Necessary conditions for inverse modeling of flow through variably saturated porous media

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Abstract
Non-unique solutions of inverse problems arise from a lack of information that satisfies necessary conditions for the problem to be well defined. This paper investigates these conditions for inverse modeling of water flow through multi-dimensional variably saturated porous media. It shows that in order to obtain a unique estimate of hydraulic parameters, along each streamline of the flow field (1) spatial and temporal head observations must be given; (2) the number of spatial and temporal head observations required should be greater or equal to the number of unknown parameters; (3) the flux boundary condition or the pumping rate of a well must be specified for the homogeneous case and both boundary flux and pumping rate are a must for the heterogeneous case; (4) head observations must encompass both saturated and unsaturated conditions, and the functional relationships for unsaturated hydraulic conductivity/pressure head and for the moisture retention should be given, and (5) the residual water content value also need to be specified a priori or water content measurements are needed for the estimation of the saturated water content.

For field problems, these necessary conditions can be collected or estimated but likely involve uncertainty. While the problems become well defined and have unique solutions, the solutions likely will be uncertain. Because of this uncertainty, stochastic approaches are deemed to be appropriate for inverse problems as they are for forward problems to address uncertainty. Nevertheless, knowledge of these necessary conditions is critical to reduce uncertainty in both characterization of the vadose zone and the aquifer, and prediction of water flow and solute migration in the subsurface.

1. Introduction
Inverse modeling exercise is a task frequently performed in many branches of science, engineering, and mathematics where the values of some model parameters are derived from observed model responses. For example, a typical inverse problem in groundwater hydrology is the determination of saturated hydraulic conductivity of a soil or a rock sample based on measured fluxes, hydraulic gradients, and Darcy’s law. Over the past decades, the inverse problem in subsurface hydrology has been extended to identification of spatially distributed hydraulic parameters, source/sink terms, boundary and initial conditions of multi-dimensional models using some observed data.

Mathematical terms, “well posedness” and “ill posedness” are widely applied to the inverse problem in subsurface hydrology. The term “well-posed” problem stems from the definition given by Hadamard [1]. He believed that a mathematical model of physical phenomena should have the properties that (1) a solution exists; (2) the solution is unique; and (3) the solution is stable, and that is to say, a small perturbation in the measurement will only cause small changes in the parameter. A problem that doesn’t follow these rules is believed to be ill posed.

Based on this definition, inverse problems in subsurface hydrology are often considered to be inherently ill posed (e.g. [2–6]). The ill-posedness issue is generally attributed to non-uniqueness of the solution to the problem, due to a lack of information on aquifer responses, initial/boundary conditions and other complications such as hysteresis in unsaturated flow problems. It is also attributed to solution instability: parameters to be estimated are highly sensitive to changes in the response of the subsurface.
Based on the Hadamard definition and the reasons discussed in the previous paragraph, forward problems in subsurface hydrology can be equally ill posed. For example, in many field studies, information about the properties and initial and boundary conditions of the aquifer is incomplete, the solution is nonunique, and the problem is therefore ill posed. Solutions to some forward problems may also encounter stability issues. For instance, nonlinear forward problems (such as some unsaturated or multi-phase flow phenomena) may inherently as well as mathematically unstable (i.e., viscous or density fingering). Therefore, ill-posedness issue is not just limited to inverse problems in subsurface hydrology.

In spite of the ill-posed nature of the inverse problems in subsurface hydrology, Nelson [7] five decades ago demonstrated mathematically that 3-D heterogeneous hydraulic conductivity distribution can be uniquely identified if some necessary conditions are given. That is, the spatial potential (head) variation must be given and the hydraulic conductivity for one point in every stream tube under a steady flow must be specified. Similar conclusions were also reached by Kitamura and Naskagiri [8] and Dietrich and Newsam [5] for parabolic partial differential equation. On the other hand, Vrugt et al. [9] emphasized that the selection of optimization methods may determine whether you can successfully find the global minimum without recognizing the requirement of necessary information. Hopmans et al. [10] suggested that the non-uniqueness may relate to the high correlation among the hydraulic parameters while van Dam et al. [11] ascribed it to low sensitivity of some parameters. The non-uniqueness also has been attributed to low quality and insufficient measurements [12,13].

As stated by Carrera and Neuman [3], “there is a general consensus among groundwater modelers that the inverse problem may, at times, result in meaningless solutions. However, the reasons for this “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.”

Such confusion, in our view, arises from misunderstanding of the Hadamard’s broad definition of well-posedness of a mathematical problem. In particular, inverse modelers in subsurface hydrology community fail to recognize that a forward or an inverse problem may be inherently ill posed due to unstable nature of the problem but it can have unique solution. To avoid such confusion, this paper proposed that a more specific term, a well- or ill-defined problem, is more appropriate for addressing the uniqueness issue of the solution to a forward or an inverse problem. That is, if a problem is well defined (if some necessary information is specified) it has a unique solution in spite of the fact the problem is ill posed in Hadamard’s sense.

