Calibration and uncertainty analysis of a regional fault zone groundwater flow and solute transport model using Nonlinear Least-Square Regression

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ABSTRACT
The Nonlinear Least-Square Regression (NLSR) approach was used to estimate model parameter values in the calibration of a transient groundwater flow and solute transport model of a heterogeneous fractured rock aquifer system. Regression statistics including sensitivity, relative composite sensitivity and correlation coefficients were calculated for analysing the parameter uncertainty. With the presented case study we demonstrated that the NLSR technique provides a simple way to quantify parameter uncertainty and to improve calibration of a groundwater flow and solute transport model of a complex fault zone system.

RÉSUMÉ
La méthode des moindres carrées non-linéaires (MCN) est utilisée afin d'estimer les valeurs des paramètres de calibration pour la modélisation du passage de la nappe phréatique et du transport d'un soluté à travers une roche fracturée de manière hétérogène, dans un système aquifère souterrain. Cette régression statistique, incluant le coefficient de sensibilité, la sensibilité relative composée et le coefficient de corrélation, fut employée pour déterminer le paramètre d'incertitude. Avec le cas d'étude d'une nappe phréatique d'un site minier, nous démontrons que la technique MCN est un moyen simple pour quantifier le paramètre d'incertitude d'une part et d'améliorer la calibration du model d'une nappe phréatique et d'un soluté transporté à travers un système de faille complexe, d'autre part.

1 INTRODUCTION

Parameter calibration in groundwater flow and solute transport modeling of heterogeneous fractured rock systems is still a challenge due to the incomplete knowledge of the flow pathways and the limitations in quantity and quality of the data available for characterising the fractured rock aquifer. In the last decade a variety of numerical approaches have been used to improve the calibration of models to simulate groundwater flow in fractured rock (Beven and Freer, 2001; Selroos, et al, 2002; Beauheim and Roberts, 2002; Kavetski and Kuczera, 2007). Though the computational aspects of such approaches are reasonably well developed, the question of confidence in parameter estimates has not been completely resolved (Seber and Wild, 2003; Hassan, 2004).

Model calibration is traditionally accomplished by manual *trial-and-error* approach with iterative selection of parameter values to improve the model results using intuition about responses of modelling results to changes in parameter values. Consequently, a calibration obtained using a trial-and-error approach alone does not guarantee the statistically best solution. Inverse model like linear least-squares regression has been widely utilised in model calibration in which the parameter values are adjusted automatically to match site observations as closely as possible (Seber and Wild, 2003; Hill and Tiedeman, 2007, Foglia et al, 2009). Linear inverse modeling can statistically give the most appropriate solution for the given input parameters, quantifies the uncertainty in parameter estimates and yield results that are not readily available through trial-and-error calibration efforts (Poeter and Hill, 1996). However, it rarely leads to optimal estimates of model parameters values in modelling of a heterogeneous groundwater system since linear inverse models frequently obtain local instead of global minima during the error estimation process, especially with small data sets of the flow observations in a fractured rock aquifer (Hassan, 2004; Moore and Doherty, 2006). Bates and Watts (1988) stated: "we hasten to warn the reader that linear approximation regions can be extremely misleading".

The nonlinear regression technique, using a much larger and more general class of objective functions to overcome the once-direct solution of Linear Least-Squares Regression (LLSR), has been used in groundwater modelling in the last decade (Yobbi, 2000; Zhang et al. 2006; Mathod et al, 2008). This approach enhances data representation in space (with weights) and optimizes the best-fit parameter values in the calibration, especially when the estimated parameter errors are uncorrelated but have different uncertainties that generally occur in the modelling of heterogeneous systems (Bate and Watts, 1988). The purpose of this paper is to present the application of nonlinear least-squares regression (NLSR) to the groundwater flow and solute transport model calibration around a fault zone in a mining area. The NLSR method is briefly described in the subsequent sections. A numerical framework including sensitivity, relative composite sensitivity and

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correlation coefficients was developed for analysing the parameter uncertainty. The groundwater flow model utilized for this study is based on the data and information presented by Coffey (2010a) for a mine site hydrogeological investigation. A short description of the hydrogeological model and regression procedure follows. The optimal set of parameter values and associated statistics finally determined by the developed NLSR framework is presented.

