AUTOMATIC CALIBRATION OF A 3D GROUNDWATER MODEL APPLIED TO THE MURAVERA-FLUMENDOSA COASTAL AQUIFER (SE SARDINIA, ITALY)

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ABSTRACT

The performance evaluation of a groundwater model is a complex task due to the large heterogeneity of hydrogeological properties, the scarcity of appropriate field data and the variability of boundary conditions. In this study an automatic calibration procedure has been developed and applied to the 3D groundwater model of the Muravera-Flumendosa coastal basin. The aquifer is threatened by seawater intrusion due to groundwater overexploitation and reduced replenishment. Aim of the study is to improve the understanding of the groundwater degradation mechanism in a complex hydrodynamic environment (diverted upstream surface waters, lagoons and channels) and to support the decision between alternative remediation scenarios. Field data are mainly represented by piezometric heads and salt concentrations and only for a very limited extent by hydraulic conductivity measurements. The finite element CODESA-3D model has been applied to simulate 3D density-dependent groundwater flow and contaminant transport in the subsurface. Inflow boundary conditions and aquifer recharge have been estimated on the basis of a distributed hydrological model calibrated against monthly streamflow data. Finally, the PEST model-independent tool has been configured to calibrate hydraulic parameters of the groundwater system against head data in an iterative fashion. Software system integration issues, on the one hand, and data uncertainty, sensitivity analysis, and calibration rules, on the other hand, are carefully reviewed and described. The model calibration procedure has shown to be a highly demanding, although computationally feasible, task.

1. INTRODUCTION

The usefulness of predictive simulations obtained by groundwater models is often hampered by the inability to quantify the reliability of model results. Uncertainty in model predictions primarily stems from a number of errors relating to the model formulation, such as inadequate concept and description of processes and interactions, of data spatial and temporal variability, of boundary conditions and stresses, and incorrect parameterisation. Significant research has been conducted in the field resulting in a variety of approaches that can be employed to incorporate these errors into the modelling process and to quantify the degree of uncertainty in model based decision making. Different techniques can be used to calibrate a model, such as inverse calibration and neural network procedures, and alternative objective functions can be defined taking into account available data and model complexity (IAHS Publ. 277, 2002).

In this study an optimization procedure has been developed to iteratively calibrate hydraulic conductivities of the groundwater system against head control data in a weighted least square sense. The calibration is carried out using the PEST model-independent calibration tool (Doherty, 2002) and the CODESA 3D groundwater model (Gambolati et al., 1999, Lecca, 2000) applied to the Muravera-Flumendosa coastal phreatic aquifer.

2. OPTIMIZATION PROCEDURE

PEST is a nonlinear parameter estimation package that can be used to calibrate parameters for any model without requiring model modifications. The tool is currently being used in many field of science and engineering and it has become a groundwater industry standard. To calibrate a given model by means of inverse modeling, PEST uses a nonlinear technique known as the Gauss-Marquardt-Levemberg (GML). A mathematical requirement of the GML method is that the dependence of model-generated observations on adjustable model parameters be continuously differentiable.

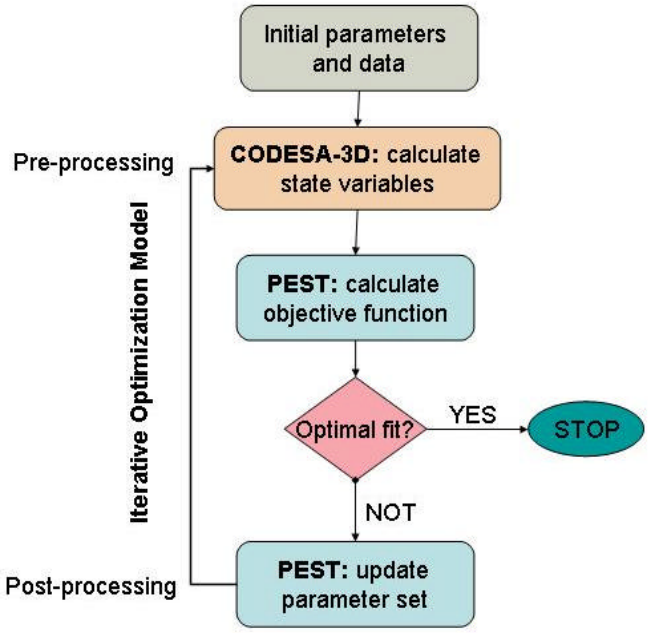

FIGURE 1. Workflow of the calibration procedure. Simulation (CODESA-3D) and optimization (PEST) modules are coupled by means of *ad hoc* processing tools.