The objective of this paper is to investigate and test the necessary conditions for inverse modeling of flow through variably saturated porous media, under isothermal conditions and omission of the gas phase, is often described by a modified Richards’ equation:

\[
\nabla : [K(h, x)] \nabla (h + z) = c_0 S_s(x) \frac{\partial h}{\partial t} + \frac{\partial h}{\partial t} = (c_0 S_s(x) + C(h, x)) \frac{\partial h}{\partial t}
\]

(1)

Where \( x \) is a position vector, \( \nabla = \left[ \frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z} \right] \), \( t \) is time, \( \theta \) represents the volumetric moisture content, and \( z \) is the positive upward vertical coordinate. The pressure head \( h \) is positive or equal to zero when the medium is saturated and negative when the medium is unsaturated. The transitioning parameter \( c_0 \) is equal to one if the medium is saturated and zero if the medium is unsaturated. The term \( S_s(x) \) represents specific storage, \( C(h, x) \) for the soil moisture capacity, and \( K(h, x) \) is the hydraulic conductivity function at location \( x \).

In this study, we will use Gardner’s model [14], a popular model because of its simplicity, to describe the \( K-h \) relation of unsaturated media:

\[
K(h) = K_s \exp(\alpha h)
\]

(2)

where \( K_s \) is the locally isotropic saturated hydraulic conductivity; and \( \alpha \) is the pore-size distribution parameter for the hydraulic conductivity function. We also assume that the \( \theta = h \) follows the Gardner exponential model, which is expressed as:

\[
\theta(h) = (\theta_s - \theta_b) \exp(\beta h) + \theta_b
\]

(3)

where \( \theta_s \) is the saturated moisture content, \( \theta_b \) is the moisture content at residual saturation and \( \beta \) is a pore-size distribution parameter for the moisture release function. The pore-size distribution parameters (\( \alpha \) and \( \beta \)) in Eqs. (2) and (3) are generally assumed to be identical, although experience indicates that they could be different [15,16]. Hysteresis behavior for these two functions is neglected in this study for the sake of simplicity. This set of exponential models is a popular choice for analytical analysis [17–19] since it makes the problem mathematically tractable.

If \( K_s, S_s, \beta, x, \theta_s, \theta_b \) are defined as parameters or primary variables, then \( h \) and \( \theta \) are state variables, secondary variables, or the system responses. A forward problem refers to solving the flow equation for the pressure head or moisture distribution in time and space for given primary variables and initial and boundary conditions. Conversely, an inverse problem refers to the estimation of the primary variables from the knowledge of secondary variables or responses of a system to known excitations.

A forward problem is well defined if the parameters and initial and boundary conditions are completely specified in the solution domain such that a particular (unique) solution exists. Otherwise, it is ill defined and has a general solution or an infinite number of solutions (i.e., there are an infinite number of global minima in terms of satisfying the equations). Similarly, an inverse problem is well defined if some necessary conditions are fully specified as explained next.

3. Inverse model of flow through variably saturated media

Eq. (1), the forward model for multi-dimensional flow in variably saturated heterogeneous media, can be rearranged to take the following form:

\[
A \nabla K(h, x) + BK(h, x) = D(c_0 S_s(x) + C(h, x))
\]

(4)

where \( A = \nabla (h + z) \) is the first-order spatial derivative of the hydraulic head, \( B = \nabla^2 (h + z) \), the second-order spatial derivative and \( D = \partial h / \partial t \), the temporal derivative of the hydraulic head. If we consider \( A, B \) and \( D \) are known coefficients, and parameter fields,
$K(h,x), S_s(x)$ and $C(h,x)$, in Eq. (4) are unknowns to be estimated, this equation becomes the partial differential equation for the inverse problem corresponding to Eq. (1). Note that $K(h,x)$ and $C(h,x)$ are functions of $h$ and $x$, implying that unsaturated hydraulic conductivity and moisture–pressure constitutive relationships of the medium vary spatially. The functional form of these constitutive relationships (i.e., Gardner’s model) is assumed to be the same everywhere, but their parameters vary in space. Again, hysteresis is not considered in this study.

In order to solve Eq. (4), coefficients $A$, $B$ and $D$ everywhere in the solution domain must be specified. This implies that the head everywhere in the domain must be known and the change of head in time everywhere must be given, which must not be zero. Furthermore, since $K(h,x)$ and $C(h,x)$ are functions of $h$, the number of the heads and head changes required at each location, $x$, would depend on the functional form of these functions (i.e., the number of parameters of the function). Additionally, Eq. (4) is a first order partial differential equation in terms of $K(h,x)$. Thus, specification of boundary conditions of the equation in terms of $K(h,x)$ at the known head is a must to guarantee a particular (unique) solution.

