This article deals with the determination of nonlinear coefficient functions in partial differential equations in the field of soil science. We consider two examples to illustrate the numerical determination of nonlinear coefficient functions. In detail, these are the determination of the sorption characteristic of a chemical and the determination of the unsaturated hydraulic properties of a porous medium from measurements obtained from suitable column experiments. This inverse problem is treated by minimizing a least square functional. To cope with the ill-posedness, we apply a parametrization of the unknown nonlinear coefficient function, which is defined by an appropriate interpolation. The parametrization does not use a priori assumptions, which are not justified by physical properties. This kind of parametrization permits a hierarchical approach in the number of the degrees of freedom used. According to the hierarchical structure, we integrate the determination of the coefficient functions into a multi-level procedure. The investigation of the stability of the parametrization is based on the singular values of the sensitivity matrix.

**Keywords:** Multi-level identification; Stability analysis; Sorption characteristics; Unsaturated hydraulic properties

1 INTRODUCTION

Reactive and nonreactive transport processes through porous media are described by models consisting of partial differential equations, see [17, 18]. Typical material properties of the porous medium or the chemical, which is transported, enter the model equation in form of coefficient functions. Often these coefficient functions depend nonlinearly on the solution of the respective differential equation.

The material properties must be known in reasonable limits for a reliable numerical simulation of the transport process. A common method to determine the material properties is the inverse modeling of suitable column experiments.
The determination of unknown nonlinearities from measured data is in general an *ill-posed* problem. Besides the question of existence and uniqueness, the missing stability complicates the solution of the inverse problem. Small measurement errors may lead to large deviations of the determined coefficient functions from the true values.

Inverse modeling is common practice for the determination of soil properties. For overviews see [19, 24]. References [9, 12, 13, 26] investigate the inverse determination of the hydraulic properties for different parametrization types and experimental setups. Reference [16] deals with the parameter identification in multiphase flow.

A method which copes with the ill-posedness is necessary to determine the nonlinearities: a generalized solution is defined by the minimum of an appropriate error functional, which indicates the difference between numerically computed and measured data. Stabilization can be achieved by replacing the infinite dimensional problem with a finite dimensional problem obtained by means of a discretization of the coefficient space.

An appropriate stability analysis detects the optimal number of degrees of freedom and a multi-level procedure stepping through the dimensions makes this information operational. Also all ingredients of such approaches are well known and partly also used for identification problems (see [1, 5–7, 27]), it is the well-tuned interplay of all these components, which provide an accurate and reliable method. This, besides the successful application of the approach to real data from geosciences application, is our new contribution.

The applied method uses only *a priori* information as monotonocity of the coefficient functions. Further information on the shape, e.g. on the curvature is not required. Occasionally, concavity can be used for an additional restriction of the coefficient space to stabilize the numerical procedure.

We illustrate the numerical determination of nonlinear material properties by means of two examples. These exemplary problems are specified in the following section. We describe the underlying model equation and the principle of the experiment used for the determination of the unknown coefficient functions. The discretization approach of the nonlinearities and the numerical procedure for solving the inverse problem are explained in the third section. In the fourth section, we present numerical results for the problems described in Section 2. The article closes with “Summary and Conclusions” in Section 5.

### 2 EXAMPLES FOR REACTIVE AND NONREACTIVE TRANSPORT PROCESSES THROUGH POROUS MEDIA

The following two examples describe fundamental problems of determining material properties in transport processes through porous media. The first one refers to reactive transport and the second one refers to fluid flow.

The necessary data for the inversion are produced from laboratory column experiments. Typically, the physical properties of these experiments allow us to assume that it is sufficient to describe the transport processes in the column in one spatial dimension. Therefore, we confine the description to the one dimensional model in space.

#### 2.1 Transport of Chemicals Coupled with Equilibrium Sorption Processes

Column breakthrough experiments serve for the identification of reactive processes of chemicals in porous media. The experimental setup consists of a vertically oriented
column filled with the porous medium. The column is initially free of contamination. Water contaminated with the chemical at a predefined concentration enters the column from the top and is pumped by a peristaltic pump into a data acquisition device. The observation takes place by measurements of the outflow concentration of the chemical – the so-called breakthrough – at the column outlet at the bottom. A sophisticated sprinkler mechanism at the top emulates natural rain infiltration and results in a vertical steady-state water flow from top to bottom. As the soil column is packed homogeneously perpendicular to the vertical flow direction, it can be modeled appropriately in one spatial dimension. Typical soil columns possess a length of about 10–20 cm. Further details on the experiment can be found, for e.g. in [32, 33, 35].