PEST has been configured to calibrate the hydraulic conductivity values of the aquifer against measured groundwater heads. In addition, a suite of pre- and post-processing tools to link together PEST outputs (hydraulic conductivity estimates) to groundwater model inputs and, in turn, CODESA-3D outputs (simulated heads) to PEST control data (measured heads) have been developed *ad hoc* (Figure 1).

The groundwater model is CODESA-3D: a three-dimensional finite element simulator for miscible flow and solute transport in variably saturated porous media on unstructured domains. The flow and solute transport modules are nonlinearly coupled through the variable density of the filtrating mixture made of water and dissolved pollutants. Another source of nonlinearity is represented by the variably saturated flow module.

The objective function (*Phi*) is the sum of the squared weighted residuals between measured and simulated groundwater heads. For linear models the GML algorithm can give the optimal parameter set in just one iteration while for nonlinear models, like CODESA-3D, parameter estimation is an iterative process. At each iteration step the relationship between adjustable model parameters and model-generated observations is linearized by means of the Taylor expansion about the current parameter set. Hence the derivatives of all outputs with respect to all parameters are calculated by means of finite differences. Then the linearized problem is solved for a better parameter set and this set is tested by a new model run. The iterative procedure is stopped when the objective function reduces to a minimum corresponding to a user-defined threshold. The adopted criterion is that the lowest three objective functions achieved in all the iterations carried out are within a distance of 0.001 relative to the lowest *Phi*.

As the calibration process proceeds, PEST continuously records the sensitivity of each adjustable parameter to the model outputs. Through this information the modeler can evaluate those parameters that influence most strongly the calibration and those that are not relevant to it. Other additional analysis comprises adjustable parameter confidence intervals, and coefficient matrices of parameter correlation and covariance.

3. THE MURAVERA-FLUMENDOSA SITE

The Muravera plain is located at the mouth of the Flumendosa river in the South-Eastern part of the Sardinia island and covers an area of about 130 km^2 (Figure 2). The population of the main centres of the plain (Muravera, Villaputzu and San Vito) is comprised of 13000 residents and dramatically increases during summer. Apart from tourism, traditional economic activities are farming, sheep and goat grazing, and citrus fruit growing. The climate of the Flumendosa watershed is Mediterranean subtropical, characterized by a strongly variable rainfall regime. Precipitation is largely confined to the winter months and the distribution is somewhat irregular, with as much as 1165 mm/year in the highest areas and 618 mm/year along the coast (Cao et al., 1996). The rainfall regime is characterized by a peak rainfall in December, a minimum in July, and an average value of about 860 mm/year. The complex stratigraphy of the plain is mainly composed of Quaternary alluvial deposits (up to a few hundreds meters thick) which overlay the Palaeozoic bedrock outcropping at the edges of the plain. Two aquifers have been identified in the plain: a shallow phreatic aquifer and a deeper semi-confined aquifer, separated by a possibly discontinuous clayey layer, which ranges from a few meters to several tens of meters thickness (Balia et al., 2003). Lagoons and natural channels (“Foxi”), covering an area of about 1.13 km^2, play an important role for the water balance of the basin. The Foxi Pedrionnas, Bau Obilu and Flumini Becciu (Figure 2) are old arms of the Flumendosa River connecting the sea to the inland territory and are used mainly as fisheries.

Saltwater encroachment in the coastal aquifer and salinisation of soils were first observed in the `50s and correlated with a significant lowering of the groundwater table. Likely causes of saltwater intrusion are both anthropic (upstream damming of the Flumendosa river and its tributaries, aquifer overexploitation, irrigation solute recycling, and fish-farming) and natural (recurrent droughts and fossil salt waters). Currently both the phreatic and the confined aquifers are heavily contaminated by saltwater and data collected during the last 20 years show a salinisation process steadily moving inland. As a result, extensive citrus plantations have been irremediably damaged and other cultivations have been severely affected. Remedial measures are being considered by the regional water agency including withdrawal rationalisation, creation of a district irrigation network, artificial recharge with treated wastewater and hydrodynamic barriers.

