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Advantages and limitation of inverse modelling (automatic calibration) applied in complex and heterogeneous groundwater conditions

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ABSTRACT

Inverse modelling is more and more proposed as a standard tool in groundwater modelling packages. However, in practice, an intelligent and adequate use of these automatic calibration techniques requires a deep understanding of (a) the underlying assumptions, (b) the minimum required data and (c) the expected confidence of results. These issues are discussed and two case studies in different groundwater conditions are analysed with regards to these three aspects.

KEYWORDS

Calibration, groundwater, hydrogeology, inverse modelling

Introduction

Numerical modelling is extensively used for groundwater resource management, aquifer remediation or protection, and for any other problems related to groundwater. Actually, groundwater systems are very complex, so that any modelling must be based on simplified assumptions. The main processes and their corresponding equations have to be determined together with other conceptual choices as boundary conditions, time and space discretizations. To have an accurate simulation model, two requirements should be verified in this conceptual step:

- equations describing the model must describe as far as possible the physical reality of the system;
- model parameters (that have consequently a physical meaning) must be assessed with accuracy.

However, the chosen equations may not be the best suitable description of the original system. Futhermore, particularities of the system, such as geometry of the different units and heterogeneity in terms of hydrogeological parameters are difficult to measure accurately in the field, so that values of the hydrodynamic parameters remain always uncertain to some extent.

Thus, before using a model for management, the model results must be compared adequately with historic data: measurements of the main variable in the 2D or 3D space domain and possibly in function of time (transient conditions).

Calibration process

Adaptation of the values of the parameters in order to find the input-output relation of the simulation model consistent with the excitation-response relation of the original system is usually called calibration of the model. To do so, piezometric heads and solute concentrations (main variables of groundwater models for respectively flow and transport problems) can be measured and historical records are collected. Then, using an observed excitation-response relation, it is possible to determine indirectly the best structure and the best parameters of a model. Unfortunately, despite the existence of a unique physic solution, a lot of inverse problems (parameter estimation) are ill-posed meaning that the problem has not, mathematically, a unique solution. Additionally, very often, these solutions are not stable. To have only one solution, a prerequisite is that the number of unknown parameters is smaller than the number of observed data. Pratically, to reduce the number of unknown parameters, two ways may be chosen: a zonation method or an interpolation method (Yeh, 1986).

The zonation method consists in subdividing the modelled domain in several zones within which parameters are supposed to be constant and representative of some equivalent value for the considered zone. This approach allows, for example, to incorporate easily geological information on lithofacies variation.

The interpolation method consists in representing the parameter spatial variation by some polynomial/spline approach including coefficients that allow for adjustment of the final parameter distribution.

In this paper, only methods for parameter estimation, that reduce the number of unknown parameters by the zonation method, are discussed. It is obvious that if parameter estimation leads to unrealistic values of the parameters, the conceptual choice (model structure) must be changed.

Two kinds of methods can be used for calibration of a model: a trial-and-error procedure or an automatic algorithm. For both methods, initial estimations of the unknown parameters are introduced in the model.

Using a trial-and-error approach, the values of the parameters are manually modified in order to obtain a better fit between observation data and model output. This step is repeated until the adjustment with observed values is considered as satisfactory. Using such methods, subjective or interpretative geological information can most often be introduced directly or indirectly in the parameters optimisation process. On the other hand, this process is often long and fastidious. In practice, for many case studies calibrated by trial-and-error, the modeller tends to introduce (consciously or not) more zones than the number of available observations. The number of unknown parameters is larger than the number of observations. This can be justified only if other information is known from geophysical data, sedimentological data, etc. This process can be considered as an input of 'soft data' in the calibration process.

To check if the parameter estimate is 'correct', a performance criterion, expressed by some weighted norm between observed data and their computed equivalent in the model, is often used. Mathematically, this criterion (often called 'objective function') can be expressed by:

$$\Phi(p) = \sum_{i=1}^{N} W_i [c_i - c_i']^2$$

where p is the set of parameters, N is the number of observations, c_i are the computed values and c_i' the observed values, W_i are the weighting factors attributed to observations c_i'.

Weights can be very useful in setting the relative importance of each measurement type. They can be used for example to discriminate between different confidence levels in measurements or to take into account in a different way integrated measurements (as base flow measurements) with regards to punctual values (as piezometric head measurements). The way of choosing the weighting factors influence the result and so this criterion (or objective function) is always chosen in a subjective way.

Use of automatic calibration tools

Automatic calibration techniques can be classified in two main categories (Neuman, 1973; Yeh, 1986).

Direct methods (or equation error criterion method) assume that the state variable and its derivative are known within the whole domain of interest (this often implies some extrapolation of measurements to unobserved locations). In that case, parameter distribution and amplitudes are progressively adapted in each cell until the equations error, which is by definition the error resulting from the substitution of the measured (and extrapolated) state variable into the state equation is minimum.

Indirect methods (or output error criterion method) minimize some objective function, usually expressed by performance criterion, as presented above.