2 NONLINEAR LEAST-SQUARES REGRESSION

The process of model calibration is essentially the same using either inverse models or the trial-and-error approach: parameter values and other aspects of the model are adjusted until the dependent variables (water levels, flows, concentrations) match field observations. The nonlinear least-squares regression method extends linear regression for use with a larger class of functions that can be written in a closed form.

2.1 NLSR Approach

Nonlinear regression attempts to fit a model function that may depend nonlinearly on the parameter vector $\hat{p}$ to a set of data with y-values at the corresponding *x*-values

$$y = f(x, \hat{p}) + \varepsilon \qquad [1]$$

where *f* is the nonlinear model function, and ε is a random error term. The nonlinear model functions are very commonly used in groundwater flow and solute transport modelling. For example flow through fractures used to be conceptualized as “cubic law” (Navier-Stokes equations) and the exponential function represents a semi infinite line dipole of decaying strength distribution (Anderson, 2000). The goal of nonlinear regression is to find the optimal values of parameter vector $\hat{p}$ that minimize the least squares function which is the sum-of-squared differences between observed and modelled quantities and is defined as

$$S(p) = \sum_{i=1}^{n} [(f(x_i, \hat{p}) - y_i)]^2 \qquad [2]$$

where $f(x_i, \hat{p})$ is the i^{th} modelled value with the parameter vector $\hat{p}$ used in the model function, y_i is the i^{th} measured value, and *n* is the number of observations. Nonlinear least squares optimization algorithm has been designed to exploit the structure of a sum of the squares objective function (Foglia et al, 2009)

$$\min S(p) = \sum_{i=1}^{n} [w_i r_i(\hat{p})]^2 \qquad [3]$$

where $r_i(\hat{p}) = f(x_i, \hat{p}) - y_i$ is the i^{th} least squares residual and w_i is the weighting factor. Optimization method used in this study is a modified Gauss-Newton method (Yobbi, 2000), the numerical framework of which is described in the following section.

2.2 NLSR Framework

The NLSR framework for estimating parameter values, including parameter sensitivities and correlation in groundwater model calibration, is developed in the six simplified stages outlined below.

(1) The parameter-estimation process is to perform one execution of the model to establish the initial differences (residuals) between simulated and measured water levels. The residuals are squared and summed to produce the sum-of-squared residuals objective function (eq. [2]), which is used by the regression to quantify the model fit to the observations.

(2) Composite sensitivity (CS) indicates the cumulative amount of information that measurements contain toward the estimation of the parameters and is quantified with the least squares residue (r_i in equation [3] using the equation:

$$CS_{kj} = \sum_{i=1}^{N_k} \partial r_i / \partial p_j \qquad [4]$$

The sensitivity coefficients $\partial r_i / \partial p_j$ are given by the Jacobian (sensitivity) matrix of the least-squares residue vector $\hat{r}$ and serve as an approximate indicator of the sensitivity of the N_k observations in the k^{th} zone with respect to the j^{th} parameter estimated.

(3) Correlation coefficients between parameters, indicates the degree of linear dependency in the sensitivity matrix and is calculated with CS vector values

$$R_k{}^2 = \frac{Cov(CS_{kj}, CS_{kl})}{(\sigma_{CS_{kj}})^{½} (\sigma_{CS_{kl}})^{½}} \qquad [5]$$

where $Cov(CS_{kj}, CS_{kl})$ is covariance of composite sensitivity of estimated *j* and *l* parameters The $\sigma_{CS_{kj}}$ and $\sigma_{CS_{kl}}$ are variances of composite sensitivity of estimated *j* and *l* parameters, respectively.

(4) The relative composite sensitivity (RCS), which is the square root of the main diagonal value of the Jacobian matrix of the least-squares residue vector divided by the maximum of the main diagonal value for each parameter, is quantified for parameter uncertainty analysis. The RCS for the j[th] parameter is qualified as:

$$RCS_j = \left(\frac{CS_{j,j}}{\max(CS_{j,j})} \right)^{\frac{1}{2}} \qquad [6]$$

(5) After the residuals and sensitivities are calculated, a single parameter-estimation iteration is performed. The arrays of sensitivity coefficients and residuals are used by a quasi-Newton procedure (Bate and Watts, 1988) to compute the parameter change for improving the model.

