Journal of Computational Physics 227 (2008) 10243–10262

Contents lists available at ScienceDirect

Journal of Computational Physics

journal homepage: www.elsevier.com/locate/jcp

Parameter estimation in flow through partially saturated porous materials

Kouroush Sadegh Zadeh *

Fischell Department of Bioengineering, University of Maryland, College Park, MD 20742, USA

ARTICLE INFO

Article history:
Received 23 March 2008
Received in revised form 1 September 2008
Accepted 8 September 2008
Available online 16 September 2008

Dedicated to Dr. Hubert J. Montas for his kindness, patience, and sense of humor

MSC:
65R32
74Pxx
76S05
65Mxx
35−xx
74G75
76M20
76B45

Keywords:
Porous media
Inverse modeling
Finite element method
Mass lumping
Richards equation
Levenberg–Marquardt algorithm

ABSTRACT

A class of numerical simulators were developed and critically evaluated to be incorporated as the solver of a forward problem in the framework of an inverse modeling strategy. The strategy couples a mass-lumped Galerkin linear finite element solution of the mixed form Richards equation with an experimental time–space series and the Osborne–Moré revised form of the Levenberg–Marquardt algorithm; to retrieve hydraulic parameters of a partially saturated porous medium. The numerical simulator shows excellent agreement with a *reference solution*, obtained on a dense grid and infinitesimal time step, in terms of fluid pressure head, fluid content, and fluid volumetric flux density and perfectly conserves the global mass. An adaptive algorithm was implemented to estimate sensitivity matrix in the inverse algorithm. A multi-criterion stopping rule was developed and successfully implemented to end the inverse code at the solution. The result of the optimization was compared with a large-scale in-situ soil moisture space–time series, measured during the course of a drainage experiment, and excellent agreements were found. Analysis of the parameter response surfaces and hyper-space plots, closeness of the gradient of the penalty function at minimum to zero, and positive definiteness of the approximation for the Hessian at the solution ($\mathrm{eigs}(H) > 0$) indicate that the obtained solution is a strong local minimum. A state-of-the-art sensitivity analysis carried out to quantify sensitivity of the state variable with respect to uncertainty and changes in different model parameters.

1. Introduction

Despite remarkable efforts to develop state-of-the-art numerical algorithms to solve systems of partial differential equations governing fluid flow and pollutant transport in variably saturated porous media, there have been relatively few attempts to calibrate and validate them against large-scale experimental data sets. The reason is large number of model parameters which requires intensive data sets that are not readily available. The success of these models and corresponding numerical simulators, in describing and understanding the real world and making predictions for them, depends largely on proper representation of relevant processes, uncertainty in model parameters [2], and parameter identification which is a critical step in modeling process [72]. Difficulties in model calibration and parameter identification are quite common in modeling flow and material transport in complex bio-environmental systems. To calibrate these models, one approach is

* Tel.: +1 301 405 0109; fax: +1 301 314 9023.
E-mail address: kouroush@umd.edu.

0021-9991/$ - see front matter
doi:10.1016/j.jcp.2008.09.007

to impose rather restrictive initial and boundary conditions on transport properties of the system that allow direct computation of the parameters. There are several laboratory and large-scale methods to measure the hydraulic and transport parameters in flow and contaminant transport through partially saturated media [9,26]. However, laboratory scale results may not be representative of large scale transport parameters. Large-scale measurements, on the other hand, are tedious, time-consuming, expensive, and often impose unrealistic and simplified initial and boundary conditions on the system. Finally, information regarding parameter uncertainty is not readily obtained from these methods unless a very large number of samples and measurements are taken at significant additional cost [40,72,74,76].

