Weierstraß–Institut
für Angewandte Analysis und Stochastik

im Forschungsverbund Berlin e.V.

Preprint ISSN 0946 – 8633

Numerical Parameter Identification in Multiphase Flow through Porous Media

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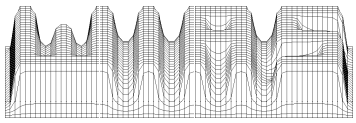
submitted: February 28th 2001

Preprint No. 644

Berlin 2001



1991 Mathematics Subject Classification. 65K05, 76T10, 65L10, 93E24.

Key words and phrases. Numerical parameter identification, multiphase flow, reduced Gauss-Newton technique, multiple shooting.

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Abstract. Multiphase flow is of high interest for the investigation of the behavior of waste in groundwater. The high nonlinearity of the model equations pose special problems. Here, a new parameter identification technique in this context is proposed which takes advantage of recently developed highly efficient numerical simulation techniques. It is based on a reduced Gauss-Newton technique in combination with an efficient gradient computation. Numerical experiments are performed for the McWhorter model problem.

1 Introduction

The study of subsurface flow and chemical transport is an important factor in view of management practice and contaminant remediation of ground water resources. Such flow and transport processes are modeled by a set of partial differential equations which involve some parameters. These parameters are used to model constitutive relationships of physical properties of the fluid, the media and their interaction.

In practical situations these parameters cannot be measured directly. Rather, they are to be determined from a set of observation data. Two types of methods have been reported, namely direct and indirect (cf., e.g., [9]). In direct methods, the parameters are determined by inverting the governing equations with simplified initial and boundary conditions using analytical or semi-analytical methods. This method has various limitations and cannot be applied to field-scale models. Indirect methods, on the other hand, are quite flexible and can be applied to practical problems. Our parameter identification technique is one of the indirect methods. In this technique, the direct problem is posed for prescribed but arbitrary initial and boundary conditions which can be solved by any appropriate analytical or numerical technique. The constitutive relationships thought to be applied are parametrized based on a-priori knowledge, and coefficients are determined by means of an optimization algorithm that extremizes some objective function. The drawback of this method is that it cannot determine the specific form of the constitutive relationships and one has to presume some formulation of these relationships which holds to a sufficient degree of approximation. Many inverse problems are ill-posed which is characterized by non-uniqueness and instability [13], and this causes uncertainty of the determined parameters. This method has also the advantage that it is possible to obtain information concerning the parameter uncertainty from the estimation analysis.

The specific problem under investigation in this paper is the determination of the parameters in the Brooks-Corey[4] capillary pressure saturation relationship and of the permeability of the soil. However, the basic methodology can be applied to more general parameter identifications in instationary multiphase models. The current inverse modeling methodology is dominated by approaches, which can be characterized by treating the multiphase simulation solver routine in the form of a black box, which just matches the unknown parameters (to be estimated) via a nonlinear process to an output least squares functional. This is the case, e.g., for ITOUGH/ITOUGH2 [6] and also in [5]. From the point of view of boundary value problems for instationary processes, this can be seen as a single shooting approach to the parameter identification problem, which, on the other hand, shares more properties with boundary value problems than pure initial value problems. As it is known that single shooting reveals instabilities for boundary value problems in ODE, a similar behaviour has been observed with these black box

approaches. Here we use a multiple shooting approach similar to [11], but generalize this approach in so far as we allow also for local adaptivity in space. That leads to a different formulation of continuity conditions. The multiple shooting by itself leads to a more robust solution behaviour than a single shooting approach. The overall multiphase system solution technology is taken from the code MUFTE-UG[7], which is enhanced by a multiple-shooting framework and computation of necessary derivatives.

The paper is organized in the following way. First we recall the governing equations considered, discretized in time and space. Afterwards we formulate the parameter identification problem in section 3 together with a numerical solution approach. Finally, section 4 presents a numerical experiment for the McWorter problem.