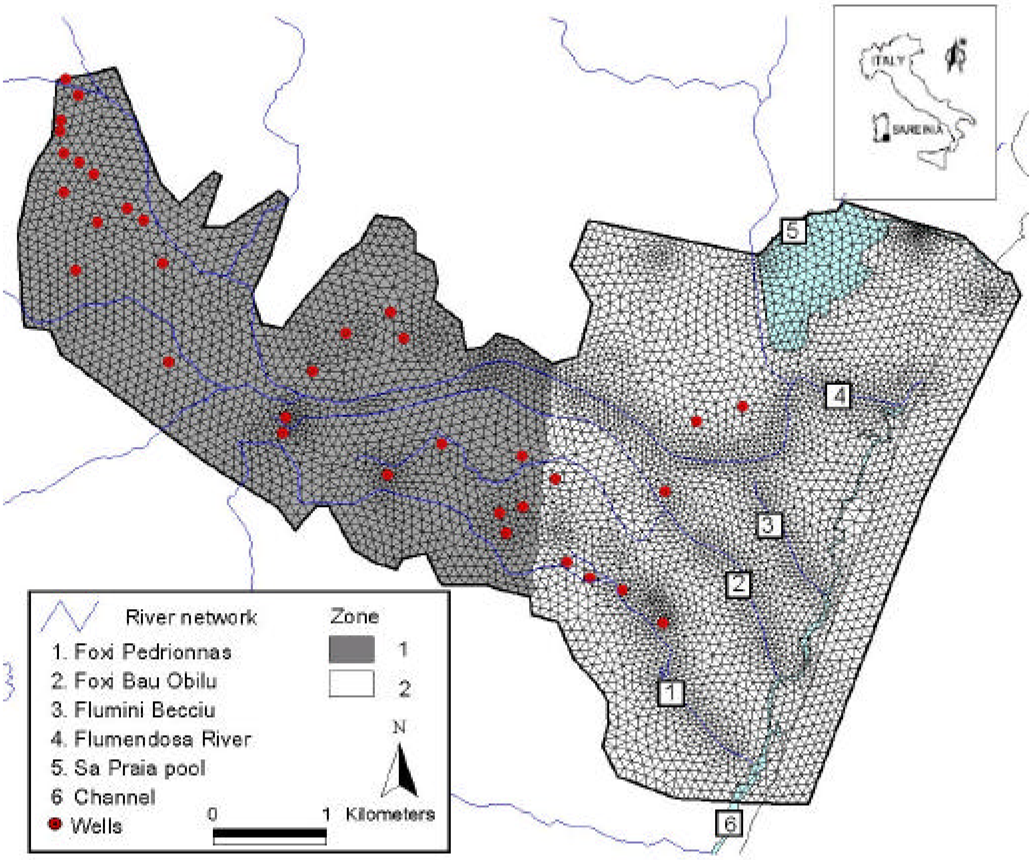

FIGURA 2. The surface triangulation of the Muravera-Flumendosa coastal aquifer (SE Sardinia, Italy) incorporates main hydrography and monitoring wells. Conductivity zones are also shown.

4. MODEL SETUP

The domain has been delimited taking into account the main geologic features, hydrogeology, internal water bodies and other territorial elements (urban areas, wells, etc.). The modelling area (25.9 km^2) is limited on the northern and southern boundaries by Paleozoic outcrops, on the East by the sea and on the West by an imaginary line parallel to the coast. The surface triangulation, containing 9839 triangles and 5105 nodes, incorporates monitoring wells and the main hydrography as grid points and lines. Mesh refinement has been introduced to have smallest triangles (175 as compared to the largest of 6619 m^2) along the coast and around zones of heavy pumping. The 3D tetrahedral mesh of the phreatic aquifer system has been obtained by vertical projection of the surface mesh with an average depth of 40 m.