4. Uniqueness of solution

In this section, we elaborate on the necessary conditions discussed above further with several cases of flow through one-dimensional homogeneous and heterogeneous media with given functional forms for $K(h,x)$ and $C(h,x)$. Note these serve as only qualitative mathematical proofs.

4.1. Saturated condition

4.1.1. Homogeneous case

Under fully saturated conditions ($\omega = 1$ everywhere in the simulation domain), the moisture capacity term in Eq. (4) is zero. Furthermore, if we assume the flow is one-dimensional in the vertical direction $z$ (positive upward), Eq. (4) is reduced to:

$$A(z,t) \frac{\partial K}{\partial z} + B(z,t)K_z = D(z,t)S_s$$

(5)

where $A(z,t) = \partial (h + z)/\partial z$, $B(z,t) = \partial^2 h/\partial z^2$, and $D(z,t) = \partial h/\partial t$. Since the medium is homogeneous, the above equation can be written as:

$$B(z,t)K_z - D(z,t)S_s = 0 \quad \text{or} \quad \frac{K_z}{S_s} = D(z,t)/B(z,t)$$

(6)

Eq. (6) shows that information about $B(z,t)$ and $D(z,t)$ at any location $z$ in the medium apparently can yield only an estimate of $K_z/S_s$ (i.e., diffusivity). For example, suppose at times, $t_1$ and $t_2$, $B$ and $D$ are known at point $z$ (i.e., no information about boundary) or everywhere in the domain (i.e., prescribed head boundaries). We have a system of equations for $K_z$ and $S_s$:

$$B(z,t_1)K_z - D(z,t_1)S_s = 0$$

$$B(z,t_2)K_z - D(z,t_2)S_s = 0$$

(7)

The determinant of the system of equations is:

$$\text{Det} = -B(z,t_1)D(z,t_2) + B(z,t_2)D(z,t_1)$$

(8)

Using the relationship of diffusivity from (6):

$$\text{Det} = \frac{S_s}{K_z} D(z,t_1)D(z,t_2) - \frac{S_s}{K_z} D(z,t_2)D(z,t_1) = 0$$

(9)

It indicates an infinite number of solutions [20]. This is also true for the case where $B$ and $D$ are known at any number of different locations and times. However, if a boundary flux at $z_0$ and any time $t$, $q_z(z_0,t) = 0$, is specified, $A(z_0,t)K_z = -q(z_0,t)$ where $A(z_0,t)$ is a non-zero gradient at the boundary at time $t$.

Or a pumping well with a pumping rate per volume $Q(t)$ at $z_p$ is known:

$$B(z,t)K_z - D(z,t)S_s = Q(t)\delta(z-z_p)$$

Since new constraints are added, the determinant of the system of Eqs. (7) will not be zero. Therefore, a unique solution of $K_z$ and $S_s$ exists. The same conclusion is made by Carrera and Neuman [3]. This also explains the reason that the analysis of aquifer tests in a 2D depth-averaged homogeneous and isotropic aquifer using their approach has a unique solution, even though the aquifer is assumes unbounded. Specifically, flow toward a well in the aquifer can be visualized as a collection of flow along axisymmetrically converging streamlines. Flow behavior along one streamline is the same as those along other streamlines, and is identical to the one-dimensional flow discussed above. Therefore, if the pumping rate is specified and the drawdown as a function of time is known at a given $r$, the necessary condition is met and the problem is well defined such that a unique solution exists.

4.1.2. Heterogeneous media

If flow is under a steady condition and the medium is heterogeneous, a general solution to the governing equation (i.e., Eq. (5) with $D(z,t) = 0$) is:

$$\ln(K(z)) = - \int \frac{B(z)}{A(z)} dz + E$$

(10)

where $A(z) \neq 0$ and that the gradient cannot be zero, which is quite obvious. $E$ is an integration constant, which can be determined by applying a boundary condition associated with the governing equation. The boundary condition can be the $\ln(K(z))$ value at any given location $z^*$ (i.e., $K(z^*)$ at any location along a streamline [7]) or specific discharge. Once $E$ is determined, the general solution, Eq. (10), becomes a particular solution (i.e., a unique solution).

For the situation where a pumping well at $z_p$ is present, the analytical solution Eq. (10) becomes:

$$K(z) = e^{\gamma \int \frac{Q(z-z_p)}{A(z)} dz + G}$$

(11)

where $y = \int \frac{B(z)}{A(z)} dz$ and $G$ is an integration constant which must be determined by applying the boundary condition. Different from the homogeneous case, if the pumping location is not at the boundary, the pumping rate of the pumping well is not sufficient to obtain a particular solution unless one $K$ value is also specified.