2 The Forward Simulation Problem

2.1 Governing Equations:

The equations for the flow of two immiscible fluid phases w (wetting) and n (non wetting) in a porous medium are given by the conservation of mass ($\alpha = w, n$)

$$\frac{\partial (\phi \rho_\alpha S_\alpha)}{\partial t} + \nabla . (\rho_\alpha v_\alpha) = \rho_\alpha q_\alpha \tag{1}$$

and the generalized Darcy Law

$$v_\alpha = -\frac{K_{r\alpha}(x, S_\alpha)}{\mu_\alpha} k \left(\nabla p_\alpha - \rho_\alpha \vec{g} \right), \tag{2}$$

with initial and boundary conditions

$$S_\alpha(x,0) = S_{\alpha 0}(x), \quad p_\alpha(x,0) = p_{\alpha 0}(x) \qquad x \in \Omega \tag{3}$$

$$S_\alpha(x,t) = S_{\alpha d}(x,t) \quad \text{on} \quad \Gamma^s_{\alpha d}, \quad p_\alpha(x,t) = p_{\alpha d}(x,t) \quad \text{on} \quad \Gamma^p_{\alpha d} \tag{4}$$

$$\rho_\alpha v_\alpha \cdot n = F_\alpha(x,t) \quad \text{on} \quad \Gamma_{\alpha n} \tag{5}$$

where ϕ is the porosity of the porous medium, ρ is the density of phase α, S_α the unknown saturation of phase α, v_α the volumetric flux vector, q_α the source/sink term, k the isotropic absolute permeability tensor, μ_α the dynamic viscosity of the fluid α, p_α the unknown pressure of phase α and $\vec{g}$ the vector of gravitational forces, $K_{r\alpha}(x, S_\alpha)$ the relative permeabilities and $S_{\alpha d}, p_{\alpha d}, F_\alpha$ appropriate boundary data.

In addition to these differential equations, we have the algebraic relations

$$S_w(x,t) + S_n(x,t) = 1, \tag{6}$$

$$p_n(x,t) - p_w(x,t) = p_c(x, S_w(x,t)). \tag{7}$$

The Brooks-Corey relationships of relative permeabilities and capillary pressure to saturation of the wetting phase are given by

$$\begin{aligned} K_{rw} &= S_e^{\frac{2+3\lambda}{\lambda}} \\ K_{rn} &= (1 - S_e)^2 \left(1 - S_e^{\frac{2+\lambda}{\lambda}} \right) \\ p_c(S_w) &= p_d S_e^{-1/\lambda}. \end{aligned}$$

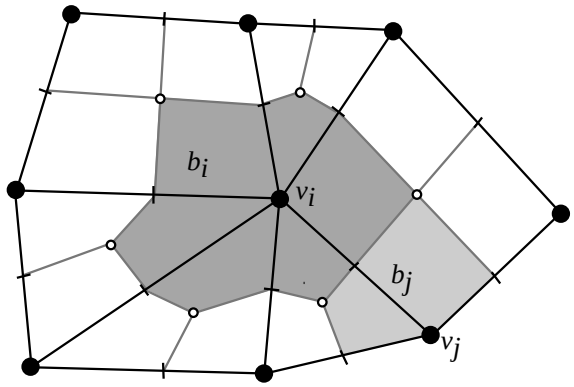

Figure 1: Control Volume

where $S_e = \frac{S_w - S_{wr}}{1 - S_{wr}}$ is the effective saturation, S_{wr} is the residual water saturation and p_d the entry pressure. The parameters to be estimated in the specific problem of this paper are λ and the absolute permeability parameter k.

Using the algebraic relations in equations (1) and (2), the simplified equations for S_n (differential variable) and p_w (algebraic variable) are given by (*phase pressure-saturation formulation*)

$$\frac{\partial\left(\phi\rho_w(1-S_n)\right)}{\partial t} + \nabla\cdot\left\{-\frac{K_{rw}(1-S_n)}{\mu_w}\rho_w k\left(\nabla p_w - \rho_w\vec{g}\right)\right\} - \rho_w q_w = 0 \tag{8}$$

$$\frac{\partial\left(\phi\rho_n S_n\right)}{\partial t} + \nabla\cdot\left\{-\frac{K_{rn}(S_n)}{\mu_n}\rho_n k\left(\nabla(p_w + p_c) - \rho_n\vec{g}\right)\right\} - \rho_n q_n = 0 \tag{9}$$

with initial and boundary conditions

$$S_n(x,0) = S_{n0}(x) \quad x\in\Omega \tag{10}$$

$$p_w(x,t) = p_{wd}(x,t) \quad \text{on} \quad \Gamma^p_{wd}, \quad \rho_w v_w\cdot n = F_w(x,t) \quad \text{on} \quad \Gamma_{wn} \tag{11}$$

$$S_n(x,t) = S_{nd}(x,t) \quad \text{on} \quad \Gamma^s_{nd}, \quad \rho_n v_n\cdot n = F_n(x,t) \quad \text{on} \quad \Gamma_{nn} \tag{12}$$

Semidiscretization of system (8,9) results in an implicit system of differential-algebraic equations (DAE) of index 1. This DAE is not fully implicit in so far as we can clearly see that S_n is the differential variable and p_w the algebraic. This helps in formulating consistent initial values (for S_n only) and in formulating consistent continuity conditions in the multiple shooting approach below.