In the two following examples, this latest approach is used with the well-known automatic calibration tool PEST (Parameter ESTimation, Doherty *et al.*, 1994). It is used in combination with MODFLOW (Mc Donald & Harbaugh, 1988) to simulate typical groundwater flow problems.

The PEST code, which can be used either in steady-state or transient conditions, uses an indirect method to solve the inverse problem. In this code, three ways can be used to constrain the solution in function of the measured information (like geological data, results of pumping test, etc). The modeller can divide the domain into zones (zonation method). For each zone, an initial value for the unknown parameters as well as their lower and upper bounds must be specified. PEST provides also the possibility for the user to introduce prior information directly or indirectly in the objective function, thus constraining the solution. This prior information may be introduced, for example, under the form of prescribed relations between values in the different zones. Using PEST, it is also important to choose an initial parameter value that is close enough to the unknown optimised value to enhance the efficiency of the automatic process. Actually, a major problem is that the objective function Φ(p) can reach more than one minimum in the admissible set of parameters: a local minimum may be computed instead of the global one. To avoid this problem, the introduction of a realistic initial parameter values is recommended.

In the following two examples, PEST was used in two very different conditions. It provides a good occasion for discussing the influence of chosen initial value for the unknown parameters and of the weighting factors. The possibility to use PEST in transient conditions was also studied. Different rules of good practice will be deduced.

Case studies

The first site is located in the alluvial plain of the Meuse river (Belgium). The studied zone cover an area of approximatively 0.045 km². The site is equipped with four pumping wells (P1, P2, P4, P6) and 10 piezometers (Pz1 to Pz10). Geological layers consist mainly of sandy gravel layers overlaid by a silty loam layer. The hydraulic conductivities of sandy gravels, as determined by pumping test, range from 10^{-5} to 10^{-2} m/s. As the water table lies in the sandy gravel layer, this aquifer system is represented by a one-layer model. This model was calibrated on piezometric heads measured in the different pumping wells and piezometers in natural flow conditions considering steady state conditions.

Step by step, by trial-and-error, the number and the shape of zones with different hydraulic conductivities were determined. The best results were found using eight zones. Then, in order to study the influence of the initial value of the unknown parameters, three automatic calibrations of the hydraulic conductivities in these eight zones were performed with uniform initial values of 0.002, 0.006, 0.05 m/s (respectively called 'INITIAL02', 'INITIAL06' and 'INITIAL5' in table 1). The same initial value of hydraulic conductivity has been chosen for all the zones. For trial-and-error calibration, the chosen initial value for each zone was determined by pumping test. Table 1 allows to compare the optimised hydraulic conductivities for these eight zones as obtained from both trial-and-error and automatic methods. Table 1 also shows that for this particular case study, the initial values of the unknown parameters have nearly no influence on the obtained value of the objective function. However, the chosen initial values can apparently influence the obtained final values for hydraulic conductivitiy in each zone. Most significant changes are observed in the zone 4. Of course it is beyond the scope of this paper to discuss more in details these results. The objective function (Φ) obtained by automatic calibration is systematically better than by trial and error method. The obtained hydraulic conductivities stay realistic compared to values measured by pumping tests.

As dynamic water levels (measured in pumping wells) are less accurate than those measured in piezometers, the influence of the weighting factor attributed to these data was studied (table 2).

Table 1. Influence of initial values on the optimized hydraulic conductivity values and comparison between automatic, manual calibration and results from pumping tests.

	Hydraulic conductivity values: pumping tests (m/s)	**Hydraulic conductivity values obtained after calibration (m/s)**			
		Trial-and-error calibration	Automatic calibration		
Zones			*INITIAL02*	*INITIAL06*	*INITIAL5*
z1	2.0 E-02	1.0 E-02	9.1 E-03	9.4 E-03	9.9 E-03
z2	9.0 E-03	2.0 E-02	4.1 E-03	4.3 E-03	4.1 E-03
z3	5.0 E-03	6.0 E-03	5.2 E-03	5.2 E-03	5.2 E-03
z4	6.0 E-04	5.0 E-04	8.2 E-05	8.6 E-05	1.2 E-04
z5	2.0 E-03	4.0 E-03	3.6 E-03	3.7 E-03	3.6 E-03
z6	5.0 E-03	5.0 E-03	2.9 E-04	2.5 E-04	2.2 E-04
z7	2.0 E-03	9.0 E-03	5.0 E-02	5.0 E-02	5.0 E-02
z8	-	1.0 E-05	2.9 E-05	3.7 E-05	3.9 E-05
Objective function Φ		0.02306	0.01201	0.01201	0.01200

Table 2. Influence of the weighting factors on the obtained values of the objective function an on the reached differences between observed and computed piezometric heads in the wells.