Likewise, in order to obtain a unique solution for $K_z(z)$ and $S_s(z)$ during transient flow in the one dimensional heterogeneous medium, the rate of head change $D(z,t)$ at every location must be given and it must be non-zero in addition to a conductivity measurement $K(z^*)$. A system of first order differential equations thus can be formed and solved for $K_z(z)$ and $S_s(z)$ values. Zhu and Yeh [21] have numerically verified these conditions. That is, all heads within a domain at two time steps and boundary fluxes or one conductivity value are the necessary conditions.

4.2. Unsaturated conditions

4.2.1. Homogeneous media

Consider the case where the medium is fully unsaturated ($\omega = 0$ everywhere in the simulation domain). Eq. (4) becomes:

$$A(z,t) \frac{\partial K(h)}{\partial z} + B(z,t)K(h) = C(h)\frac{\partial h}{\partial t}$$

(12)

with a boundary condition at $z = 0$:
If the flow is steady, Eq. (12) can be reduced to:

\[ \frac{dK(h)}{K(h)} = \frac{B(z)}{A(z)} \, dz \quad \text{or} \quad \ln K(h) = - \int \frac{B(z)}{A(z)} \, dz + G \]

(14)

where \( G \) is an integration constant, which can be determined by the application of the boundary condition. Afterward, Eq. (14) becomes

\[ \ln K(h) = - \int \frac{B(z)}{A(z)} \, dz + \ln K(h_0) + \int \frac{B(z)}{A(z)} \, dz \bigg|_{z=0} = F(z) \]

(15)

where \( h_0 \) denotes \( h \) at \( z = 0 \). Substitution of the hydraulic conductivity and pressure relation, Eq. (2), into the left-hand side of Eq. (15) yields

\[ \ln K_s + z h = F(z) \]

(16)

In order to determine \( K_s \) and \( z \) of Eq. (16), two independent equations based on Eq. (16) must be formed. This system of equations can be derived if \( A, B, h \) and \( z \) at two locations, \( z_1 \) and \( z_2 \) are known such that \( F(z_1) \) and \( F(z_2) \) can be determined. Therefore, we have two independent equations:

\[ \ln K_s + h_1 z = F(z_1) \]
\[ \ln K_s + h_2 z = F(z_2) \]

(17)

The determinant of the equations is:

\[ \text{Det} = h_2 - h_1 \]

(18)

and it will not be zero as long as \( h_1 \neq h_2 \). Two possible physical situations can lead to a non-zero determinant: (1) two unit-gradient conditions with different specific discharges, \( q_1 \neq q_2 \), then \( h_1 \neq h_2 \); (2) one steady-flow, non-unit gradient profile where \( z \) is constant along the flow path. If two head measurements are taken at different elevations \( z_1 \) and \( z_2 \), and \( h_1 = h_2 \), thus the determinant is non-zero.

Once we determine the parameters for \( K(h) \), we can proceed to estimate soil-moisture capacity term. Suppose \( A, B, h \) and \( \partial h/\partial t \) at all \( z \)'s at a given \( t \) in the flow domain are known. We can rewrite Eq. (12) as:

\[ A(z, t) \frac{\partial k(h)}{\partial z} + B(z, t) K(h) \bigg|_z = A(z, t) \frac{\partial k(h)}{\partial z} \bigg|_z = C(h) \]

(19)

where terms on the left hand side of Eq. (19) are known. If the moisture retention curve takes an exponential form, Eq. (3), then the moisture capacity term is:

\[ C(h) = \frac{dh}{dh} \right\} = (\theta_s - \theta_i) \beta \exp(\beta h) \quad \text{or} \quad \ln C(h) \]
\[ = \ln(\theta_s - \theta_i) + \ln \beta + \beta h \]

(20)

Eq. (20) implies that two different pressure heads are necessary to determine \( \beta \) and \( (\theta_s - \theta_i) \). Note that in order to estimate \( \theta_i \) or \( \theta_s \), one of them must be given a priori or moisture content measurements. The solution to the inverse equation is again unique.