(6) The model is updated to reflect the latest parameter estimates and a new set of residuals is calculated. The entire process of changing a parameter in the model, calculating new residuals, and computing a new value for the parameter is continued iteratively until the model error change is reduced to a specified level or until a specified number of iterations are made.

The criteria of uncertainty analysis based on statistical parameters from the above described framework are:

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(1) The CS values are used for assessing the relative sensitivity of the model (either as a whole or locally) to each parameter.
(2) Correlation between parameters indicates whether or not the parameter estimates are unique with the given model construction and observations. It is an indicator of the degree of linear dependency in the sensitivity matrix and reflects the redundancy of the problem. Correlation coefficients greater than 0.95 usually indicate a pair of parameters that are highly correlated (Hill and Tiedeman, 2007). These highly correlated parameters are not desirable because they cannot be independently estimated.
(3) The most sensitive parameter has an RCS equal to 1.00 and the RCS of all other estimated parameters is less than one. The larger the value of the RCS, the more sensitive the model is to that parameter, as a whole. Parameters with smaller RCS values also tend to have higher parameter uncertainty and broader confidence intervals.

3 CASE STUDY

In Australia mined out ore pits have been used increasingly for the storage of mining process residue. As part of approval requirements, a three-dimensional FEFLOW finite element groundwater flow and solute transport model was developed for simulating the effects of in-pit filling on the groundwater environment at a mine site in Victoria, Australia.

Fault zones, disrupting Ordovician meta-sandstone and meta-siltstones, are understood to be the controlling hydrogeological structures at the site. Abandoned and partially flooded mine workings are aligned along these fault zones with the active underground mining following the fault zones to depth in the south of the workings. The country rock is overlain by a thin cover of alluvial sediments with cover thickness increasing to the east towards a river valley. Groundwater in the alluvial sediments is considered to be relatively fresh with a low salinity of 50 to 100 mg/L Total Dissolved Solids (TDS). In contrast, the salinity of groundwater in the fractured country rock ranges from 2,000 to 10,000 mg/L TDS.

The groundwater environment across the site was conceptualized as consisting of three zones with relatively small groundwater head gradients in broad areas to the West and the East of the pits and an area between fault zones, where water levels drop over a very short distance. The conceptual site model is shown in Figure 1.

Based on the fracture density and frequency of fault structures observed in exploration boreholes the central zone was subdivided into two zones with Zone 1 representing intensely fractured and faulted rocks and Zone 2 characterised by numerous faults but less intensely fractured rock. The back fill in the pits were conceptualised by a zone of Rock Fill in the South of the southern pit and a zone filled with process residue (RSF).

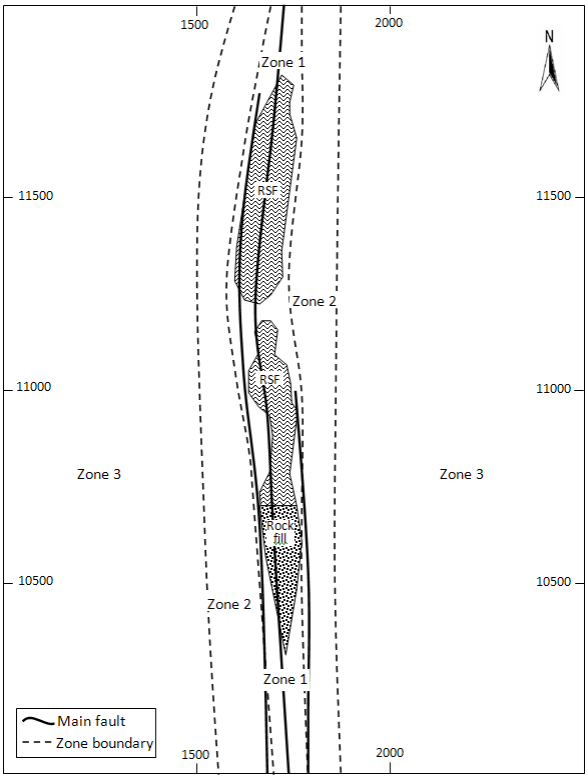

Figure 1 Location of study area and parameter zonation. Numbers at the figure frame represent mine coordinates in metres.