The transport of a sorbing chemical through the column is modeled by a convection–diffusion equation for $x \in (0, L)$ and $t \in (0, T]$:

$$\partial_t c(x, t) + \theta \partial_x c(x, t) - \partial_x (D \partial_x c(x, t) - qc(x, t)) = 0$$

(1)

$$c(x, 0) = 0$$

(2)

$$-(D \partial_x c(0, t) - qc(0, t)) = qc_0(t)$$

(3)

$$\partial_x c(L, t) = 0$$

(4)

where $L$ is the length of the column and $T$ the time of complete breakthrough of the dissolved chemical. $c(x, t)$ denotes the dissolved concentration of the chemical, $s(x, t)$ the concentration of the chemical sorbed to the immobile phase, $\theta$ the volumetric water content, $\rho$ the mass fraction of the sorption site, $D$ the diffusion–dispersion and $q$ the Darcy flow velocity. The inflow and outflow boundaries of the column are described by a flux boundary condition (3) and a homogeneous Neumann boundary condition (4), respectively.

The reactive interaction is given by the sorption of the dissolved chemical to the surface of the porous medium. Here, the sorption process is confined to the equilibrium case, where the sorbed concentration is described by a (nonlinear) sorption characteristic in dependence on the dissolved concentration:

$$s(x, t) = \varphi(c(x, t)).$$

The sorption characteristic $\varphi : \mathbb{R}^+ \rightarrow \mathbb{R}^+$ is assumed to be monotone increasing with $\varphi(0) = 0$. This assumption is justified by physical reasons. Occasionally, concavity of the sorption characteristic is supposed. A more detailed consideration of transport and sorption models can be found in [22].

The observation of the breakthrough can be interpreted as an additional boundary condition:

$$c(L, t) = w(t)$$

(5)

for $t \in (0, T]$.

The determination of the sorption characteristic $\varphi$ ($\theta$, $\rho$, $D$ and $q$ are assumed to be known) from measured $w$ denotes the inverse problem, whereas the corresponding direct problem consists of the computation of $w$ for given $\varphi$.

Igler [20, 21] shows that the sorption characteristic $\varphi$ is identifiable from the observation $w$ in the following sense: the direct mapping $\varphi \mapsto w$ is injective in the space of piecewise analytic functions $\varphi$ if $c_0(t)$ is monotone increasing and $w$ is obtained by
exact, error-free measurements. This statement was proven by means of the method of
integral identities originated by DuChateau [10]. The identifiability domain is given by
\[ [0, \max_{x \in [0, L]} c(x, t)] . \]

The experiment does not provide information about the sorption characteristic outside
of this domain.

2.2 Unsaturated Water Flow

The second example concerns the determination of the hydraulic properties of porous
media. The hydraulic properties consist of the water retention curve, which relates the
capillary pressure to the volumetric water content in the pore volume, and the hydraulic
conductivity also depending on the capillary pressure.

To determine these two nonlinearities, column outflow experiments were developed. A
precise description of the experimental setup can be found e.g. in [12, 31]. The
principle of a column outflow experiment is as follows: a vertically oriented and
initially saturated column is drained by decreasing the pressure applied at the bottom
of the column. Water flow across the top of the column is not allowed. The water
outflow at the bottom is retained in a burette, such that the cumulative water outflow
can be measured. Additionally, the pressure at (or near) the top can be measured by a
tensiometer. The soil column is packed homogeneously perpendicular to the vertical
flow direction, hence we can confine the description of the experiment to one spatial
dimension.

The water flow in the column is described by the Richards equation in the pressure
form for \( x \in (0, L) \) and \( t \in (0, T) \):

\[
\frac{\partial}{\partial t} \Theta(\psi(x, t)) - \frac{\partial}{\partial x}(K(\psi(x, t))(\frac{\partial}{\partial x} \psi(x, t) - 1)) = 0 \tag{6}
\]

\[ \psi(x, 0) = x \tag{7} \]

\[ \frac{\partial}{\partial x} \psi(0, t) - 1 = 0 \tag{8} \]

\[ \psi(L, t) = \psi_L(t), \tag{9} \]

where again \( L \) is the length of the column and \( T \) is the end time of the experiment.
\( \psi(x, t) \) denotes the pressure, \( \Theta(\psi) \) the retention curve and \( K(\psi) \) the hydraulic
conductivity. The upper boundary is modeled by a no flow boundary condition. A
Dirichlet boundary condition is used for describing the outflow boundary.