Suppose steady flow information is not available. From Eq. (19) we have:

\[ A(z, t) \frac{\partial k(h)}{\partial z} + B(z, t) = D(z, t) C(h) / K(h) \]

(21)

After using the exponential relationship, further simplification leads to:

\[ A \frac{\partial h}{\partial z} + B = D(\theta_i - \theta_s) / K_s \]

(22)

If we assume that \( \alpha = \beta \) for mathematic simplicity, then we have:

\[ A \frac{\partial h}{\partial z} x + B = D(\theta_i - \theta_s) \]
\[ A \frac{\partial h}{\partial z} + B(x)^{-1} = D(\theta_i - \theta_s) \quad \text{or} \quad \Omega + BY = DX \]

(23)

where \( \Omega = (\partial h/\partial z + 1) / \partial h/\partial z, X = (\theta_i - \theta_s) / K_s \), and \( Y = \alpha^{-1} \). If \( \partial h/\partial z, B = \partial^2 h/\partial z^2 \) and \( D = \partial h/\partial t \) are specified at two different times or locations, a system of two linear equations is formed.

\[ D_x X - B Y = \Omega_1 \]
\[ D_x X - B Y = \Omega_2 \]

(24)

The determinant is non-zero, and there is a unique solution for \( X = (\theta_i - \theta_s) / K_s \) and \( Y = \alpha^{-1} \). With a given flux boundary condition:

\[ K(h)|_{z=0} = -q / [\partial h(t) / \partial z] \bigg|_{z=0} = -q / A_0 \]

\[ A_0 = \left[ \frac{\partial h(t) / \partial z} {\partial h(t) / \partial z} \right]_{z=0} \]

(25)

The value of \( K_s \) can then be determined and in turn, the value of \( (\theta_i - \theta_s) \). Again, in order to obtain the value of \( \theta_i \) or \( \theta_s \), one of them must be specified a priori. For cases where \( \alpha = \beta \), an analytical analysis is difficult but should lead to the same result (see the numerical example section).

4.2.2. Heterogeneous media

The aforementioned necessary conditions hold for the heterogeneous medium if the constitutive relationship everywhere in the media is described by the same model. An analytical analysis may be possible for this case but it can be intractable at this moment. As a result, we use numerical examples to demonstrate validity of these necessary conditions.

4.3. Variably saturated conditions

The necessary conditions for flow through media under variably saturated conditions are the combination of the necessary conditions for saturated flow and those for unsaturated flow situations. That is, the pressure head measurements must register both changes in positive and negative pressures such that the value of the parameters, \( K_s, S_x, \alpha, \beta \), and \( \theta_s \), can be uniquely estimated if \( \theta_i \) is given.

4.4. Summary

The above analysis corroborates the fact that in order to obtain a unique solution: (1) the spatial derivatives \( A \) and \( B \) and the temporal derivative \( D \) of head everywhere in the medium or the spatial and temporal head distributions must be known and non-zero, (2) the number of spatial and temporal head data equals to the number of unknowns, (3) one \( K \) value or flux at the boundary must be specified, (4) for unsaturated and variably saturated conditions, the mathematical model for \( K(h) \) and \( \partial h/\partial t \) or \( \partial h/\partial z \) relationships must be given and (5) \( \theta_i \) must be specified a priori or water content data are needed.

5. Numerical experiments

Numerical experiments are conducted to further illustrate the validity of the necessary conditions for three cases: Case 1, flow through a saturated homogenous medium, Case 2, flow through a variably saturated homogenous medium and Case 3, flow through a variably saturated heterogeneous medium. The unsaturated flow experiment is skipped since it is just a part of the variably saturated experiment. All these experiments involve a one-dimensional, vertical, uniform flow in a two-dimensional soil
column with height of 60 cm and width of 1 cm. The column is discretized into 60 elements; each of them is 1 cm \times 1 cm in dimension. The two sides of the column are considered to be impermeable. For the homogeneous medium, the unsaturated hydraulic conductivity curve and the moisture release curve of the medium are assumed to follow the Gardner exponential model. Specific values of parameters are: $K_s = 0.495$ cm/min, $S_s = 0.0005$ cm, $\alpha = 0.15$ cm, $\beta = 0.15$ cm, $\theta_i = 0.35$ and $\theta_f = 0.045$.

For the case where flow through a fully saturated medium (Case 1) is considered, the following initial and boundary conditions are used. A total head of 200 cm is assigned as the initial condition throughout the entire medium. At the top boundary condition, a total head of 200 cm is specified at all times and a constant flux of 0.12 cm/min discharging from the medium is assigned to the bottom boundary.

In the case where variably saturated flow is considered (Case 2), the initial condition in terms of the total head is assumed to be 60 cm (a hydrostatic condition with the water table initially at the top boundary). The top boundary is considered to be impermeable, and a constant flux of 0.12 cm/min discharging from the bottom of the medium is assigned.

In Case 3, the same soil column is used but is divided into four layers. Each layer is 15 cm thick and has its own hydraulic properties as specified in Table 1. The boundary and initial conditions are the same as those in Case 2.

For all these cases, VSAFT2 is used to simulate pressure head, moisture content, and velocity fields at different times. VSAFT2 is a FORTRAN program for simulating variably saturated flow and transport in two-dimensional media, using a finite element approach [22] (available at www.hwr.arizona.edu/yeh).