The seawater intrusion simulation has been organized in two subsequent stages: 1) steady state freshwater flow and 2) transient state seawater intrusion. Flow initial condition (IC) at the 1st stage is assumed fully saturated hydrostatic pressure head distribution. In turn, simulated steady state pressure heads are assumed as IC for the seawater intrusion simulation

(2^{nd} stage, not shown). Southern and northern domain boundaries are set impervious to groundwater flow at the contact with rock outcrops. Also aquifer bottom is assumed impervious. Western boundary of the aquifer system is allowed to receive some groundwater flow from uplands. The volume *Q* recharging all the aquifer systems of the Flumendosa watershed is estimated equal to 65 Mm^3/year according to calculations of the SWAT hydrological model (Neitsch et al., 2000) calibrated against monthly streamflow data (Cau et al., 2003). Seaside eastern boundary, transversal channel and lagoons (Figure 2) are assumed fixed head with reference to mean sea level. Using SWAT also vertical recharge *q* is estimated up to 2.0 10^{-9} m/s. Calibration has been performed in steady state condition without pumping.

Very few measures of hydraulic conductivities, which are characteristics of highly permeable alluvia, are available (Ardau et al., 1996). Horizontal (K_h) and vertical (K_v) hydraulic conductivity initial estimates are 10^{-4} and 10^{-5} m/s, respectively, both for the western (1) and eastern (2) zones depicted in Figure 2. Porosity is set to 0.3 and elastic storage to 10^{-2} m^{-1}.

Control data (piezometric heads [m]) were measured in June 1999 (Barrocu et al., 1999) in the 34 surface agricultural wells scattered in the plain (Figure 3). Observation error, related to any aspect of the observation not accounted for by the model (measuring device, spatial location, seasonally and inter-annual fluctuations in head measurements, etc.), is set to 1 m. Weights of measured heads, that should be inversely proportional to the standard deviation of observations, are assumed all equal to unity.

5. RESULTS

With the initial model setup the simulated groundwater heads are higher then the measured ones (Figure 3-A panel). After calibration only few control points exhibit residuals outside the observation error bar (Figure 4). This may be due either to the low quality of control data or to the lack of model details. Indeed, the conceptual model does not take into account local pumping, recharge spatial and temporal variability and small scale heterogeneity. Figure 3-B panel shows the groundwater head contour lines for the calibrated system along with residuals at the monitoring wells. Closer to the sea the simulated water table is generally depressed and has a very low gradient due to the flat topographic surface and the boundary conditions imposed on the sea, the channel and the lagoon.

Best estimates of adjustable parameters are listed in Table 1 along with initial values allowed range and increment. Calibrated parameters K_{1h}, K_{1v}, K_{2h} and K_{2v} read as follows 7.8 10^{-6}, 1.2 10^{-6}, 1.4 10^{-5}, and 4.2 10^{-6} m/s, resulting in zone 2, closer to the sea, more permeable then zone 1. The 95% confidence intervals of adjustable parameters are [6.61–9.29], [0.41–3.37], [5.63–35.12], [1.01–17.39] multiplied by a factor of 10^{-6}, respectively.

TABLE 1. Initial and best estimates for hydraulic conductivity K values [m/s].

Zone	Initial K_h	Initial K_v	Lower bound	Upper bound	Increment	Calibrated K_h	Calibrated K_v
1	10^{-4}	10^{-5}	10^{-7}	10^{-2}	10%	7.8 10^{-6}	1.2 10^{-6}
2	10^{-4}	10^{-5}	10^{-7}	10^{-2}	10%	1.4 10^{-5}	4.2 10^{-6}

