

# Environment Canada

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Technology Directorate

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Direction générale des sciences  
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## Environnement Canada

Adding Inverse Analysis Functionality to an  
Existing Computer Model

By:

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### Management Perspective

Computational modelling has become a component of a wide range of geotechnical investigations; for example, groundwater flow and contaminant transport modelling is frequently used to investigate groundwater management and remediation strategies. Often, the objective of the modelling exercise is either to calibrate the model to match in situ conditions or to estimate the properties of the geologic formation from a set of observed data. Both pursuits are forms of inverse analysis, a method of analysis that reverses the conventional direction of forward analysis. The interpretation of data using inverse analysis significantly reduces the effort and subjectivity of the analysis relative to the analogous, manual procedures that are more frequently invoked. This paper outlines an approach to developing an inverse analysis algorithm from an existing forward model that has proven to be successful in numerous modelling scenarios. The intent of this paper is to assist in the technology transfer of inverse analysis to the geotechnical community by stating the inverse analysis methodology in brief and highlighting the advantages of the approach through the presentation of an example of inverse analysis of hydrogeological testing data.

## **Adding Inverse Analysis Functionality to an Existing Computer Model**

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Computational modelling of processes such as groundwater flow and contaminant transport has become an important component of many geotechnical investigations. This popularity appears to be due to increased access to computing facilities and software, and perhaps also to increased appreciation for the value of modelling results. As computer modelling has migrated towards more practical applications, there has been a corresponding trend toward functionality that is particularly suited to applied modelling scenarios. The emergence of pre- and post-processors and graphical interfaces is characteristic of this trend.

In many cases, the objective of a modelling effort is to match calculated results to in situ data. This may be required to calibrate a model relative to in situ conditions, or to estimate the parameters that regulate the process at hand. Model calibration and parameter estimation are both forms of inverse analysis, which reverses the conventional direction of analysis to determine input data from output results. Our experience in developing inverse analysis functionality for various forward models (Piggott et al., 1992, 1994, 1995) indicates that this task can be accomplished by geotechnical practitioners with some experience in computer programming and applied mathematics. This paper describes a simple approach to developing an inverse analysis algorithm. It is hoped that this description will encourage practitioners to consider inverse analysis as a component of their modelling efforts. While groundwater terminology and a hydrogeological example are cited, other types of geotechnical models are equally well suited to this approach.

Using a computer model to predict in situ conditions (e.g., groundwater levels) from a set of input parameters (e.g., hydraulic conductivity) may be expressed in a symbolic fashion as

$$\underline{y} = F(\underline{x}) \quad (1)$$

where  $\underline{x}$  is an array containing the input parameters,  $\underline{y}$  is an array containing the output results, and  $F(\underline{x})$  represents the mathematics entrained in the forward analysis. The mathematics expressed in  $F(\underline{x})$  can vary from simple closed-form solutions to detailed numerical solutions such as finite element approximations. Regardless, forward modelling involves the input of parameters and the output of calculated results.

Inverse analysis is the reciprocal of Equation (1) where the output results are replaced by measured data and the input parameters are replaced by a best estimate of the in situ values of the parameters. Thus, following the syntax of Equation (1), inverse analysis may be expressed as

$$\underline{x}^* = F^{-1}(\underline{y}) \quad (2)$$

Here,  $\underline{x}^*$  is an array containing the best estimates of the input parameters,  $\underline{y}^*$  is an array containing the measured data, and  $F^{-1}(\underline{y}^*)$  represents the mathematics entrained in the inverse analysis. In practice, an iterative approach is used to achieve the result indicated in Equation (2). This approach is as follows:

1. Input the measured data,  $\underline{y}^*$ , constraints that define the values of  $\underline{x}$  that are reasonable for the problem at hand, and an initial estimate of  $\underline{x}^*$ . It may also be necessary to configure the forward model for the problem at hand; for example, specifying confined or unconfined groundwater flow.
2. Execute the forward model using the current estimate of  $\underline{x}$  and record the calculated results in  $\underline{y}$ .
3. Compare  $\underline{y}^*$  and  $\underline{y}$  using an error function; for example

$$E(\underline{x}) = \sum_{i=1}^n (y_i^* - y_i)^2 \quad (3)$$

The minimum value of the error function implies the optimal match between the measured data and calculated results; the corresponding estimate of the input parameters forms the best estimate of the in situ values. A residual discrepancy between the measured data and calculated results indicates measurement errors or the failure of the forward model to fully represent in situ conditions.