### 6. Numerical inverse solution

Based on the above analysis, the necessary conditions are a must for a unique solution to the inverse problem. Once they are fully specified in spite of accuracy of the conditions, the problem is deterministic (well defined). A deterministic inverse problem can be solved directly based on a system of Eq. (4) and associated boundary conditions using analytical methods as illustrated previously. Alternatively, one can employ an optimization approach based on the least squares method (see [23,24]). In the following numerical experiments, we demonstrate the necessary conditions using the widely employed PEST. Equal weights are assigned to all the observation data. No regularization scheme is used in PEST and only the ordinary iterative parameter estimation method is applied.

The least squares approach iteratively adjusts parameters and solves the forward equation to match observed heads. Since the solution to the forward problem requires specification of the associated boundary and initial conditions. Knowledge of the flux boundary condition for the forward problem and matching observed heads is equivalent to specification of spatial derivatives $A, B$ and $D$ as required for the necessary conditions. Once the initial condition is given, the head distribution in the entire domain at time zero is known. Therefore, head values at one additional time will be necessary to satisfy the requirement of the temporal derivative $D$. Furthermore, the number of head observations needed in each medium would depend on the number of parameters to be sought as discussed previously.

### 7. Results

#### 7.1. Noise free

**7.1.1. Saturated flow**

Fig. 1 shows the total head as a function of time at four elevations ($Z = 8$ cm, $20$ cm, $30$ cm and $50$ cm) of Case 1. Symbols (circle) indicate observed heads at $t = 0.5$ min and $t = 3.0$ min at $Z = 20$ cm, which were used in the inverse model. Estimated $K_s$ and $S_s$ values based on three different initial guess values as a function of iteration are plotted in Figs. 2a and b. According to these figures, all estimates converge to the same values after the 7th iteration. The estimated $K_s$ and $S_s$ converge to the true value. The result confirms the theoretical analysis. That is, observed heads at two different times at one location and a specified flux are the necessary conditions for unique identification of $K_s$ and $S_s$ values for flow through homogeneous medium under saturated conditions. Likewise, head observations at two different locations at a given time and a specified flux allow unique identification of $K_s$ and $S_s$ values.

**7.1.2. Variably saturated flow**

Simulated total heads as a function of time at three elevations under the variably saturated flow condition (Case 2) are plotted in Fig. 3. Total head data at five observation times (i.e., $t = 0.7$ min, 2 min, 40 min, 55 min, and 70 min, circle symbols in the figure) at a given elevation $Z = 40$ cm and the flux information were used for identifying five parameters. That is, we established five equations for five parameters. The estimated values for parameters, $K_s, S_s, \alpha$, and $\beta$ are required for the necessary conditions. Once the initial condition is given, the head distribution in the entire domain at time zero is known. Therefore, head values at one additional time will be necessary to satisfy the requirement of the temporal derivative $D$. Furthermore, the number of head observations needed in each medium would depend on the number of parameters to be sought as discussed previously.

### Table 1

Lists of hydraulic properties of the composite soil column.

<table>
<thead>
<tr>
<th>Medium</th>
<th>$K_s$ (cm/min)</th>
<th>$S_s$ (1/cm)</th>
<th>$\alpha$ (1/cm)</th>
<th>$\beta$ (1/cm)</th>
<th>$\theta_i$</th>
<th>$\theta_f$</th>
<th>Location (cm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Medium 1</td>
<td>0.20</td>
<td>0.0002</td>
<td>0.10</td>
<td>0.20</td>
<td>0.35</td>
<td>0.045</td>
<td>0–15</td>
</tr>
<tr>
<td>Medium 2</td>
<td>0.35</td>
<td>0.0005</td>
<td>0.15</td>
<td>0.25</td>
<td>0.20</td>
<td>0.045</td>
<td>15–30</td>
</tr>
<tr>
<td>Medium 3</td>
<td>0.55</td>
<td>0.0008</td>
<td>0.30</td>
<td>0.40</td>
<td>0.25</td>
<td>0.045</td>
<td>30–45</td>
</tr>
<tr>
<td>Medium 4</td>
<td>0.45</td>
<td>0.0006</td>
<td>0.20</td>
<td>0.35</td>
<td>0.30</td>
<td>0.045</td>
<td>45–60</td>
</tr>
</tbody>
</table>
and $h$ as a function of iteration using three initial guess values for each parameter are shown in Fig. 4a–e. According to these figures, all estimates converge to corresponding true values after the 20th iteration. Again, these results suggest that these parameters can be uniquely identified as demonstrated in the above theoretical analysis, in spite of high or low degree of sensitivity of head to changes of parameters.