An alternative approach is parameter estimation by inverse modeling. Model calibration, history matching, nonlinear regression, and optimization are equivalent terms for inverse modeling [7,8,15,16,23,29,31,35,43,45–48,50,58,59,64,71,73,77]. Inverse modeling may be viewed as a procedure for converting more easily measured data such as fluid content, fluid pressure head, and concentrations into harder to obtain transport parameters such as kinetic rate constants, hydraulic conductivity of the media, hydrodynamic dispersion coefficient, retardation factor, degradation and production coefficients, and pore water velocity. Unlike direct inversion methods, inverse modeling does not impose any constraints on the form or complexity of the forward model, on the choice of initial and boundary conditions, on the constitutive relationships, or on the treatment of heterogeneities via deterministic or stochastic formulations [76]. Therefore, experimental conditions can be chosen based on convenience rather than by a need to simplify the mathematics of the process. Additionally, if information regarding parameter uncertainty and model accuracy is needed, it can be obtained from the parameter optimization procedure [40,72,76,80].

A general problem in parameter estimation by inverse modeling is ill-posedness [83,72]. Generally, ill-posedness arises from non-uniqueness and instability. Instability occurs when the estimated parameters are excessively sensitive to the input data. Any small errors in measurements will then lead to significant error in estimated values of parameters. If boundary conditions are improperly formulated appreciable errors in parameter optimization may arise. Non-uniqueness occurs when there are multiple parameter vectors that can produce almost the same values of the objective function thus making it impossible to determine the unique solution [81,87,76]. This problem is closely related to parameter identifiability. Parameter identifiability depends on both the structure of the mathematical model and the experimental input data. A common cause for non-identifiability of model parameters is high intercorrelation among parameters. In these situations a change in one parameter generates a corresponding change in the correlated parameter making it impossible to obtain accurate estimate for either of them. Furthermore, even when parameters in a mathematical model are independent of each other, the experimental data may produce an objective function that is not sensitive enough to one or more parameters. The characteristics of the second situation are wide confidence regions on the estimated parameters and large estimation variance. Where a possible solution for the first case is fixing one of the parameters and estimating the other one, in the second case performing multi-objective optimization by coupling different kinds of experimental data may lead to unique solution [40,72].

The goal of this study is to develop, implement, and evaluate an efficient inverse modeling strategy to estimate hydraulic parameters of in partially saturated porous media. A mass-conservative numerical simulator is first developed to solve the initial-boundary value *direct problem* which simulates flow through partially saturated porous media. Neumann boundary conditions are imposed at either ends of the spatial domain. A realistic initial condition in which fluid content of the porous medium varies as a function of the vertical coordinate, is implemented in the numerical simulator and the corresponding physical model to gather the experimental data. To reduce CPU time and maintain small truncation error, an adaptive time-stepping strategy is developed and implemented. The nonlinear matrix equations are solved using the modified Picard iteration scheme. To solve the inverse problem, the Osborne–Moré [54,61] modified version of the Levenberg–Marquardt method [49,52] is used. A switching technique is proposed to calculate the sensitivity matrix (Jacobian matrix) in the inverse code. During each iteration, the algorithm solves the forward problem $p+1$ times (p is number of model parameters being estimated) in the early stages of the optimization by calculating the partial derivatives of the state variable with respect to model parameters by *one-sided finite difference approximation*. As the iteration proceeds and the search approaches the minimum, the algorithm solves the direct problem $2p+1$ times by switching to a *two-sided finite difference scheme* which is more accurate in comparison with the former.

The plan of the paper is as follow: in Section 2 we present a partial differential equation governing fluid flow through partially saturated porous media and the corresponding numerical simulator followed by formulation of the inverse problem in Section 3. Section 4 describes the design of the physical model used to obtain experimental data needed to verify the proposed strategy. Implementation, model verification and calibration, results, and analysis of the developed methodology are also presented in Section 4 followed by concluding remarks in Section 5.

2. Formulation of the forward problem

2.1. Mathematical model

Historically, Richards equation [70], which derives from mass conservation and Darcy–Buckingham law [11,18], has been used to simulate fluid flow in partially saturated porous media:

$$\frac{\partial\theta}{\partial t} - \frac{\partial}{\partial z}\left[K(h)\left(\frac{\partial h}{\partial z} - 1\right)\right] = 0 \quad (1)$$