The unsaturated zone is characterized by negative pressure values (\( \psi < 0 \)). A non-
negative pressure (\( \psi \geq 0 \)) indicates the saturated zone, where the atmospheric pressure
is assumed being scaled to 0. The saturated zone need not be taken into account, because the hydraulic properties are constant there:

\[
\Theta(\psi) = \Theta_{sat}, \quad K(\psi) = K_{sat} \quad \text{for } \psi \geq 0 . \tag{10}
\]
In addition, the functions \( \Theta: \mathbb{R} \to \mathbb{R}_+ \) and \( K: \mathbb{R} \to \mathbb{R}_+ \) must be monotone increasing for physical reasons.

As we have to determine two different functions, we also use two different kinds of observations, measurements of the pressure and the cumulative outflow. These observations yield the following conditions:

\[
\psi(0, t) = w_0(t) \quad (11)
\]

\[
\int_0^t K(\psi(L, \tau)) \left( \partial_x \psi(L, \tau) - 1 \right) d\tau = w_L(t). \quad (12)
\]

Analogously to the first example, the inverse problem consists of the determination of the hydraulic properties \( \Theta \) and \( K \) from given measurements of \( w_0 \) and \( w_L \). The computation of \( w_0 \) and \( w_L \) for given \( \Theta \) and \( K \) is the corresponding direct problem.

By means of the method of integral identities, DuChateau has proven the identifiability of the hydraulic properties from the observations \((w_0, w_L)\) in above sense (injectivity of the mapping \((\Theta, K)\) \(\mapsto (w_0, w_L)\)) if the Dirichlet boundary value is monotone decreasing \((\psi_L(t) \leq 0 \text{ with } \psi_L(0) = L)\) and if the saturated water content \( \theta_{\text{sat}} \) is known. The maximum identifiability domain is given by (see [11])

\[
[\psi_L(T) - L, 0].
\]

### 3 Solution of the Inverse Problem

#### 3.1 Least Squares Approach and Parametrization

First, we note that in practice the observations cannot be measured continuously in time. Therefore, we assume in the following that the observations are given as a finite dimensional vector \( w \in \mathbb{R}^n \).

Let \( \mathbf{f} \) denote the coefficient function (or the vector of the coefficient functions, respectively), which is to be determined and let \( w(\mathbf{f}) \) be the corresponding observation computed by solving the direct problem for given \( \mathbf{f} \). The measured observations possibly disturbed by measurement errors are denoted by \( \mathbf{w}^* \).

Now, our inverse problem reads as: find a coefficient function \( \mathbf{f} \), which solves

\[
w(\mathbf{f}) = \mathbf{w}^*. \quad (13)
\]

As a solution \( \mathbf{f} \) of (13) does not exist in general, we define a generalized solution by a least squares approach: Find \( \mathbf{f}^* \) which minimizes

\[
J(\mathbf{f}) = \|w(\mathbf{f}) - \mathbf{w}^*\|_2^2. \quad (14)
\]

Here, \( \| \cdot \|_2 \) denotes the Euclidian norm. The generalized solution \( \mathbf{f}^*(w^*) \) defined by the minimum of the error functional (14) need not depend continuously on \( w^* \). We regularize the inverse problem by a discretization of the coefficient space.

In accordance with the remarks of the previous section concerning identifiability, it is sufficient to describe a single-valued function \( f \) only on the respective identifiability domain, which is in the following denoted by \([u_{\text{min}}, u_{\text{max}}]\). (Outside of this domain, \( f \) can be assumed to be constant if it is necessary.)
A coefficient function \( f \), which is continuous and piecewise analytic on \( [u_{\text{min}}, u_{\text{max}}] \), is replaced by a parametrization \( f(u) = f_p(u) \) defined by a finite number of parameters – also called degrees of freedom – in the following way: We define a partition of \( [u_{\text{min}}, u_{\text{max}}] \):

\[
  u_{\text{min}} = u_1 < u_2 < \cdots < u_{r-1} < u_r = u_{\text{max}},
\]

where each node \( u_j \) is supplied with a degree of freedom \( p_j \) (\( j = 1, \ldots, r \)). We use the degrees of freedom as values of \( f_p \) at the nodes \( u_j \):

\[
  f_p(u_j) := p_j \quad \text{for} \quad j = 1, \ldots, r .
\]

For \( u \in (u_j, u_{j+1}) \), \( j \in \{1, \ldots, r-1 \} \), we determine the value \( f_p(u) \) by interpolation between \( p_j \) and \( p_{j+1} \). Appropriate approaches are piecewise linear interpolation and piecewise cubic Hermite interpolation.