The transient groundwater flow and solute transport model was calibrated with groundwater level recorded in 2009 over 2 ½ months at 20 monitoring bores and with concentrations of selected solutes obtained from groundwater and in-pit water sampled over the same time period. Calibration was conducted using both methods: LLSR and NLSR, and results obtained with both methods were compared. The general results from the analysis described in the following sections indicate that there is insufficient observation data to independently estimate all model parameter values given the present zonation.

3.1 Relative Composite Sensitivities for zone specific hydraulic conductivities

Changes to horizontal hydraulic conductivity (K_h) and to the anisotropy factor for hydraulic conductivity K_h/K_v that defines the ratio of horizontal hydraulic conductivity and

vertical hydraulic conductivity were found to have the most significant effect on computed groundwater heads. Except for the residue fill in the pits (RSF zone in Figure 1), RCS values computed for the remaining hydraulic conductivity zones are shown in Table 1. NLSR analysis results indicate that the available groundwater level data provide sufficient information to reliably estimate hydraulic conductivity of the fractured country rock for two of the four parameter zones (RCS > 0.5). Relative Composite Sensitivity is highest for the Zone 1 and is lowest for the Zone 3. The low sensitivity for Zone 3 and the Rock Fill zone is primarily due to the lack of monitoring data within these zones.

Table 1 Relative Composite Sensitivity (RCS) of horizontal hydraulic conductivity adopted for four parameter zones during model calibration.

Zone	K_h (m/d)	RCS	Number of bores
Zone 1	0.12	1.000	6
Zone 2	0.015	0.749	5
Rock Fill	0.26	0.227	1
Zone 3	0.002	0.013	8

The parameter zones are not highly correlated to one another, except for Zone 1 and Zone 2 that show high correlation with a correlation coefficient R^2 of 0.93. The high correlation between Zone 1 and Zone 2 indicates that with respect to the hydraulic conductivity these zones may not be separable. The lowest degree of correlation occurred between Zone 3 and the Rock Fill (r = 0.28). Additional groundwater-level monitoring data in these zones would be beneficial for improving the model calibration.

RCS values for the anisotropy factor of hydraulic conductivity are summarised in Table 2. With RCS values for Zone 1 and Zone 2 anisotropy factors of hydraulic conductivity exceeding 0.5 estimates are considered to be reliable. However, the RCS is very low for the Rock Fill zone (RCS<0.1) indicating low reliability of the calibration result for the anisotropy factor of this zone. Improvements of the reliability of the parameter estimate for this zone could be achieved with additional observation locations in the Rock Fill.

Table 2 Relative Composite Sensitivity (RCS) of anisotropy factor of hydraulic conductivity adopted for four parameter zones during model calibration.

Zone	K_h/K_v	RCS	Number of bores
Zone 2	2	1.000	6
Zone 1	2	0.773	5
Zone 3	5	0.185	8
Rock fill	1	0.006	1

3.2 Assessment of zone specific absorption coefficient estimates

The RCS values of arsenic absorption coefficients (c_a) computed for each parameter zone are shown in Table 3. The RCS values indicate that the water quality data used for model calibration provides sufficient information to estimate the absorption coefficients for two of the four parameter zones (RCS > 0.5). The lowest RCS value computed for the Rock Fill zone is basically due to the lack of water quality data within the Rock Fill zone while the second lowest sensitivity for Zone 3 is possibly due to very low solute concentrations observed in Zone 3.

Table 3 Relative Composite Sensitivity (RCS) of arsenic absorption coefficients adopted for four parameter zones during model calibration.

Zone	c_a	RCS	Number of bores
Zone 1	0.18	1.000	6
Zone 2	0.12	0.557	5
Rock Fill	0.22	0.083	1
Zone 3	0.05	0.008	8

Most of the estimated absorption coefficients are highly correlated. As shown in Table 5, the most highly correlated zones are Zone 1 and Zone 2 with a correlation coefficient (R^2) of 0.97. The lowest correlated pair of zones is adjacent Zones 3 and Rock Fill with a correlation coefficient of 0.37. These relationships reflect the less dependency of model results on the observation data set and the high uncertainty within the parameter-zonation of absorption coefficient.

