



Uniqueness, scale, and resolution issues in groundwater model parameter identification

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Abstract

This paper first visits uniqueness, scale, and resolution issues in groundwater flow forward modeling problems. It then makes the point that non-unique solutions to groundwater flow inverse problems arise from a lack of information necessary to make the problems well defined. Subsequently, it presents the necessary conditions for a well-defined inverse problem. They are full specifications of (1) flux boundaries and sources/sinks, and (2) heads everywhere in the domain at at least three times (one of which is $t = 0$), with head change everywhere at those times being nonzero for transient flow. Numerical experiments are presented to corroborate the fact that, once the necessary conditions are met, the inverse problem has a unique solution. We also demonstrate that measurement noise, instability, and sensitivity are issues related to solution techniques rather than the inverse problems themselves. In addition, we show that a mathematically well-defined inverse problem, based on an equivalent homogeneous or a layered conceptual model, may yield physically incorrect and scenario-dependent parameter values. These issues are attributed to inconsistency between the scale of the head observed and that implied by these models. Such issues can be reduced only if a sufficiently large number of observation wells are used in the equivalent homogeneous domain or each layer. With a large number of wells, we then show that increase in parameterization can lead to a higher-resolution depiction of heterogeneity if an appropriate inverse methodology is used. Furthermore, we illustrate that, using the same number of wells, a highly parameterized model in conjunction with hydraulic tomography can yield better characterization of the aquifer and minimize the scale and scenario-dependent problems. Lastly, benefits of the highly parameterized model and hydraulic tomography are tested according to their ability to improve predictions of aquifer responses induced by independent stresses not used in the inverse modeling efforts.

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1. Introduction

The need of using inverse models to determine the spatial distribution of hydraulic properties has been well recognized for decades. Nevertheless, as stated by [Carrera and Neuman \(1986\)](#), “There is a general consensus among groundwater modelers that the inverse problem may, at times, result in meaningless solutions. However, the reasons for this

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“misbehavior” of the inverse solution are not always well understood: some hydrologists attribute them to nonuniqueness, some to nonidentifiability, and others to instability. This misunderstanding has led to a controversy in the literature regarding the question whether the inverse problem is at all solvable; if so, under what circumstances and in what manner. There are those who argue that this problem is hopelessly ill-posed and, as such, intrinsically unsolvable.” After more than two decades, arguments remain. This controversy mainly stems from the definition of a well-posed mathematic problem given by Hadamard (1902): mathematical models of physical phenomena should have the properties that (1) a solution exists, (2) the solution is unique, and (3) the solution depends continuously on the data, in some reasonable topology. The last condition implies that if the solution depends in a discontinuous way on the data, then small errors, whether rounding-off errors, measurement errors, or perturbations caused by noise, can create large deviations. Most of the inverse models in science exhibit this unstable nature. The inverse problem in subsurface hydrology is therefore commonly perceived as an ill-posed problem.

In spite of the ill-posed nature of inverse problems, Nelson (1960) demonstrated mathematically five decades ago that three-dimensional (3D) heterogeneous hydraulic conductivity distribution can be uniquely identified if the spatial potential variation is known, and the hydraulic conductivity at one point in every stream tube under a steady flow is given. While recognizing that an insufficient amount of Cauchy data causes the inverse problem of steady flow to be non-unique, Neuman (1973) attributed an infinite number of possible solutions of the inverse problem to errors in data and governing equations. Because the inverse modeling efforts are non-unique, Emsellem and de Marsily (1971) and Neuman (1973) emphasized the need for multiple objectives in dealing with groundwater parameter identification problems: calibration error and physical plausibility of the estimate.

An extensive discussion on the uniqueness, identifiability, and stability associated with inverse modeling of transient and steady groundwater flow equations was provided by Carrera and Neuman (1986). They stated that identifiability is ensured if the rank of the Jacobian matrix is equal to the number of unknown parameters. They concluded, however, that “The large number of flow situations that can arise from governing groundwater flow equations prevents us from developing detailed rules about uniqueness.” They further stated that “No parameter estimates must be accepted at face value without subjecting them first to a thorough sensitivity analysis ... Concerning the sensitivity of heads to model parameters, the issue is strongly problem-dependent and can be resolved only through a prior and/or post-optimal sensitivity analysis.”

Likewise, McLaughlin and Townley (1996) and Carrera et al. (2005) stressed that the low sensitivity of head to the hydraulic conductivity is the cause of the difficulties in solving groundwater inverse problems. In particular, McLaughlin and Townley (1996) stated “In many situations where parameters are difficult to identify it is easier to improve sensitivity by

introducing new kinds of information than by simply adding more measurements of the same variable. This is particularly true in the groundwater flow inverse problem. Since steady state heads are relatively insensitive to spatial variations in hydraulic conductivity, estimation performance may not improve dramatically when more head measurements are included.” They also suggested inverse experiments should be designed so as to maximize the sensitivity of measurements to estimated parameters (Knopman and Voss, 1988). More recently, the role of different statistics based upon sensitivity in parameter identifiability have been discussed by Doherty and Hunt (2009), Hill (2010), and Doherty and Hunt (2010).

Stallman (1956) noted that his inverse solutions tended to be unstable. He suggested that this instability problem can be prevented by treating transmissivity as a constant over large segments of the aquifer (zones) and using least squares to estimate transmissivity over such zones. The zone must not be too large. Otherwise, important information about spatial variability is lost and one may be unable to obtain a satisfactory match between computed and measured heads (a sparsely parameterized approach). This is basically a block parameterization or zonation approach (Neuman, 1973; Hill, 2006; Sun and Yeh, 1985; Eppstein and Dougherty, 1996; McLaughlin and Townley, 1996). In particular, McLaughlin and Townley (1996) stated “If the actual spatial distribution of hydraulic conductivity is not blocked or if the block boundaries are incorrectly specified, the inverse algorithm may be forced to generate unrealistic estimates in order to provide a good fit to head measurements. So, although the inverse problem may be well-posed in the sense that it yields a stable solution, the estimates it provides may not properly characterize the subsurface environment.” They further suggested that “when geological structure is apparent and formation boundaries are distinct a blocked approach to parameterization is probably the best choice.”

On the other hand, highly parameterized approaches such as geostatistical approaches (e.g., kriging, cokriging, conditional simulations, and geostatistics-based inverse models) have been used extensively over the past few decades (Zimmerman et al., 1998). Hunt et al. (2007) recently emphasized the need for increasing parameterization in groundwater model calibrations with the use of a regularized inverse approach.

The objective of this paper is not to provide a review of mathematical methods for solving groundwater inverse problems as there are already many review articles. Rather, it is to emphasize the fact that non-unique solutions in either a forward or an inverse problem are a result of the lack of data that satisfy necessary conditions for a well-defined problem. Mathematical stability issues or high or low measurement sensitivity to the estimated parameters are not the cause. The non-uniqueness of forward and inverse problems should be addressed as uncertainty in the solutions.

In this paper, we first visit the forward groundwater flow model, the necessary conditions for a forward solution to be well defined, and the process scale implied in the conceptual model. We then emphasize the fact that forward modeling of

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