Additionally, we integrate the monotonicity into the parametrization by simple restrictions for the degrees of freedom:

\[
  p_j \leq p_{j+1} \quad \text{for} \quad j = 1, \ldots, r - 1.
\]

These constraints are used to a further stabilization of the minimization of the error functional. The condition (17) implies that \( f_p \) is monotone increasing on \( [u_{\text{min}}, u_{\text{max}}] \) in the case of piecewise linear interpolation. If the piecewise cubic Hermite interpolation is used, the derivatives of \( f_p \) at the nodes of the partition (15) must be prescribed for a unique definition of \( f_p \). The values of the derivatives \( f'_p(u_j) \) (\( j = 1, \ldots, r \)) can be computed in dependence on \( p_j \) (\( j = 1, \ldots, r \)), such that the function \( f_p \) is monotone increasing, if the condition (17) is satisfied. Details on piecewise monotone cubic interpolation can be found in [14].

The main difference of the two interpolation methods consists of the available smoothness. The parametrization by means of piecewise cubic Hermite interpolation provides continuously differentiable coefficient functions, whereas piecewise linear interpolation ensures only continuity of the coefficient functions. However, the computational effort for cubic Hermite interpolation is slightly higher.

The identification problem is thus reduced to the determination of a parameter vector \( p \in \mathbb{R}^{v \cdot r}_+ \), where \( v \) is equal to the number of unknown coefficient functions (\( v = 1 \) for our first example and \( v = 2 \) for our second example). The resulting constrained minimization problem can be written as: Find a parameter vector \( p^* \in \mathbb{R}^{v \cdot r}_+ \) which minimizes

\[
  J(p) = \|w(p) - w^*\|^2
\]

under the restriction

\[
  p_{(k-1) \cdot r+j} \leq p_{(k-1) \cdot r+j+1} \quad \text{for} \quad k = 1, \ldots, v \quad \text{and} \quad j = 1, \ldots, r - 1 .
\]

In the case of piecewise linear interpolation, we can achieve concavity of the coefficient functions by considering the following additional constraints for the degrees of freedom:

\[
  \frac{1}{2}(p_{(k-1) \cdot r+j-1} + p_{(k-1) \cdot r+j+1}) \leq p_{(k-1) \cdot r+j} \quad \text{for} \quad k = 1, \ldots, v \quad \text{and} \quad j = 2, \ldots, r - 1 .
\]
3.2 Stability Analysis and Multi-level Procedure

In order to investigate the stability of the inverse problem we perform a linear error analysis similar to [8]. Let \( \mathbf{p}^* \) be the parameter vector which minimizes the error functional (18) corresponding to the observation \( \mathbf{w}^* \). The constraints (19) and (20) are disregarded in the following.

If we add a small value \( \delta \mathbf{w} \) to the observation \( \mathbf{w}^* \), the minimization of the error functional (18) for \( \mathbf{w}^* + \delta \mathbf{w} \) results in a perturbation of the parameter vector \( \mathbf{p}^* \):

\[
\mathbf{p}^* + \delta \mathbf{p}.
\]

\( \delta \mathbf{p} \) denotes the parameter deviation caused by the measurement deviation \( \delta \mathbf{w} \). A first order expansion of \( \mathbf{w}(\mathbf{p}^* + \delta \mathbf{p}) \) leads to

\[
J(\mathbf{p}^* + \delta \mathbf{p}) = \| \mathbf{w}(\mathbf{p}^* + \delta \mathbf{p}) - (\mathbf{w}^* + \delta \mathbf{w}) \|_2^2
\]

1. order

\[
= \left\| \mathbf{w}(\mathbf{p}^*) + \frac{\partial \mathbf{w}}{\partial \mathbf{p}}(\mathbf{p}^*)\delta \mathbf{p} - \mathbf{w}^* - \delta \mathbf{w} \right\|_2^2
\]

\[
\leq \left( \| \mathbf{w}(\mathbf{p}^*) - \mathbf{w}^* \|_2^2 + \left\| \frac{\partial \mathbf{w}}{\partial \mathbf{p}}(\mathbf{p}^*)\delta \mathbf{p} - \delta \mathbf{w} \right\|_2^2 \right). \quad \text{(21)}
\]

The equality sign in the last line of Eq. (21) is valid if \( \frac{\partial \mathbf{w}}{\partial \mathbf{p}}(\mathbf{p}^*) = \mathbf{w}^* \). We conclude that we have to minimize

\[
\left\| \frac{\partial \mathbf{w}}{\partial \mathbf{p}}(\mathbf{p}^*)\delta \mathbf{p} - \delta \mathbf{w} \right\|_2^2
\]

(22)

to reduce the value of the error functional as best as possible.