2.2 Discretization

The set of equations (8,9) together with the initial and boundary conditions (10-12) is solved using a cell centered finite volume method with fully implicit time discretization on unstructured meshes [2]. The polyhedral domain Ω is divided in meshes $E_h = \{e_1, e_2, \cdots, e_k\}$ consisting of elements e_i with mesh width h. The set of vertices

are denoted by $V = \{\nu_1, \nu_2, \cdots, \nu_n\}$, the location of vertex ν_i is X_i and the barycenter of element e_k is X^k. Furthermore, $V(k)$ denotes the set of all indices i where ν_i is a corner of the element e_k and conversely $E(i)$ is the set of all indices k such that $i \in V(k)$. The secondary or dual mesh is constructed from E_h by connecting the element barycenters to the edge midpoints (Fig.1). The secondary mesh $B_h = \{b_1, b_2, \cdots, b_n\}$ consists of polyhedral regions b_i called *boxes* or *control volumes*. Each control volume is naturally associated with vertex ν_i in the primary mesh. Interior vertices are approximately in the center of their associated control volume while boundary vertices are at the boundary of their control volume.

The semi-discretization of equations (8) and (9) implies that the corresponding weak form of the equations are valid in each of the control volumes which are given by

$$\frac{d}{dt}\int_{b_i} \phi_h \rho_{wh}(1 - S_{nh})dV + \int_{\partial b_i \cap \Omega} \rho_{wh} v_w \cdot n ds + \int_{\partial b_i \cap \Gamma_{wn}} F_w ds - \int_{b_i} \rho_{wh} q_w dV = 0 \quad (13)$$

$$\frac{d}{dt}\int_{b_i} \phi_h \rho_{nh} S_{nh} dV + \int_{\partial b_i \cap \Omega} \rho_{nh} v_n \cdot n ds + \int_{\partial b_i \cap \Gamma_{nn}} F_n ds - \int_{b_i} \rho_{nh} q_n dV = 0. \quad (14)$$

Using the basis function representation, this semidiscrete formulation leads to a system of DAE in the incompressible case. That is, for 0<t<T find $\mathbf{p_w(t)}, \mathbf{S_n(t)}$, such that for $\alpha = w, n$:

$$\frac{d}{dt}\mathbf{M}_\alpha(\mathbf{p_w(t)}, \mathbf{S_n(t)}) + \mathbf{A}_\alpha(\mathbf{p_w(t)}, \mathbf{S_n(t)}) + \mathbf{Q}_\alpha(\mathbf{t}, \mathbf{p_w(t)}, \mathbf{S_n(t)}) = \mathbf{0}. \quad (15)$$

The vector $\mathbf{M}_\alpha$ represents the accumulation term, $\mathbf{A}_\alpha$ the flux term and $\mathbf{Q}_\alpha$ the source/sink and boundary flux terms. This system can be formally rewritten as

$$\begin{pmatrix} M_{ww} & M_{wn} \\ M_{nw} & M_{nn} \end{pmatrix} \begin{pmatrix} \frac{\partial \mathbf{p_w(t)}}{\partial t} \\ \frac{\partial \mathbf{S_n(t)}}{\partial t} \end{pmatrix} + \begin{pmatrix} \mathbf{A_w}(\mathbf{p_w}, \mathbf{S_n}) + \mathbf{Q_w}(\mathbf{t}, \mathbf{p_w}, \mathbf{S_n}) \\ \mathbf{A_n}(\mathbf{p_w}, \mathbf{S_n}) + \mathbf{Q_n}(\mathbf{t}, \mathbf{p_w}, \mathbf{S_n}) \end{pmatrix} = 0, \quad (16)$$

with the (solution-dependent) submatrices given by

$$(M_{\alpha w})_{ij} = \frac{\partial \mathbf{M_{\alpha w,i}}}{\partial \mathbf{p_{w,j}}}, \qquad (M_{\alpha n})_{ij} = \frac{\partial \mathbf{M_{\alpha n,i}}}{\partial \mathbf{S_{n,j}}}.$$

In the incompressible case this results into a system of DAE which is characterized by the matrix in the left hand side being singular.