3.3 Comparison of NLSR and LLSR model calibration results

Two different approaches, LLSR and NLSR, were implemented for the analysis of parameter uncertainty as part of the model calibration. Tables 4 and 5 show the adopted values for hydraulic conductivities and absorption coefficients for the two calibration approaches.

Table 4 Horizontal hydraulic conductivities derived from initial (LLSR) and optimal (NLSR) calibration approaches.

Zone	Initial (m/d)	Optimal (m/d)	RCS	The most correlated
Zone 1	0.1	0.12	1.000	Zone 2 (.93)
Zone 2	0.01	0.015	0.749	Zone 1 (.93)
Zone 3	0.001	0.002	0.013	Zone 2 (.87)
Rock Fill	0.12	0.26	0.227	Zone 1 (-.79)

Table 5 Absorption coefficients derived from initial and optimal calibration approaches.

Zone	Initial	Optimal	RCS	The most correlated
Zone 1	0.15	0.18	1.000	Zone 2 (.97)
Zone 2	0.15	0.12	0.557	Zone 1 (.97)
Zone 3	0.05	0.05	0.008	Zone 2 (.92)
Rock Fill	0.20	0.22	0.083	Zone 1 (-.85)

The optimized hydraulic conductivities (K) shown in Tables 4 were increased by 20% to 100% from the initial estimated parameter values while the final arsenic absorption coefficients (c_a) shown in Table 5 were adjusted by 10% to 20% from the initial estimated values. As indicated previously, parameters (K and c_a) with higher RCS values for Zone 1 and Zone 2 are likely to have lower parameter uncertainty and the parameters with smaller RCS values in Zone 3 and Rock Fill zone are likely to have higher parameter uncertainty.

Most of the estimated K-values are not highly correlated to one another. However, as indicated by correlation coefficients in Table 4, the zones with the most highly correlated pair are adjacent fractured Zones 1 and 2 with a correlation coefficient of 0.93. Similarly the zones with the most highly correlated pair in c_a-values shown in Table 5 are also adjacent fractured Zone 1 and Zone 2 with a correlation coefficient of 0.97. These values reflect the high uncertainty in the parameter-zonation of the model.

Table 6 summarises statistical parameters of the simulation results in a period of 4 months from the models calibrated using LLSR and NLSR approaches. The results demonstrate that the improvement of the model calibration achieved by using NLSR approach compared to the LLSR calibration is essential with the diminution of 30% of groundwater level residual. Correlation coefficient between measured water level values and values computed with the NLSR calibrated models increased by 2% when compared to the correlation coefficient computed with results of the LLSR calibrated model.

Table 6 Statistical summary of groundwater flow model simulations

	R^{2} +)	MSE++)	Residue
Initial	0.96	0.007	-0.42 (m)
Optimal	0.98	0.005	-0.34 (m)

+) Correlation coefficient between measured and modelled water level; ++) Mean square error

Statistical parameters obtained from arsenic concentration simulations using absorption coefficients (c_a) calibrated with LLSR and NLSR approaches are shown in Table 7. The improvement of the solute transport model calibration made by NLSR compared with the results from the LLSR approach is significant with a 40% reduction of arsenic concentration residual and a 25% reduction of Mean Square Error (MSE). Also the correlation coefficient between measured and computed arsenic concentration values slightly increased by about 0.5% when compared to the LLSR calibrated model.