The minimization of (22) can be viewed as a generalized solution of the following system of \( n \) linear equations for \( v \cdot r \) unknowns:

\[
\frac{\partial \mathbf{w}}{\partial \mathbf{p}}(\mathbf{p}^*)\delta \mathbf{p} = \delta \mathbf{w}. \quad \text{(23)}
\]

The sensitivity matrix \( \frac{\partial \mathbf{w}}{\partial \mathbf{p}}(\mathbf{p}^*) \in \mathbb{R}^{n \times v \cdot r} \) containing the partial derivatives of the observations with respect to the degrees of freedom at the point \( \mathbf{p}^* \) relates the measurement deviations \( \delta \mathbf{w} \) to the corresponding parameter deviations \( \delta \mathbf{p} \). Due to (21) the generalized solution of (23) is given by the generalized inverse. If we assume \( v \cdot r \leq n \) and \( \frac{\partial \mathbf{w}}{\partial \mathbf{p}}(\mathbf{p}^*) \) to have full rank \( v \cdot r \) (otherwise \( v \cdot r \) must be replaced by the rank of the sensitivity matrix), it can be expressed as (e.g. see [25])

\[
\delta \mathbf{p} = \sum_{j=1}^{v \cdot r} \frac{1}{\sigma_j} [\delta \mathbf{w}, a_j] b_j, \quad \text{(24)}
\]

Here, \( \{\sigma_j; a_j, b_j\}_{j=1,\ldots,v \cdot r} \) denotes a singular value decomposition of the sensitivity matrix. The singular values \( \sigma_j \) \( (j = 1, \ldots, v \cdot r) \) determine the transfer of measurement errors to identification errors of the determined parameters. Accordingly, the ill-posedness of the
The inverse problem is characterized by the (spectral) condition number of the sensitivity matrix

$$\mu_{\text{cond}}(r) = \max_{i,j=1,\ldots,r} \frac{\sigma_i}{\sigma_j}$$

(25)

and the maximum error amplification

$$\mu_{\text{max}}(r) = \max_{j=1,\ldots,r} \frac{1}{\sigma_j}$$

(26)

in dependence on the level of the parametrization, i.e. the number $r$ of degrees of freedom for each unknown coefficient function. The stability decreases for increasing characteristic numbers $\mu_{\text{cond}}$ and $\mu_{\text{max}}$.

Finally, we integrate the determination of coefficient functions coupled with the stability analysis into a multi-level procedure: The determination of the unknown functions is started with the minimization of the error functional (18) for the least possible number of degrees of freedom ($r = 2$). Next, the optimization is successive continued for an increasing number of degrees of freedom. A finer parametrization with a larger number of degrees of freedom is obtained by refining the underlying partition (15) by adding one or more extra nodes. The already existing nodes are not modified. The initial values for the new parameter vector are set to be equal to the values of the optimized coefficient function of the previous level at the nodes of the refined partition.

The stopping criterion of the multi-level procedure is formed by means of the characteristic numbers $\mu_{\text{cond}}$ and $\mu_{\text{max}}$. The numerical determination of the coefficient functions is stopped, if a maximum fineness of the parametrization is reached or one of the characteristic numbers exceeds a given tolerance value $\mu_{\text{cond}}^{\text{tol}}$ and $\mu_{\text{max}}^{\text{tol}}$:

$$\begin{cases} r \geq r_{\text{max}} \\ \epsilon \cdot \mu_{\text{cond}}(r) \geq \mu_{\text{cond}}^{\text{tol}} \\ \epsilon \cdot \mu_{\text{max}}(r) \geq \mu_{\text{max}}^{\text{tol}} \end{cases}$$

(27)

The parameter $\epsilon > 0$ is included in the condition (27) to take different noise level of the measured data into account. We know appropriate tolerance values from experience. In practice, the increasing of the characteristic numbers $\mu_{\text{cond}}(r)$ and $\mu_{\text{max}}(r)$ is observed. In the beginning of the multi-level procedure, the number of degrees of freedom must be increased as long as the necessary flexibility of the parametrization is achieved. Then the determination is stopped if the characteristic numbers show a strong increase taking the noise level into account.