2.3 Implicit Time Discretization

For the time discretization, we use an implicit scheme. For notational ease, the evaluation of any quantity at time level t^n is denoted by a superscript n e.g., $p_{wh}(t^n) = p^n_{wh}$, $S_n(t^n) = S^n_n$ etc. The notation for a time step is

$$\Delta t^n = t^{n+1} - t^n.$$

The one step θ-scheme [8] applied to the semi-discrete system (16) yields p^n_w, S^n_n such that for $\alpha = w, n$

$$\mathbf{M^{n+1}_\alpha} - \mathbf{M^n_\alpha} + \Delta t^n \theta \left(\mathbf{A^{n+1}_\alpha} + \mathbf{Q^{n+1}_\alpha}\right) + \Delta t^n (1-\theta)(\mathbf{A^n_\alpha} + \mathbf{Q^n_\alpha}) = 0 \quad (17)$$

with $\mathbf{M}_\alpha^{\mathbf{n}} = \mathbf{M}_\alpha\left(\mathbf{p}_{\mathbf{w}}^{\mathbf{n}}, \mathbf{S}_{\mathbf{n}}^{\mathbf{n}}\right)$, etc. For $\theta = 1$, we obtain the first order accurate backward Euler scheme and for $\theta = 1/2$ the Crank-Nicolson scheme which is second order accurate in time. Here, we use the backward Euler scheme since Crank-Nicolson has only weak damping properties which may cause stability problems as the equations are of mixed parabolic and hyperbolic types. For details of the step selection process, see [2].

3 The Parameter Estimation Problem

3.1 Least-Squares Formulation

In order to perform a maximum likelihood estimation with respect to the output errors in measured data Z_{ij} of functions ϕ_{ij} of the variables $S_n and p_w$ we formulate a pointwise weighted least squares function to be minimized,

$$\min \frac{1}{2} \sum_{i,j} \left(\phi_{ij}(S_n, \beta) - Z_{ij}\right)^2 / \sigma_{ij}^2. \tag{18}$$

Here, Z_{ij} are measurements of the capillary pressure taken at the j-th measurement time $(\hat{t}_j)$ and the i-th measurement position in space $(\hat{x}_i)$ and

$$\phi_{ij}(S_n, \beta) = p_d \left(\frac{1 - S_n(\hat{x}_i, \hat{t}_j) - S_{wr}}{1 - S_{wr}} \right)^{1/\lambda},$$

where we remind that λ is one of the parameters to be estimated and p_d and S_{wr} are constants given a priori. The measurement errors are assumed to be independently normally distributed with expectation 0 and standard deviation $\sigma_{i,j}$. This objective functional is subjected to the conditions that the DAE (8,9) together with initial and boundary conditions (10-12) are solved over the time horizon $[0, T] \ni \{\hat{t}_j\}_j$.

The vector β collects the unknown parameters to be estimated. Of course, the set of unknown parameters considered in this paper can be enlarged by, e.g., porosity, permeability.

3.2 The multiple shooting parameter estimation approach

We subdivide the time interval under consideration, $(0, T)$ into subintervals with the grid points $0 = \tau_0 < \tau_1 < \tau_2 < \cdots < \tau_m = T$, where in general the nodes τ_j are independent from the measurement points in time. For ease of presentation, however, we let the measurement time-grid coincide with the multiple shooting time-grid, since the necessary generalizations are obvious. At these nodes the initial values of the differential variables S_j, are introduced as unknowns in addition to the parameter vector β. In a standard multiple shooting formulation, these additional degrees of freedom are constrained by explicitly formulating continuity equations. Thus we arrive at the (time-)discretized least-squares problem

$$\min_{\{S_j\}_j, \beta} \frac{1}{2} \sum_{i,j} \left(\phi_{ij}(S_j, \beta) - Z_{ij}\right)^2 / \sigma_{ij}^2 \tag{19}$$

subject to the continuity conditions

$$S_{j+1} - S_n(\tau_{j+1}; S_j, \beta) = 0, \quad j = 0, 1, \cdots, m-1, \tag{20}$$

where $S_n(\tau_{j+1}; S_j, \beta)$ denotes the solution at time τ_{j+1} of the multiphase DAE (8, 9) with its boundary conditions (11,12) together with the initial condition $S_n(\tau_j) = S_j$. Additionally, the initial condition

$$S_n(0) = S_0 \tag{21}$$

has to hold.