Table 7 Statistical summary of arsenic solute transport model simulations

	R^{2} +)	MSE++)	Residue
Initial	0.948	0.0093	0.0071 (mg/L)
Optimal	0.953	0.0072	0.0038 (mg/L)

+) Correlation coefficient between measured and modelled As concentration; ++) Mean square error

3.4 Model validation

The calibrated model was validated with monitoring data recorded in 2009 and 2010 over a period of 14 months during the pre-filling and the filling of the residue storage facility (Coffey, 2010b). For the model validation the modelling efficiency index (IA) was used to analyse the correspondence between model results and observations. The IA is commonly used as a goodness-of-fit measure and is defined as:

$$IA = 1 - \frac{\sum_{i=1}^{n}(Y_i^m - Y_i^o)^2}{\sum_{i=1}^{n}[|Y_i^m - \overline{Y^m}| + |Y_i^o - \overline{Y^o}|]^2} \qquad [7]$$

Where Y^m and Y^o are the modelled and observed variables, n is the number of data, and $\overline{Y^m}$ and $\overline{Y^o}$ are the corresponding mean values. The IA is defined in a range between 0 and 1, and the closer it is to 1, the better is the fit between modelled and observed variables and the validity of the model (Hassan, 2003).

Modelling efficiency index between observed and computed water level and arsenic concentration for each parameter zone were calculated and are summarised in Table 6.

Based on an IA threshold value of 0.8 which was initially adopted for this case study, the parameters, hydraulic conductivity and anisotropy factor of hydraulic conductivity for all zones were assessed to be valid. However, the absorption coefficient of all material zones required re-calibration.

A comparison between the IA computed for parameter values obtained with the LLSR and the NLSR method showed that the IA values for parameters adopted during calibration using the NLSR method are slightly higher. In particular the IA computed for Zone 1 and Zone 2 absorption coefficients are by 10% to 20% higher for the NLSR method compared to the LLSR method (Table 6).

Table 6 Statistical summary of two model validations

Zone	IA for groundwater head		IA for arsenic concentration	
	LLSR	NLSR	LLSR	NLSR
Zone 1	0.913	0.937	0.698	0.773
Zone 2	0.908	0.932	0.427	0.515
Zone 3	0.871	0.884	0.163	0174
Rock Fill	0.895	0.903	0.259	0.272

4 CONCLUSION

This paper presents the results of a study on the application of nonlinear least-squares regression to a groundwater flow and solute transport model of an in-pit residue storage facility located in a regional fault zone. The main advantages of using nonlinear least-squares regression for model calibration are the ability to estimate parameter values more accurate when compared to parameter estimation with LLSR and to quantify the quality of model calibration using more

general statistical measures for both model sensitivity and uncertainty.

The quality of model calibration and uncertainty in simulation results has been demonstrated with regression statistics like Relative Composite Sensitivity (RCS), correlation coefficient and IA values. With calculated RCS, it could be demonstrated that the quality of the calibration highly relied on the density of monitoring locations for each parameter zone. Calibration of hydraulic conductivities for highly fractured rock zones (Zone 1 and Zone 2) showed a high value of RCS indicating that the sensitivity of computed groundwater heads to changes in hydraulic conductivity is very high. However, the uncertainty of the calibrated parameters of these zones is not higher than that of the others zones. The high correlation between Zone 1 and Zone 2 RCS suggest that the differentiation between the two zones is arbitrary and cannot be justified by the limited monitoring data used in the calibration. The uncertainty of the calibrated parameters for Rock Fill and Zone 3 tends to be very high possibly due to limited monitoring data available for this units and less well defined unit boundaries.

The validation of the NLSR calibrated model showed an approximately 20% reduction in groundwater level residual and 40% reduction in solute concentration residual when compared to the LLSR calibrated model. The IA values for model parameters estimated with the NLSR method were up to 20 % higher when compared to IA values obtained for the LLSR parameter values. These results suggest that the NLSR technique can improve the quality of groundwater flow and solute transport models and yield results of a quality that are not readily achievable with linear regression calibration.

Consequently, NLSR approaches could be used to determine strengths and weaknesses of the model and measures of parameter uncertainty in a heterogeneous aquifer system. Furthermore, the model is likely to be able to obtain a unique set of parameter values if the inverse model converges. The stability of algorithm used in this study for NLSR model calibration are affected by the number of parameters and observations with some instabilities encountered when the number of observation is small compared to the model parameter numbers to be calibrated. Nevertheless the statistical framework of the NLSR method provides an effective way to improve the calibration of groundwater flow and solute transport models.

ACKNOWLEDGEMENTS

The authors are grateful for the support from Northgate Australia Ventures, Fosterville Gold Mine. The authors also would like to acknowledge the contribution of Coffey employees who have been working on the project.

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