The minimization with a large number of degrees of freedom depends critically on the initial value due to local minima. The risk that the minimization is stopped in a local minimum increases with the number of degrees of freedom. The multi-level procedure eliminates the problem to find appropriate initial values. An initial value must be only prescribed for the first parametrization level explicitly, where we start with a linear function. The final result of the multi-level procedure is nearly independent of this initial value. As we apply an iterative optimization technique, it is important that the optimum is well-approximated by using a sufficient number of iterations in each level of the multi-level procedure.
4 RESULTS

We illustrate the numerical determination of the nonlinear coefficient functions for the two examples introduced in Section 2 by means of synthesized data. For this we have simulated the respective column experiment for given coefficient functions. The simulated observations were disturbed by a 5% Gaussian noise.

The minimization problem is solved by the sequential quadratic programming method, as implemented by Schittkowski (see [28]). This method involves the computation of the gradient of the error functional with respect to the degrees of freedom. Efficient methods for the computation of the gradient and the sensitivity matrix can be found in [4, 20].

To refine the parametrization we insert a new node $\bar{u}_r$ into the partition of the identifiability domain $[u_{\min}, u_{\max}]$ successively by a dyadic strategy with $r_{\max} = 33$. That means the new node $\bar{u}_r$ is given as displayed in Table I. One could also think of coarsening strategies removing “unnecessary” nodes. To put this and also the question of where to put new nodes on firm grounds, local a posteriori error indicators would be necessary. Meanwhile, as is common for (well-posed) boundary value problems, we are not aware of such results for nonlinear ill-posed problems as treated here. Heuristic approaches in these directions will be presented elsewhere.

Note that the number of observation data, i.e. the dimension of the vector $w$, influences the identification. The identification results become more reliable if the number of observation data increases. The appropriate number of observation data depends on the data noise level and the extent of the identifiability domain. In general, the number of degrees of freedom should not exceed the number of observation data. This must be taken into account by defining the maximum number of degrees of freedom $r_{\max}$. We use in the following examples 50 different points in time for the measurements. In practice, this number can be increased.

4.1 Sorption Characteristics

The solution of the direct problem of the convection–diffusion equation is numerically computed by a conforming finite element method with backward Euler steps in time (see [20, 21, 23]). The approximation by conform finite elements is reasonable, because the column Peclet number ranges typically from $1/100$ to $100$.

To generate the data we have used the function $\varphi(c) = 20c/(1 + 2c)$ as sorption characteristic. This is a sorption characteristic of the Langmuir type, which is one of the parametrizations frequently used in the geoscience. The inflow concentration was chosen to be constant ($c_0(t) = 1$). Thus the identifiability domain is given by $[0, 1]$.

<table>
<thead>
<tr>
<th>$r$</th>
<th>$u_{\max}$</th>
<th>$10$</th>
<th>$(1/16)u_{\max}$</th>
<th>$18$</th>
<th>$(1/32)u_{\max}$</th>
<th>$26$</th>
<th>$(17/32)u_{\max}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$2$</td>
<td>$u_{\max}$</td>
<td></td>
<td>$(1/16)u_{\max}$</td>
<td></td>
<td>$(1/32)u_{\max}$</td>
<td></td>
<td>$(17/32)u_{\max}$</td>
</tr>
<tr>
<td>$3$</td>
<td>$(1/2)u_{\max}$</td>
<td>$11$</td>
<td>$(3/16)u_{\max}$</td>
<td>$19$</td>
<td>$(3/32)u_{\max}$</td>
<td>$27$</td>
<td>$(19/32)u_{\max}$</td>
</tr>
<tr>
<td>$4$</td>
<td>$(1/4)u_{\max}$</td>
<td>$12$</td>
<td>$(5/16)u_{\max}$</td>
<td>$20$</td>
<td>$(5/32)u_{\max}$</td>
<td>$28$</td>
<td>$(21/32)u_{\max}$</td>
</tr>
<tr>
<td>$5$</td>
<td>$(3/4)u_{\max}$</td>
<td>$13$</td>
<td>$(7/16)u_{\max}$</td>
<td>$21$</td>
<td>$(7/32)u_{\max}$</td>
<td>$29$</td>
<td>$(23/32)u_{\max}$</td>
</tr>
<tr>
<td>$6$</td>
<td>$(1/8)u_{\max}$</td>
<td>$14$</td>
<td>$(9/16)u_{\max}$</td>
<td>$22$</td>
<td>$(9/32)u_{\max}$</td>
<td>$30$</td>
<td>$(25/32)u_{\max}$</td>
</tr>
<tr>
<td>$7$</td>
<td>$(3/8)u_{\max}$</td>
<td>$15$</td>
<td>$(11/16)u_{\max}$</td>
<td>$23$</td>
<td>$(11/32)u_{\max}$</td>
<td>$31$</td>
<td>$(27/32)u_{\max}$</td>
</tr>
<tr>
<td>$8$</td>
<td>$(5/8)u_{\max}$</td>
<td>$16$</td>
<td>$(13/16)u_{\max}$</td>
<td>$24$</td>
<td>$(13/32)u_{\max}$</td>
<td>$32$</td>
<td>$(29/32)u_{\max}$</td>
</tr>
<tr>
<td>$9$</td>
<td>$(7/8)u_{\max}$</td>
<td>$17$</td>
<td>$(15/16)u_{\max}$</td>
<td>$25$</td>
<td>$(15/32)u_{\max}$</td>
<td>$33$</td>
<td>$(31/32)u_{\max}$</td>
</tr>
</tbody>
</table>