The standard formulation of the continuity equations (20) is typically used in the context of DAE for ordinary differential equations. If the instationary state equation is constructed from a partial differential equation, this formulation may be no longer appropriate, at least if adaptivity in space is necessary, which means, that, as long as the solution is not yet reached, the space grid on the "right hand side" of the continuity conditions need not coincide with the grid on the "left hand side". Therefore, we apply a strategy similar to mortar element discretizations and formulate instead of that weak continuity conditions in the computational domain Ω at the multiple shooting node τ_{j+1}:

$$\int_\Omega \left(S_{j+1} - S_n(\tau_{j+1}; S_j, \beta)\right) \psi = 0, \quad \forall \psi \in V_{j+1} \tag{22}$$

where V_{j+1} is the space of spatial ansatz functions at node τ_{j+1}. The local shooting solution $S_n(\tau_{j+1}; S_j, \beta)$ coming from "left" may, of course, use a different ansatz space $\bar{V}_{j+1}$. In the sequel, we use a basis representation of the form

$$\begin{aligned} S_{j+1} &= \sum_{\psi \in V_{j+1}} S_{j+1}^{\psi} \psi, \\ S_n(\tau_{j+1}; S_j, \beta) &= \sum_{\bar{\psi} \in \bar{V}_{j+1}} S_n^{\bar{\psi}}(\tau_{j+1}; S_j, \beta) \bar{\psi}, \end{aligned}$$

and the mass matrices

$$\begin{aligned} (M_{j+1})_{k,l} &:= \int_\Omega \psi_k \psi_l, \quad \psi_k, \psi_l \in V_{j+1}, \\ (\bar{M}_{j+1})_{k,l} &:= \int_\Omega \psi_k \bar{\psi}_l, \quad \psi_k \in V_{j+1}, \bar{\psi}_l \in \bar{V}_{j+1}. \end{aligned}$$

Note that in general M_{j+1} is quadratic and $\bar{M}_{j+1}$ only rectangular. With these definitions and using the same symbol S_{j+1} again, now denoting the vector consisting of the scalars $\{S_{j+1}^{\psi}\}_\psi$ (S_n analogously), we can rewrite the weak continuity conditions (22) in discretized form as

$$M_{j+1} S_{j+1} - \bar{M}_{j+1} S_n(\tau_{j+1}; S_j, \beta) = 0.$$

3.3 A reduced generalized Gauss-Newton approach

An efficient numerical solution technique for the discretized parameter identification problem described in the previous section is the application of generalized Gauss-Newton

methods as introduced in [3]. Increments to be added in each iteration are computed by solving the linearized constrained least squares problem

$$\min_{\{\Delta S_j\}_j, \Delta\beta} \frac{1}{2} \sum_{i=1}^{N} \sum_{j=0}^{m} \{\phi_{ij}(S_n(S_j,\beta)) - Z_{ij} + \left(\frac{\partial \phi_{ij}}{\partial S_j} \quad \frac{\partial \phi_{ij}}{\partial \beta}\right) \begin{pmatrix} \Delta S_j \\ \Delta\beta \end{pmatrix} \Big\}^2 / \sigma_{ij}^2 \tag{23}$$

subject to

$$\bar{M}_{j+1} G_j \Delta S_j - M_{j+1} \Delta S_{j+1} + \bar{M}_{j+1} G_j^{\beta} \Delta\beta = d_j, \tag{24}$$

for $(j = 0, 1, 2, \ldots, m)$, where

$$G_j = \frac{\partial S_n(\tau_{j+1}; S_j, \beta)}{\partial S_j} \quad \text{and} \quad G_j^{\beta} = \frac{\partial S_n(\tau_{j+1}; S_j, \beta)}{\partial \beta}.$$

and

$$d_j = M_{j+1} S_{j+1} - \bar{M}_{j+1} S_n(\tau_{j+1}; S_j, \beta).$$

The Wronskians G_j and G_j^{β} cannot be computed practically or even stored in the case of PDE. In order to avoid that, we apply a reduction technique, first proposed in [10]. For the application to our case, we first have to define

$$\bar{G}_j := M_{j+1}^{-1} \bar{M}_{j+1} G_j, \quad \bar{G}_j^{\beta} := M_{j+1}^{-1} \bar{M}_{j+1} G_j^{\beta}, \quad \bar{d}_j := M_{j+1}^{-1} d_j.$$

Then we can solve the recursion (24) for ΔS_{j+1} as

$$\Delta S_{j+1} = -\sum_{l=1}^{j} \left(\prod_{i=l+1}^{j} \bar{G}_i \right) d_l + \left\{ \sum_{l=1}^{j} \left(\prod_{i=l+1}^{j} \bar{G}_i \right) \bar{G}_l^{\beta} \right\} \Delta\beta + \prod_{i=0}^{j} \bar{G}_i \Delta S_0 \tag{25}$$