More realistic $K(h)$ and $h(h)$ relationships such as van Genuchten model [25] have also been tested although the results are not shown here. Similarly, unique and accurate estimates for all the parameters can be obtained if the necessary conditions are met.

7.2. Effects of data noise

Effects of white noise on the estimates of a well-defined inverse problem were investigated using observed heads corrupted with white noise with a standard deviation of 2.0 cm. We investigated only the case where the flow is under variably saturated conditions. First, we assumed that observations were made at the three elevations as in the previous case, and at each observation elevation head values were sampled at 45 different time steps. Random noises are then added to these data. As expected, with the necessary conditions given, three different initial guess values for each parameter converge to the same final value. However, the value of the final estimate deviates significantly from the true value due to the noise.

If the number of spatial observations is increased to 8 ($z = 5$ cm, 15 cm, 25 cm, 35 cm, 40 cm, 45 cm, 50 cm and 55 cm) and the number of temporal samples remains the same: 45 time steps, we have 360 head data with noise for the inverse modeling effort. The final estimate of each parameter approaches its true value with slight differences as illustrated in Figs. 5a–e. Fig. 6 shows the simulated total heads vs. observed heads as a function of time at the eight locations.

Apparently, as long as the necessary conditions are met, the estimates are unique in spite of the presence of measurement errors. However, quality of the estimate will vary with the accuracy of the head observations. Nevertheless, since a least squares approach is used and the errors are uncorrelated white noises, the quality of the estimate improves as the number of observations in time and space increases.

7.3. Effects of heterogeneity

Fig. 7 shows simulated total head at four sampling elevations (13 cm, 22 cm, 37 cm, and 48 cm) as a function of time in the column of Case 3. Each of the four sampling elevations is located in one of the four layers. To meet the requirement of the necessary condition, five pressure head measurements, ranging from saturated to unsaturated conditions (see symbols in Fig. 7) are sampled at each elevation to estimate five parameters ($K_s$, $S_s$, $a$, $b$, and $h_s$) of each medium. A uniform initial guess value for each of the five parameters is used for the four layers to find the true values of the parameters. The estimated results using three different sets of initial guess values for the five parameters are shown in Figs. 8. All estimates, regardless of different initial guess values, converge to their corresponding true values. Unsaturated parameters $a$ and $b$ shows a relatively slow convergence speed. It may be attributed to their small sensitivity to observed heads. Although only four media are considered here, this principle applies to any number of media. These results therefore substantiate the necessary conditions for heterogeneous media we established in the previous section.

8. Discussion and conclusion

This study shows that an inverse model of flow through porous media under variably saturated conditions can be well defined and has a unique solution if the necessary conditions are met. These necessary conditions are as follows. Along any streamline (1)
spatial and temporal head observations must be specified of which temporal change must be non-zero for transient problem. The number of temporal head measurements required depends on the number of unknown parameters at each location; (2) for homogeneous model, flux boundary condition or the pumping rate at the pumping well must be specified; and both flux boundary condition and pumping rate are needed for heterogeneous case; (3) head data must cover both saturated and unsaturated conditions; (4) mathematical model for $K(h)$ and $h(h)$ or $C(h)$ relationships must be given, and (5) $h_s$ must be specified a priori or water content data are needed for the estimation of $h_s$. Once these conditions are met, the solutions always converge to the true values regardless of initial guess values if head measurements and fluxes are free of errors. Under situations where the measurements are infested with noise, the solutions are unique but may be incorrect. The discrepancies between the correct values and the solutions diminish as the number of head measurements in time and space increases.

These necessary conditions are developed based on the governing equation for flow through multi-dimensional media under variably saturated conditions. The validity of these conditions is tested using one-dimensional example due to our limited computational resources. Nevertheless, as long as flow through porous media obeys Darcy’s law, a multi-dimensional problem is merely a collection of many one-dimensional flow tubes. Therefore, one-dimensional examples are deemed to be sufficient for demonstrating the validity of the necessary conditions.

The necessary conditions for inverse modeling are critical for field data collections. For instance, if a confined aquifer is conceptualized as a 2-D depth averaged, homogeneous and isotropic aquifer, then the pumping rate and drawdown-time data (a well hydrograph) at one location of the aquifer are sufficient to make the inverse modeling of the pumping test well defined. As a well-defined problem, its solution is unique. On the other hand, the same aquifer subjected to the same pumping test may be

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**Fig. 4.** The figure shows estimates of (a) $K_s$, (b) $S_s$, (c) $a$, (d) $b$ and (e) $h_s$ as a function of iteration using noise-free head data with different initial guess values and the corresponding true values for the variably saturated medium.
conceptualized as a heterogeneous one with several parameter zones. In this case, knowledge of well hydrographs at each zone and the pumping rate are however not sufficient to make the inverse problem well defined. The problem becomes well defined if the flow rate at each of the observation wells (boundary flux) is known during the pumping test. This implies that groundwater flow rate at the monitoring wells should be collected. The necessary conditions thus provide some insight to the design of data collection schemes.