TABLE I Refinement strategy.

MATERIAL PROPERTIES IN SOIL SCIENCE 369
The other physical properties was set as follows: $\theta = 1.0$, $\rho = 1.0$, $D = 0.402$ and $q = 1.0$. Complete breakthrough can be achieved under this condition for $T = 20$.

The piecewise linear approach is appropriate to determine the sorption characteristics by our free-form parametrization. As $\varphi(0) = 0$ must be valid, we fix the degree of freedom corresponding to $u_{\min} = 0$: $p_1 = 0$.

The Figs. 1–5 show the results for 3, 8, 13, 17 and 33 degrees of freedom. Strictly speaking, we must subtract one degree of freedom each, because of the fixing of $p_1$.
The determined (solid line) and original (dotted line) sorption characteristics are displayed on the left hand side and the corresponding reconstructed (solid line) and measured (points) breakthrough on the right hand side.

The results show the typical behavior of the solution of an inverse problem. First, the identification error (measured in the maximum norm) decreases as a result of the increasing flexibility of the parametrization. Afterwards the identification error increases again influenced by the measurement errors (see Fig. 6). The determined sorption characteristic is perturbed by small oscillations more and more for an increasing number of degrees of freedom as it can be seen in Fig. 5.

The singular values of the sensitivity matrix indicates the decreasing stability by increasing values $\mu_{\text{cond}}(r)$ and $\mu_{\text{max}}(r)$. Especially, the values of the condition number $\mu_{\text{cond}}(r)$ and the maximum error amplification $\mu_{\text{max}}(r)$ heavily increase for a number of degrees of freedom greater than 13 (see Fig. 7).

So far we have only used the monotonicity constraints to stabilize the numerical minimization. If we include the concavity constraints (20) into the minimization as additional a priori information for the sorption characteristic, we can improve the obtained identification results. Figure 8 shows the result for $r = 33$, where the same data were used as previously. The defect of the sorption characteristic is clearly smaller (see Fig. 6). But in general, the concavity cannot a priori be assumed for real data (e.g. see [21]).
FIGURE 6 Identification error of sorption characteristic.

FIGURE 7 Condition number (left) and maximum error amplification (right).

FIGURE 8 Sorption characteristic and breakthrough for $r = 33$ with consideration of the concavity.
4.2 Unsaturated Hydraulic Properties

The Richards equation is numerically solved in the pressure form by a hybrid mixed finite element method in space and backward Euler steps in time (see [29, 30]). The volumetric flow rate

\[ q(x, t) = -K(\psi(x, t))(\partial_x \psi(x, t) - 1) \]  

(28)

for \( x \in [0, L] \), \( t \in [0, T] \) is introduced as additional unknown, which must be approximated explicitly. The cumulative outflow (12) is computed from \( q \) by applying the trapezoidal rule.

Numerical test runs show that the weak smoothness of the piecewise linear parametrization critically affects the smoothness of the volumetric flow rate \( q \). Therefore we prefer a parametrization, which is at least continuously differentiable, e.g. piecewise cubic Hermite interpolation. (Quadratic B-splines provides another possibility for a free-form parametrization of the hydraulic properties, see [2–4].) Moreover, we have detected that the hydraulic properties cannot be uniquely identified in free-form parametrization if only cumulative outflow measurements are used (see [3]).

In addition to the monotonicity constraints, we prescribe the saturation values of the hydraulic properties for the optimization. In any case, the saturated water content \( \theta_{\text{sat}} \) can anyway not be identified by our column experiments. The fixing of the saturated conductivity \( (\psi = \theta_{\text{sat}}) \) stabilizes the determination, especially it reduces the identification error of the conductivity. The values \( \theta_{\text{sat}} \) and \( K_{\text{sat}} \) are usually known from independent experiments. Consequently, the number of degrees of freedom is reduced to \( r - 1 \) if \( r \) is the number of nodes used for the parametrization.

