	LVA*	MC†
Analytical	0.1495	0.008138‡	–	–
Coarse	0.18		0.0081	0.0055
Fine	0.15		0.0078	0.0107

* LVA = linear variance analysis (TriConf)
† MC = Monte Carlo analysis (TraConf)
‡ $\frac{\partial\varphi}{\partial[{}^{10}\log(k)]} = 27.64;\ \frac{\partial\varphi}{\partial[{}^{10}\log(c)]} = -0.6013$

outcome TRIWACO. The fact that the MC results are worse shows the underestimation of the true values due to the linearity assumption in both the analytical and the LVA calculation.

The analytical radius of the capture zone is 559.8 m. The derivative of the radius with respect to the logs of the hydraulic conductivity k and resistance c are respectively –37.50 and 487.2. This results in a variance of 3649 or standard deviation of 60.41 m for the capture zone radius. TRIWACO does not calculate the radius of the capture zone itself. The radius follows from path line calculations. For this purpose path lines are traced forward from the surface in each node of the finite element mesh. The trace program produces a destination code for each path line (or node). The perimeter of all nodes with the code of the well is the capture zone. The fact that the radius of the capture zone is based on an "indicator" value (true/false) for the nodes implies that the linear variance module is not appropriate for the confidence determination of the capture zone radius. The Monte Carlo module can determine the probability of reaching the well in a straightforward manner. The results of the analytical linear variance calculations and the Monte Carlo runs with TRIWACO are presented in Fig. 3.

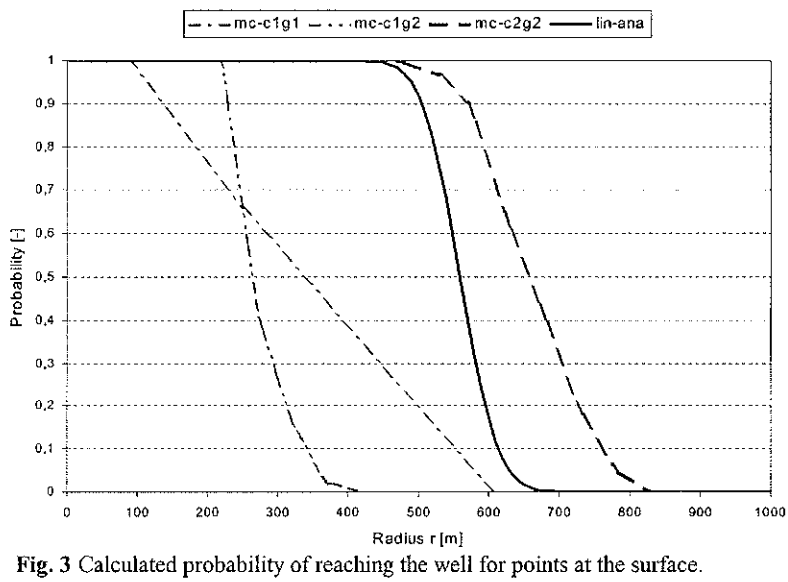

Fig. 3 Calculated probability of reaching the well for points at the surface.

The coarse grid clearly is too coarse for the calculation (mc-c1g1). The results are not good, even when the fine grid is used for starting points of the path lines in the flow field of the coarse grid (mc-c1g2). The graph of the analytic solution is calculated with the probability function of the normal distribution: $p = \frac{1}{2}\left[1 - \mathrm{erf}\left(\frac{r-\mu}{\sigma}\right)\right]$ with the analytical capture zone radius as average μ and the value mentioned above for the standard deviation σ. The fine grid produces a graph that has the expected shape and is worse than the analytical result as was expected since the latter is based on a linearity assumption.

CONCLUSION

The problem of a well in the centre of a circular island with a semi-confined aquifer allows testing of automatic parameter optimization with parameter covariance calculation and confidence calculations of model output based on the parameter covariance matrix. TrCalCon, the Calibration and Confidence module of the groundwater flow simulation package TRIWACO, produces good test results.

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APPENDIX

Derivative of the piezometric head φ with respect to the logarithm (base 10) of the resistance, ${}^{10}\log c$:

$$\frac{\partial\varphi}{\partial\, {}^{10}\log c} = \frac{Q\mathrm{K}_1(R/\lambda)Rc\ln(10)}{4\pi\lambda^3\,\mathrm{I}_0(R/\lambda)}\mathrm{I}_0\left(\frac{r}{\lambda}\right) - \frac{\left(h - p + \frac{Q}{2\pi kH}\mathrm{K}_0(R/\lambda)\right)\ln(10)}{2\lambda\mathrm{I}_0(R/\lambda)} r\mathrm{I}_1\left(\frac{r}{\lambda}\right)$$
$$+ \frac{\left(h - p + \frac{Q}{2\pi kH}\mathrm{K}_0(R/\lambda)\right)\mathrm{I}_1(R/\lambda)R\ln(10)}{2\lambda\mathrm{I}_0(R/\lambda)^2}\mathrm{I}_0\left(\frac{r}{\lambda}\right) - \frac{Qc\ln(10)}{4\pi\lambda^3} r\mathrm{K}_1\left(\frac{r}{\lambda}\right)$$

where ln denotes the natural logarithm (base e).

Derivative of the piezometric head φ with respect to the logarithm (base 10) of the hydraulic conductivity ${}^{10}\log k$:

$$\frac{\partial\varphi}{\partial^{10}\log k}=\frac{\left(\frac{-Q}{2\pi kH}\mathrm{K}_0(R/\lambda)+\frac{QRc}{4\pi\lambda^3}\mathrm{K}_1(R/\lambda)\right)\ln(10)}{\mathrm{I}_0(R/\lambda)}\mathrm{I}_0\left(\frac{r}{\lambda}\right)$$

$$-\frac{\left(h-p+\frac{Q}{2\pi kH}\mathrm{K}_0(R/\lambda)\right)\ln(10)}{2\lambda\mathrm{I}_0(R/\lambda)}r\mathrm{I}_1\left(\frac{r}{\lambda}\right)$$

$$+\frac{\left(h-p+\frac{Q}{2\pi kH}\mathrm{K}_0(R/\lambda)\right)\mathrm{I}_1(R/\lambda)R\ln(10)}{2\lambda\mathrm{I}_0(R/\lambda)^2}\mathrm{I}_0\left(\frac{r}{\lambda}\right)$$

$$+\left(\frac{Q}{2\pi kH}\right)\ln(10)\mathrm{K}_0\left(\frac{r}{\lambda}\right)-\frac{Qc\ln(10)}{4\pi\lambda^3}r\mathrm{K}_1\left(\frac{r}{\lambda}\right)$$