Since we assume to have full information on the initial data $S_n(0)$, we know $\Delta S_0 = 0$ and it can be neglected in what follows. Now the linear quadratic problem can be reformulated as an unconstrained quadratic problem,

$$\min_{\Delta\beta} \left[\sum_{i=1}^{N} \sum_{j=0}^{m} \left\{ \phi_{ij}(S_n(S_j,\beta)) - Z_{ij} - \frac{\partial \phi_{ij}}{\partial S_j} g_j^s + \left(\frac{\partial \phi_{ij}}{\partial S_j} g_j^{\beta} + \frac{\partial \phi_{ij}}{\partial \beta} \right) \Delta\beta \right\}^2 \right], \tag{26}$$

where

$$g_j^s = \sum_{l=1}^{j} \left(\prod_{k=l+1}^{j} \bar{G}_k \right) \bar{d}_l \tag{27}$$

$$g_j^{\beta} = \sum_{l=1}^{j} \left(\prod_{k=l+1}^{j} \bar{G}_k \right) \bar{G}_{\beta}^{l} \tag{28}$$

The vectors g_j^s, g_j^{β} can be computed in parallel to the solution of the forward multiple shooting sweep in each nonlinear iteration. This QP is solved for the parameter vector increment $\Delta\beta$. Afterwards, the increments in S_n can be obtained from the recursion

$$\Delta S_{j+1} = \bar{G}_j \Delta S_j + \bar{G}_j^{\beta} \Delta\beta - \bar{d}_j,$$

These increments are then scaled by a line-search parameter and added to the current iterate.

3.4 Computation of Derivatives

For the solution of the linear quadratic subproblems of the previous section, we need the matrix-vector products with the Wronskians G_j, G_j^β. These can be carried out "on the fly" (*Internal Numerical Differentiation* [3, 11]) by solving linear systems of equations with the same linear solver, which is used for the integration of the DAE. The differentiation of the DAE (8,9) with respect to S_n leads to the same matrix, which is used in the formulation of linear systems resulting from the application of a Newton method to the implicit equation defined by, e.g., an implicit Euler method. Therefore, the necessary computations to be done in each integration step for the computation of G_j, G_j^β are $\dim(\beta)$ additional solutions of linear systems after each completed nonlinear Newton solve with the same matrix as used in the last Newton step and with the same linear solver (here a multigrid solver).

In order to clarify this, we consider equation (16) for the incompressible case, which we write in a more abstract and therefore a more simple form

$$M_{wn}\frac{d\mathbf{S}_n}{dt} = f(\mathbf{S}_n, \mathbf{p}_w, \beta)$$
$$M_{nn}\frac{d\mathbf{S}_n}{dt} = g(\mathbf{S}_n, \mathbf{p}_w, \beta),$$

within the shooting interval $[\tau_j, \tau_{j+1}]$, where we have the initial condition $S_n(\tau_j) = S_j$. An implicit Euler step computing S_j^{i+1} as an approximation of $S_n(t_{i+1})$ from $S_j^i = S_n(t_i)$ with $t_i, t_{i+1} \in (\tau_j, \tau_{j+1})$ is of the form

$$M_{wn}\frac{S_j^{i+1} - S_j^i}{h} = f(S_j^{i+1}, p_j^{i+1}, \beta) \tag{29}$$
$$M_{nn}\frac{S_j^{i+1} - S_j^i}{h} = g(S_j^{i+1}, p_j^{i+1}, \beta), \tag{30}$$

with appropriate time-stepsize h. The principle of internal numerical differentiation is based on a computation of the exact derivative of the approximating discretization scheme (in contrast to computing an approximation of an exact derivative of the nondiscretized solution). Therefore we obtain by differentiating (29, 30) w.r.t. S_j the recursion

$$[M_{wn} - hf_{S_n}]\frac{\partial S_j^{i+1}}{\partial S_j} - hf_{S_n}\frac{\partial p_j^{i+1}}{\partial S_j} = M_{wn}\frac{\partial S_j^i}{\partial S_j}$$
$$[M_{nn} - hg_{S_n}]\frac{\partial S_j^{i+1}}{\partial S_j} - hg_{S_n}\frac{\partial p_j^{i+1}}{\partial S_j} = M_{nn}\frac{\partial S_j^i}{\partial S_j}$$

for

$$G_j^i := \frac{\partial S_n(t_i; S_j, \beta)}{\partial S_j} \quad \text{and} \quad \Pi_j^i := \frac{\partial p_w(t_i; S_j, \beta)}{\partial S_j}$$

where

$$G_j = G_j^n \quad \text{and} \quad \begin{bmatrix} G_j^0 \\ \Pi_j^0 \end{bmatrix} = \begin{bmatrix} I \\ 0 \end{bmatrix},$$

if n implicit Euler steps are performed in interval $[\tau_j, \tau_{j+1}]$. Thus we obtain the following lemma.