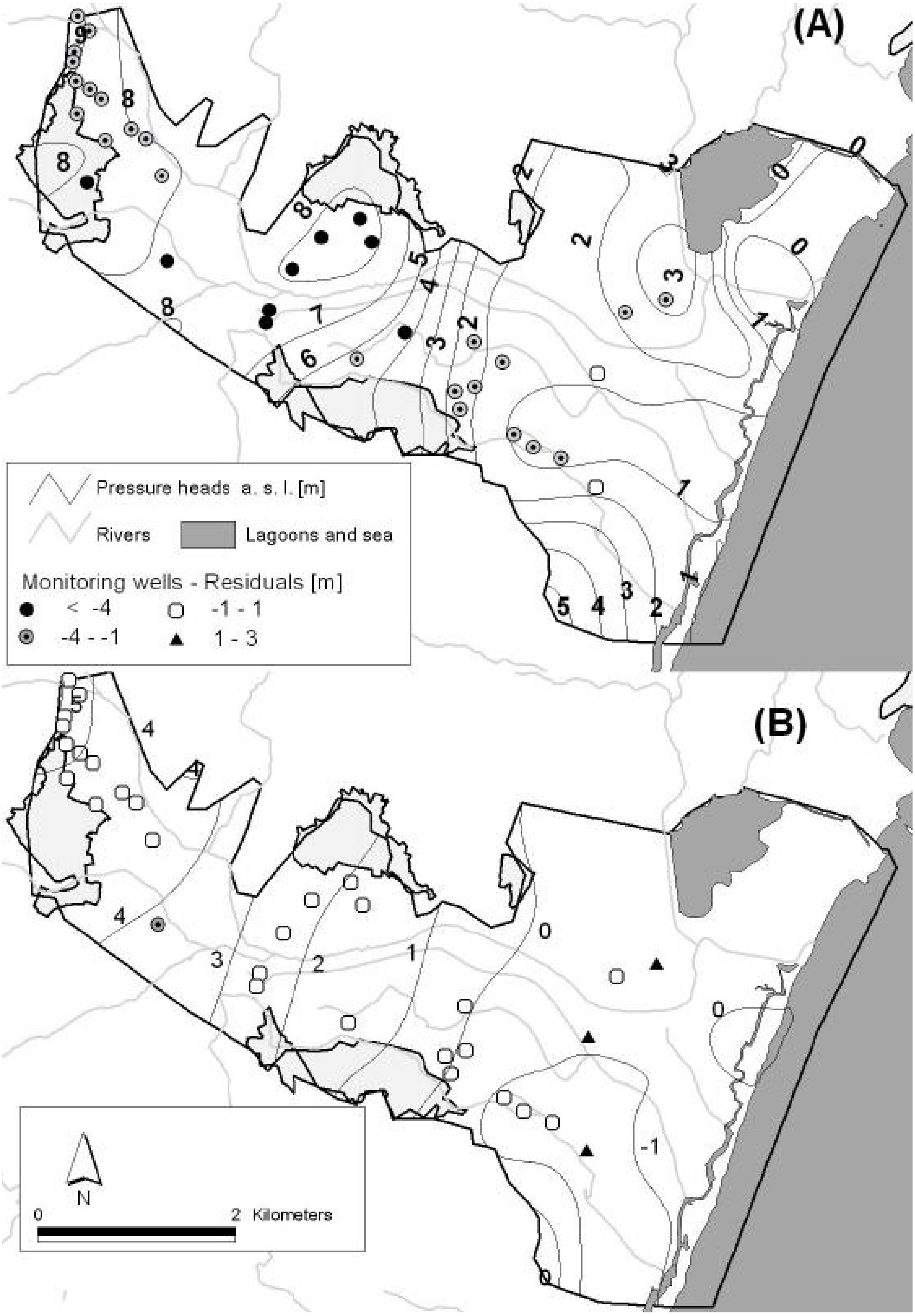

FIGURE 3. Groundwater head contour lines in meters a.s.l. of the no-calibrated (A) and calibrated (B) models. Residuals [m] at the monitoring wells are also shown.

TABLE 2. Residual analysis.

Number. of residuals	*Phi*	Maximum Residual	Minimum Residual	Mean value	Standard variance	Standard error
34	16.81	1.45	-1.71	0.11	0.56	0.75

The extent to which model outputs honor field-measured counterparts is measured by the value of the objective function. In this case *Phi* is equal to 16.81 corresponding to a standard error of 0.75 m (Table 2). Such error is consistent with the observation accuracy. The goodness of fit is also demonstrated by the correlation coefficient (R) of 0.95. Coefficient R allows the modeler to directly compare different calibration exercises, being independent of the number of observations.

TABLE 3. Composite parameter sensitivities.