The uniqueness of the solution of an inverse problem nevertheless is not the cure to all issues of aquifer/vadose zone characterization as is the uniqueness of the solution of a forward problem to prediction of flow and solution transport. The unique solution of a well-defined inverse problem is accurate only in terms of given model assumptions or input information. Inaccurate solutions to the inverse problem arise from inaccuracy, inconsistency or non-representativeness of the model as well as the input information. That is, while the solution to an inverse problem is mathematically unique, it may be uncertain. Uncertainty means that there are many possible solutions. For example, geologic media are inherently heterogeneous at multiple scales, and homogeneous assumption is intrinsic in any mathematical model over certain volume (control volume) or the entire domain of the media. As a result, observed heads in a field or laboratory experiment are expected to be different from the simulated based on a model (see [26,27]). Effect of such differences on the estimate is similar to that of noisy data. That is, unless representative head samples in time and space are used in the estimation, the estimates likely will vary with the number of head samples used. Huang et al. [28], Straface et al. [29], Xiang et al. [30] and Berg and Illman [31] also reported that the equivalent homogeneous transmissivity and storage coefficient identified from well-defined inverse problems associated with pumping tests vary.

**Fig. 5.** It shows plots of different initial guess values for (a) $K_s$, (b) $S_s$, (c) $\alpha$, (d) $\beta$ and (e) $\theta_s$ and their estimates as a function of iteration using noisy data and their corresponding true values for the variably saturated medium.
with the pumping well location, and that they yield biased predictions of flow fields if pumping location is changed. These issues are attributed to nonrepresentativeness of the estimated effective homogeneous transmissivity and storage parameters [26,28].

If the necessary conditions are not met (information is lacking), the inverse problem becomes ill defined and has mathematically nonunique solutions. This is also true for any forward problem. For ill-defined forward problems, techniques have been employed to fill in the missing information. For example, inverse distance method or linear or nonlinear functions or others has been used to estimate hydraulic parameter values at locations where measurements are not available to satisfy the necessary condition.

Fig. 6. It shows plots of simulated total heads vs. observed heads as a function of time at the eight sampling locations for the variably saturated flow case where standard deviation of noise is 2.0 cm.
Consequently, the forward problem can be solved, and a unique solution can be derived. This solution however may not be the correct solution and thus, it is uncertain. Similarly, to deal with ill-defined inverse problems, regularization approaches have been developed to obtain mathematically unique solutions (e.g., [6]). Again, the unique solutions may not be the true solutions and thus are uncertain.

Because of uncertainty of solutions to either forward or inverse problems, stochastic methods have emerged over the past decades to derive statistically unbiased solution and to quantify its uncertainty (likely deviation from the true field). Specifically, for ill-defined forward problems where our knowledge of hydraulic properties of geological media is not available or incomplete, unconditional and conditional effective parameter approaches have been developed. The goal of the unconditional approaches is to derive homogeneous effective properties that facilitate prediction of most probable flow field at the lowest spatial resolution and is to quantify its uncertainty (e.g., [32–35] and others for saturated flow; [36–38] for unsaturated flow). On the other hand, conditional approaches (e.g., kriging or conditional simulations using measurements of hydraulic parameters) aims to derive the most probable flow field at a high resolution with less uncertainty (e.g. [39–42] for aquifers, and [43–46] for the vadose zone).

Stochastic conditional approaches have also been developed using measurements of parameters as well as aquifer responses (such as heads or concentrations) to cope with ill-defined inverse problems (e.g. [47–59] and many others) for saturated flow and [44,60–62] for variably saturated flow). To reduce uncertainty in the solution, recently joint interpretation of sequential pumping tests have been developed (e.g. [21,30,63–73]) and tested in fields (e.g. [28,29,74–78]).

While the stochastic approaches are useful to deal with ill-defined inverse problems, the necessary conditions provide valuable guidance for collecting appropriate data that are necessary to reduce uncertainty of its solution. For example, knowledge of the pumping rate of a pumping test or boundary fluxes in aquifers is essential to narrow the range of the conductivity value of an aquifer. Likewise, knowledge of the infiltration rate is necessary to reduce the range...
of possible values of parameters for the vadose zone. This necessary information also explains the reason why active and passive hydrologic tomography (i.e. hydraulic and river stage tomography, [79,80]) should yield more robust characterization of aquifers than geophysical methods in terms of their hydraulic property values. Finally, we emphasize that understanding of the necessary conditions would lead to more accurate characterization of the vadose zone and the aquifer and in turn, prediction of flow and solute transport in the subsurface become possible.

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