4. Examine the current and past estimates of  $\underline{x}$  and the corresponding values of  $E(\underline{x})$  to determine if the minimum value of the error function has been located and if the estimates of  $\underline{x}$  have converged.
5. Output the current estimate of  $\underline{x}$  as the best estimate of  $\underline{x}^*$  if the termination conditions have been achieved, otherwise select a new estimate of  $\underline{x}$  and return to Step 2.

This procedure is an automated equivalent of the trial-and-error methods used in numerous geotechnical analyses. The advantage of automating the procedure is that, once initiated, no additional intervention of the analyst is required. Further, the automated approach continues until a quantitative, optimal match between the measured data and calculated result is obtained. Trial-and-error methods are often terminated when the match is deemed "good enough" where this distinction is both qualitative and subjective.

Generally speaking, a limited amount of programming is required to develop an inverse analysis algorithm from an existing forward model provided that the source code for the forward model is available. The most complex component of the algorithm, the determination of the minimum value of the error function and the corresponding values of the input parameters, may be performed using any of the numerous optimization algorithms that appear in texts on applied mathematics (e.g., Press et al., 1992) and in libraries of mathematical subroutines (e.g., IMSL, 1992). It is important to select an optimization algorithm that is robust relative to inconsistencies in the calculated results as this is a characteristic of many numerical solutions. Also, many optimization algorithms require differentiation of the calculated results with respect to the input parameters. This information is not typically computed by forward models, so the selection of an

optimization algorithm should proceed accordingly.

As an example of the performance of inverse analysis, Figure 1 depicts the results of manual and automated type-curve matching of data collected during a tracer test conducted on a single fracture in rock. Fracture aperture, dispersivity, and matrix porosity were extracted using conventional, type-curve matching and the inverse analysis approach described in Piggott et al. (1995). Clearly, the automated match better represents the measured data than does the manual match. The manual match was obtained by an experienced analyst and therefore the reduced precision of the manual match reflects the inherent limitations of the manual type-curve matching procedure relative to the inverse analysis procedure. Figure 2 illustrates the variation of the error function and input parameters during the inverse analysis of the data. The parameter estimates converge toward the final, best estimates as the error function approaches the apparent minimum value. A total of 99 forward analyses were completed in determining the minimum value of the error function.

The approach to inverse analysis described in this paper tends to be computationally intensive as the time required to complete an analysis is proportional to the time required to complete each forward analysis and the number of forward analyses required to locate the minimum value of the error function. The computational resources allocated to an inverse analysis should be considered relative to the effort associated with the analogous manual operation. The cost of dedicating a computer to even a lengthy analysis is likely to be much less than the cost of completing the manual equivalent. Whatever savings can be realized in applying inverse analysis can then be assigned to important supporting exercises such as determining the sensitivity of the inverse analysis results to the assumptions invoked in the analysis.

In conclusion, adding inverse analysis functionality to an existing computer model increases the utility of the model in interpretive efforts, for example, in calibration and in parameter estimation. Every model is unique and even the most robust models occasionally "crash" when subjected to the rigors of inverse analysis. Thus, attention should be applied to ensuring that the results of an analysis are reasonable in light of confirming observations. Inverse analysis, properly applied, extracts increased value from costly in situ measurements while reducing the effort applied to the analysis and ensuring consistent and thorough

treatment of the data. Most importantly, inverse analysis is not a substitute for geotechnical expertise, it is simply a tool that assists in the analysis of data. Numerous opportunities for the application of geotechnical expertise exist in configuring the forward model, selecting the parameters for determination and applying constraints to the parameters, and assessing the results of the inverse analysis.