Parameter name	K_{1h}	K_{1v}	K_{2h}	K_{2v}
Sensitivity	1.23	0.12	0.21	0.18
Relative sensitivity	6.27	0.73	1.04	1.00

The PEST tool has been used to exploit the effect of possible hydraulic connections between the Foxi and the groundwater basin by imposing fixed heads on the grid nodes that fall within these superficial water bodies. This alternative conceptualization proved to be less effective (R = 0.85) although some control wells near the coast were better simulated.

Table 3 shows the composite sensitivities of adjustable parameters to model outputs for the overall optimization. Those parameters with lowest sensitivities are the most likely to cause trouble to the inversion process giving rise to slow convergence. Modeler can take control over this unwanted behavior temporarily freezing insensitive parameters for one or two optimization iterations when needed.

The number of optimization iterations required by the Muravera-Flumendosa steady state model to converge was 15 for a total of 132 CODESA-3D runs. The average elapsed times for a single model run and the whole optimization procedure are 4.7 and 1238 s, respectively on a AMD Opteron 246 processor (2000 MHz clock) machine equipped with 2Gbyte RAM.

6. CONCLUSIONS

The study presents and demonstrates how an automatic calibration can be carried out based on a nonlinear model-independent parameter estimation package coupled to a 3D groundwater model. Hydrologists can benefit of statistical analysis available by means of such model inversion procedure to refine the conceptual model of the system under study, to exploit available data, and to estimate the uncertainty associated with model predictions. Future application to transient-state seawater intrusion simulation will include the use of PEST parallel option on networked PCs.

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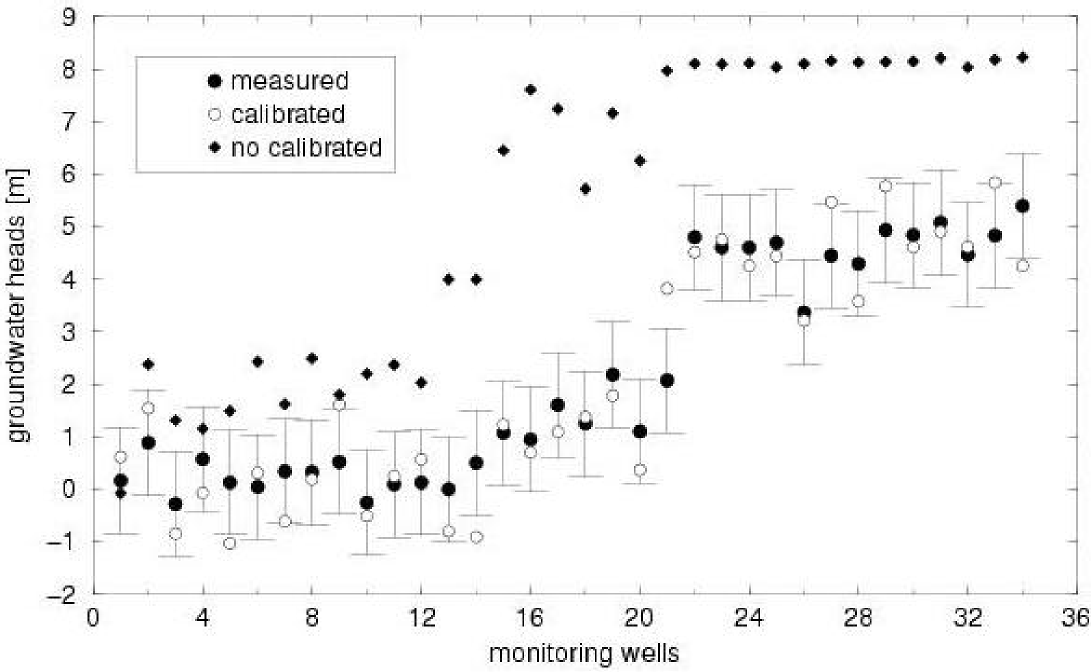

FIGURE 4. Calibration graph showing measured (*black circle*), calibrated (*opaque circle*) and no calibrated (*diamond*) groundwater heads (June 1999) at the 34 monitoring wells ordered according to sea distance. Field measure error bars are also shown.

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