Lemma 3.1 *The matrix-vector product $G_j d$ is the result of n recursion steps for $\gamma^i := G_j^i d$ and $\pi^i := \Pi_j^i d$.*

$$\begin{bmatrix} (M_{wn} - hf_{S_n}) & -hf_{S_n} \\ (M_{nn} - hg_{S_n}) & -hg_{S_n} \end{bmatrix} \begin{pmatrix} \gamma^{i+1} \\ \pi^{i+1} \end{pmatrix} = \begin{bmatrix} M_{wn} & 0 \\ M_{nn} & 0 \end{bmatrix} \begin{pmatrix} \gamma^i \\ \pi^i \end{pmatrix}, \quad \gamma^0 := d.$$

Hence, $G_j d = \gamma^n$. □

All matrices mentioned are already assembled in the last Newton step of each implicit Euler step for the nominal trajectory S_n, p_w; and also the same linear solver as they can be used for the matrix on the left hand side. In fact, the whole recursion can be considered an implicit Euler discretization of the corresponding variational DAE.

Similarly we obtain by differentiating (29, 30) w.r.t. β the recursion

$$[M_{wn} - hf_{S_n}] \frac{\partial S_j^{i+1}}{\partial \beta} - hf_{S_n} \frac{\partial p_j^{i+1}}{\partial \beta} = M_{wn} \frac{\partial S_j^i}{\partial \beta} + hf_\beta$$
$$[M_{nn} - hg_{S_n}] \frac{\partial S_j^{i+1}}{\partial \beta} - hg_{S_n} \frac{\partial p_j^{i+1}}{\partial \beta} = M_{nn} \frac{\partial S_j^i}{\partial \beta} + hg_\beta$$

for

$$G_j^{\beta,i} := \frac{\partial S_n(t_i; S_j, \beta)}{\partial \beta} \quad \text{and} \quad \Pi_j^{\beta,i} := \frac{\partial p_w(t_i; S_j, \beta)}{\partial \beta}$$

where

$$G_j^\beta = G_j^{\beta,n} \quad \text{and} \quad \begin{bmatrix} G_j^{\beta,0} \\ \Pi_j^{\beta,0} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}.$$

Analogously, the following lemma holds.

Lemma 3.2 *$G_j^\beta \Delta\beta$ is the result of the recursion for $\gamma_\beta^i := G_j^{\beta,i} \Delta\beta$ and $\pi_\beta^i := \Pi_j^{\beta,i} d$,*

$$\begin{bmatrix} (M_{wn} - hf_{S_n}) & -hf_{S_n} \\ (M_{nn} - hg_{S_n}) & -hg_{S_n} \end{bmatrix} \begin{pmatrix} \gamma_\beta^{i+1} \\ \pi_\beta^{i+1} \end{pmatrix} = \begin{bmatrix} M_{wn} & 0 \\ M_{nn} & 0 \end{bmatrix} \begin{pmatrix} \gamma_\beta^i \\ \pi_\beta^i \end{pmatrix} + \begin{pmatrix} hf_\beta \Delta\beta \\ hg_\beta \Delta\beta \end{pmatrix}, \quad \gamma_\beta^0 := 0.$$

Hence $G_j^\beta \Delta\beta = \gamma_\beta^n$. □

One should note that the system matrices in this recursion are identical to the ones above - with obvious consequences for the computer implementation. In complete analogy, more complicated products, as in (27,28), are carried out with identical recursions but different starting data γ^0 and γ_β^0 for different multiple shooting intervals.

4 Numerical results and discussion

We consider the **McWhorter Problem** in the domain $\Omega = [0, 2.6] X [0, 1.0]$ and time interval $(0, 1000[s])$. as a test case to verify our algorithm. In this problem, the instationary displacement process of oil by water is computed, taking into account the capillary effects in a two-dimensional horizontal system (Fig.2). The fluid and solid matrix properties, constitutive relationships and simulation parameters are given as follows.