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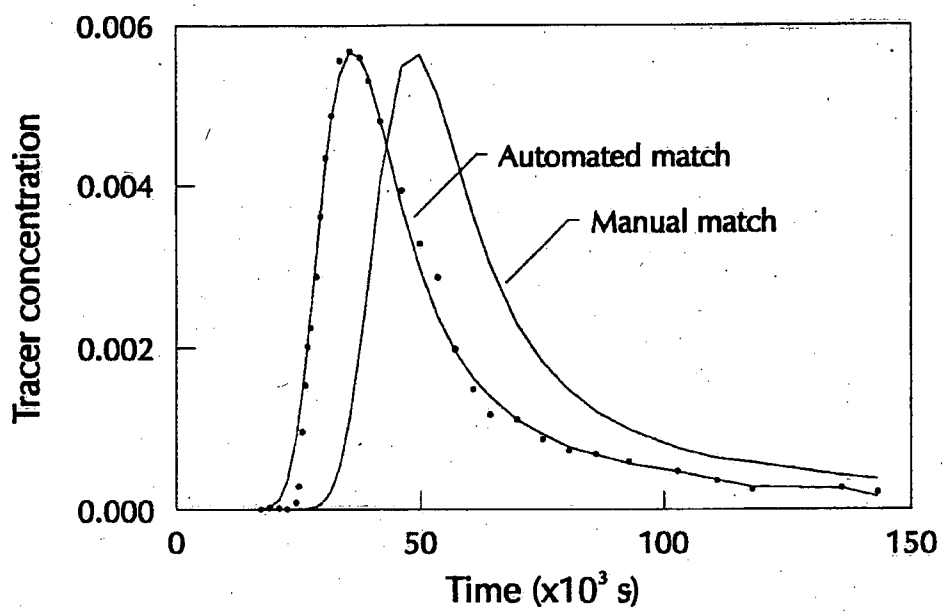


Figure 1. Comparison of manual and automated type-curve matches for a tracer test conducted on a single fracture in rock.



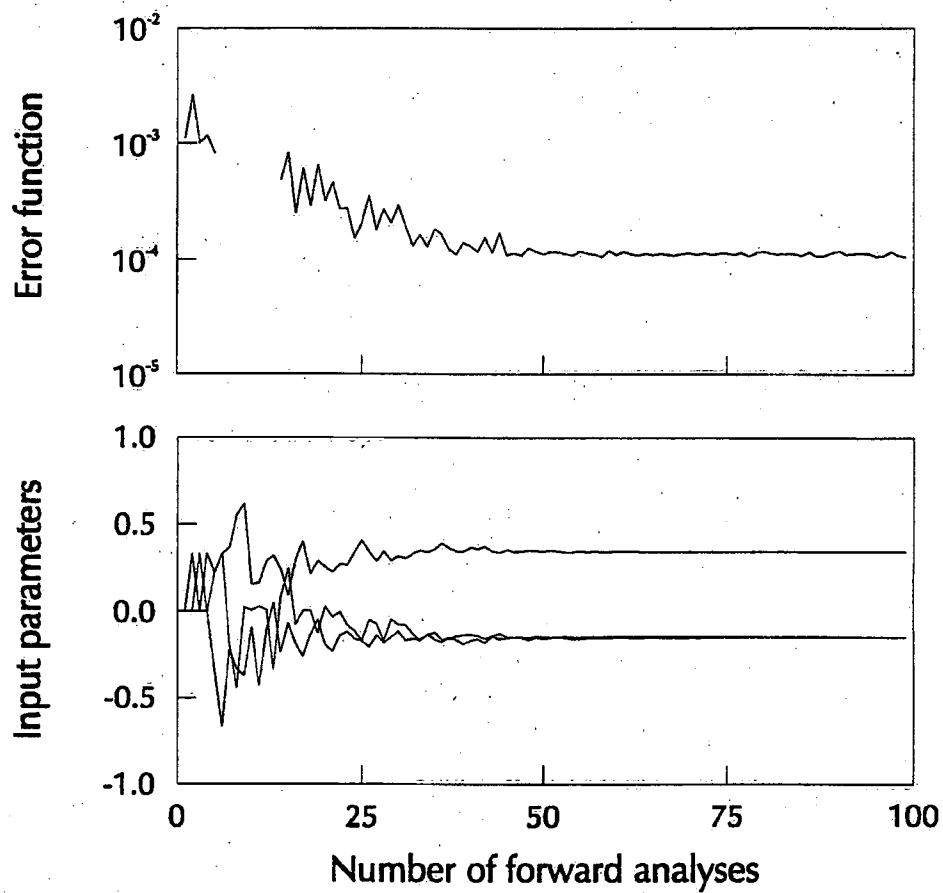


Figure 2. Variation of the error function and input parameters during inverse analysis of the data shown in Figure 1. Parameter magnitudes are stated relative to the initial estimates and permissible ranges of values assigned to the parameters. The discontinuity in the error function indicates parameter estimates that violate the permissible ranges of values.

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