	Trial-and-error calibration	**Automatic calibration**			
		DEFAULT	WEIGHT1	WEIGHT2	WEIGHT3
	$W_{pumpwells}=1$	$W_{pumpwells}=1$	$W_{pumpwells}=0.1$	$W_{pumpwells}=0.2$	$W_{pumpwells}=0.3$
Pz5	6.13 cm	6.3 cm	7.1 cm	7.1 cm	7 cm
Pz6	-1.87 cm	-2.3 cm	-1.8 cm	-1.6 cm	-1.4 cm
Pz7	2.33 cm	1.9 cm	0.1 cm	0 cm	0.4 cm
Pz8	0.51 cm	-0.4 cm	2.4 cm	-0.2 cm	-0.8 cm
Pz9	-5.38 cm	-6.1 cm	-2.7 cm	-2.7 cm	-3.3 cm
Pz10	-1.62 cm	-3.2 cm	1.5 cm	1.4 cm	0.6 cm
P1	**-11.08 cm**	**3 cm**	**23 cm**	**13 cm**	**12 cm**
P2	-6.46 cm	-5.1 cm	-5.2 cm	-6.2 cm	-6.7 cm
P4	**-25.86 cm**	**-1.8 cm**	**-22 cm**	**-11 cm**	**-6 cm**
P6	**-10.82 cm**	**0.2 cm**	**-4 cm**	**0.2 cm**	**1.4 cm**
ϕ (m^2)	0.02306	0.01687	0.01142	0.01149	0.01257

A reference automatic calibration (called 'DEFAULT') with a weight factor of 1 for all the observations was computed. Then three other automatic calibrations were performed with weighting factors of 0.1, 0.2 and 0.3 for the pumping wells P1, P4 & P6 (respectively called 'WEIGHT1', 'WEIGHT2', 'WEIGHT3'). The objective function for the trial-and-error calibration was computed with weighting factors of 1 for all the observations. Results of table 2 show the influence of the weighting factors on the objective function and on the reached differences between observed and computed piezometric heads. However, due to changes in weighting factors, the computed objective functions can not be compared anymore because they are not calculated in the same way.

The second site consists in an area of approximately 0.5 km^2, located in Gaume (South of Belgium), in the North-East of the geological Paris basin. Secondary sub-horizontal layers are overlying a Primary bedrock. These sub-horizontal layers consist mainly of three sandy layers (aquifers) separated by two clayey layers (aquitards). 23 piezometers were drilled in the three sandy aquifers. Different pumping tests were performed in different wells in each aquifer. During pumping tests, the drawdown was measured in the tested aquifer as well as in the other aquifers. Hydraulic conductivity values of the aquifers range from 1.10^{-6} to 1.10^{-4} m/s. The hydraulic conductivity values of the clayey aquitards, measured on samples in laboratory are approximatively 10^{-9} m/s. Suspecting a scale effect leading to an underestimation of the actual hydraulic conductivity values of the aquitards, interpretation of these pumping tests is performed using a quasi-3D model in order to fit by calibration the vertical leakance factors through the aquitards. In a first step, local models (0.04 km²) were built around each piezometer. Hydraulic conductivity for aquifers and vertical leakance C for aquitards were considered to be uniform in each considered layer. PEST was here only used to optimise the vertical leakance values, the K values for aquifers being considered as known. Calibrations in steady state conditions, using measured drawdowns in the three aquifers, have provided results of table 3. It shows the influence of the initial value ($C1_{initial}$) for the vertical leakance of the upper aquitard on the corresponding optimised value ($C1_{optimized}$), the value for the second aquitard being always the same. It appears that in a situation where high contrasts in hydraulic conductivity values are found between the different layers of the modelled domain, optimised parameters can be very influenced by initial values (table 3). Also, if the C-values are very low, a change induces nearly no influence on the computed piezometric heads. The optimisation process stops at a local minimum because the change of the parameter value induces a so small change in results (main variable) than the stopping criteria is reached.

Table 3. Influence of initial values on the optimised vertical leakance C.

$C1_{initial}$	1.37E-09	1.00E-10	9.00E-08
$C1_{optimized}$	1.37E-09	1.30E-10	8.99E-08
Φ	-	0.001152	0.001689

In a second step, a global model was developed for the whole area. For this site, many piezometric data were available for the different pumping tests. A lot of parameters (hydraulic conductivities, storage coefficients, vertical leakances) could be optimised in transient conditions. It is not the aim of this paper to describe this case that has shown in practice that for a complicated case, an automatic calibration procedure can also be very time consuming.

Conclusion

The two examples, described here above, show that precautions must be taken when inverse modelling is performed. An automatic procedure provides an optimised set of parameters only for the initially chosen spatial distribution. If no information is available for determining a realistic initial spatial distribution of the parameters, it could be important to perform a sensitivity analysis to this initial distribution of zones. It has been shown also that the initial value introduced in each zone could have a strong influence on results. There also, a sensitivity analysis can be useful to be sure to reach the global mimimum of the objective function.

Chosen weighting factors of the objective function can influence the obtained calibration. In that way, the objective function can always be considered as 'subjective' to some extent. Two objectives functions calculated with different weighting factors cannot be compared.

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