Figures 9–11 present the results for the parametrization levels with \( r = 3, 5, 9 \) and 33. The pictures on the left hand side show the hydraulic properties \( \Theta \) and \( K \) and the pictures on the right hand side the corresponding observations (pressure at the upper boundary and cumulative outflow at the lower boundary) in the same representation as in the previous subsection. As the observation \( w_0 \) and \( w_L \) are of different orders of magnitude, we apply a scaling of the observations by weighting \( w_0 \) and \( w_L \) with the inverse of the respective mean value (see [15, 24]).

The used data was generated by using the van Genuchten–Mualem model (cf. [34]) for the unsaturated hydraulic properties \( \psi < 0 \):

\[
\Theta(\psi) = \theta_{\text{res}} + (\theta_{\text{sat}} - \theta_{\text{res}}) \left( \frac{1}{1 + (-\alpha \psi)^n} \right)^{(n-1)/n}
\]

\[
K(\psi) = K_{\text{sat}} \frac{(1 - (-\alpha \psi)^n)(1 + (-\alpha \psi)^n)^{1-n/n})^2}{(1 + (-\alpha \psi)^n)^{(n-1)/2n}}.
\]

\( \theta_{\text{res}} \) is the residual water content and \( \alpha \) and \( n \) are empirical parameters. Here we have used one of the parameter sets presented in [34]: \( \theta_{\text{sat}} = 0.52 \), \( \theta_{\text{res}} = 0.218 \), \( K_{\text{sat}} = 1.3167 \), \( \alpha = 0.0115 \) and \( n = 2.03 \). The pressure at the outflow boundary was linearly decreased from \( \psi_L(0) = 15 \) to \( \psi_L(T) = -200 \) with \( T = 40 \). Thus the maximum identifiability domain is \([-215, 0]\). As the pressure does not yet exceed the value \(-200\) for \( t \leq 40 \), we have plot the hydraulic properites only for the interval \([-200, 0]\), but for the parametrization, we have used \([-215, 0]\). The identification errors are shown in Fig. 12. The condition number of the sensitivity matrix and the maximum error amplification are presented in Fig. 14.
FIGURE 9  Hydraulic properties (left) and corresponding observations (right) for $r = 3$.

FIGURE 10  Hydraulic properties (left) and corresponding observations (right) for $r = 5$. 
FIGURE 11  Hydraulic properties (left) and corresponding observations (right) for $r = 9$.

FIGURE 12  Hydraulic properties (left) and corresponding observations (right) for $r = 33$. 
The determination of the hydraulic properties shows a similar behavior as the determination of the sorption characteristics, especially concerning the retention curve. The identification error of the hydraulic conductivity is essentially larger than the identification error of the retention curve. This is caused by a small sensitivity of the hydraulic conductivity, and so the reproduction of small measurement errors does not evidently influence the hydraulic conductivity (see Figs. 12 and 13).

The two considered examples show that the parametrization with about 8–16 degrees of freedom ensures a sufficient flexibility of the parametrized functions. For this range of the parametrization level we obtain the minimum of the maximum identification error. A further increase of the degrees of freedom does not improve the identification results. On the contrary, the identification errors partly increase again. This result was also obtained for further numerical case studies.

5 SUMMARY AND CONCLUSIONS

We have presented a numerical approach for the determination of nonlinear coefficient functions of partial differential equations. The numerical procedure was illustrated on the basis of two examples concerning flow and transport problems in porous media.
The basic idea of our method is using a free-form parametrization of the unknown nonlinearities by polynomial functions. The determination of the unknown functions is done by minimizing a least squares functional. The minimization is stabilized by including a priori information on the unknown functions, which are well-founded physically (e.g. monotonocity). The hierarchical concept of the parametrization allows an embedding of the determination into a multi-level procedure. Considering the singular values of the sensitivity matrix provides a possibility to find an appropriate fineness of the parametrization.

Our method was able to determine sorption characteristics of chemicals and the hydraulic properties of porous media. A sorption characteristic can be determined by using the simplest free-form parametrization by piecewise linear functions. The determination of the hydraulic properties is more difficult, because two functions must be simultaneously determined there. Moreover, the hydraulic conductivity shows a weak sensitivity with respect to the degrees of freedom close to the saturated zone.

However, the free-form parametrization offers a possibility to determine material properties without precise a priori assumptions on the shape of the unknown functions which are included in fixed-form models.

References