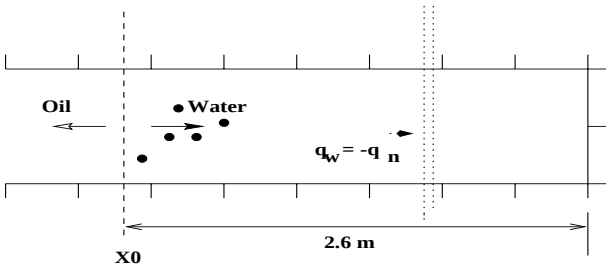

Figure 2: McWhorter Problem

Boundary conditions:
water saturation $S_w = 1.0$ [-], oil pressure $p_n = 2.10^5$ [Pa] at x=0
$F_\alpha(x,t) = 0$ at $y = 0$ and $y = 1.0[m]$
$F_\alpha(x,t) = 0$ at $x = 2.6[m]$
Initial Condition:
water saturation $S_w(x,0) = 0.01$ [-] for $x \in \Omega$

	Water	Oil
(1) Fluid properties		
density	1000 [kg/m^3]	1000 [kg/m^3]
dyn. viscosity	0.001 [kg/(ms)]	0.001 [kg/(ms)]
(2) Solid matrix properties and constitutive relationships		
abs. permeability k	[m^2]	$a * 10^{-10}$ a: to be estimated
porosity ϕ	[-]	0.30
pore size distr. index λ	[-]	to be estimated
entry pressure p_d	[Pa]	5000
residual saturation $s_{\alpha r}$	0.00	0.00
rel. permeability $k_r(S_w)$	[-]	Brooks-Corey model
capillary pressure $pc(S_w)$	[Pa]	Brooks-Corey model

Table 1: Fluid and Solid matrix properties and constitutive relationships

We identify the parameter λ, in the Brooks-Corey relationship for capillary pressure and relative permeabilities, and a, the scaling factor in the absolute permeability. The capillary pressure values obtained by the numerical computation using $\lambda = 2$ and $a = 1$ have been used as measurement values for this case. Five such measurement points (marked in black in Fig.2) and two shooting intervals are used for the computation at times $3.75[s]$ and $31.15[s]$. All the measurement points are taken within the region between the boundary at $x = 0$ and the 'free boundary' (which moves with time) at time 31.15[s]. We use the MUFTE-UG [7] software tool for solving the above mentioned set of partial differential equations on a grid with 1305 grid points. The least-squares problem is solved using reduced Gauss-Newton technique and this is incorporated in MUFTE-UG.

Each iteration of the multiple-shooting takes about 2 seconds of CPU time for the above grid size on an SGI machine. The iterations are stopped as soon as $\|(\Delta\lambda, \Delta a)\|_2 < 10^{-3}$.

The solution is independent of the initial guess of the saturation. Table 2 presents the results of the computation using the actual measurements and with measurements having random error of 5% and 10% with starting values of $\lambda = 1.6$ and $a = 0.5$. As we see the change in the final value of the parameter is also approximately 5% and 10% respectively. Figure 3 presents the results of the saturations of two shooting intervals in different iterations. The defects in computations are large initially and are reduced in subsequent iterations, as expected. Since the term

$$\left(\frac{\partial \phi_{ij}}{\partial S_j} g_j^{\beta} + \frac{\partial \phi_{ij}}{\partial \beta}\right)$$

in (26) is computed in each iteration, all information necessary for the computation of linearized covariances for the parameters are available if the parameter identification algorithm is converged (and therefore $d_j = 0, \forall j$). From that we compute 95% confidence intervals and display them in Table 2, as well.

Data set	# Iter.	Value of λ	Value of a
Actual Data	7	2.000 ± 0	0.999 ± 0
Data with 5% error	7	1.987 ± 0.014	0.973 ± 0.030
Data with 10% error	7	1.979 ± 0.027	0.979 ± 0.055

Table 2: Stability of Solution for the Estimation of λ and a

5 Conclusions

An algorithm has been developed for parameter identification in multi-phase flow through porous media. It employs the reduced Gauss-Newton method to an output least squares minimization problem in an efficient implementation. Special care has been taken concerning the proper formulation of continuity conditions and the computation of derivatives. The numerical studies show that the method is comparatively stable (small changes in experimental data results similar changes in the solution).

Acknowledgements

This research was supported by the German National Science Foundation (DFG). The authors are indebted to invaluable comments and suggestions from P. Bastian, R. Helmig, and G. Wittum.

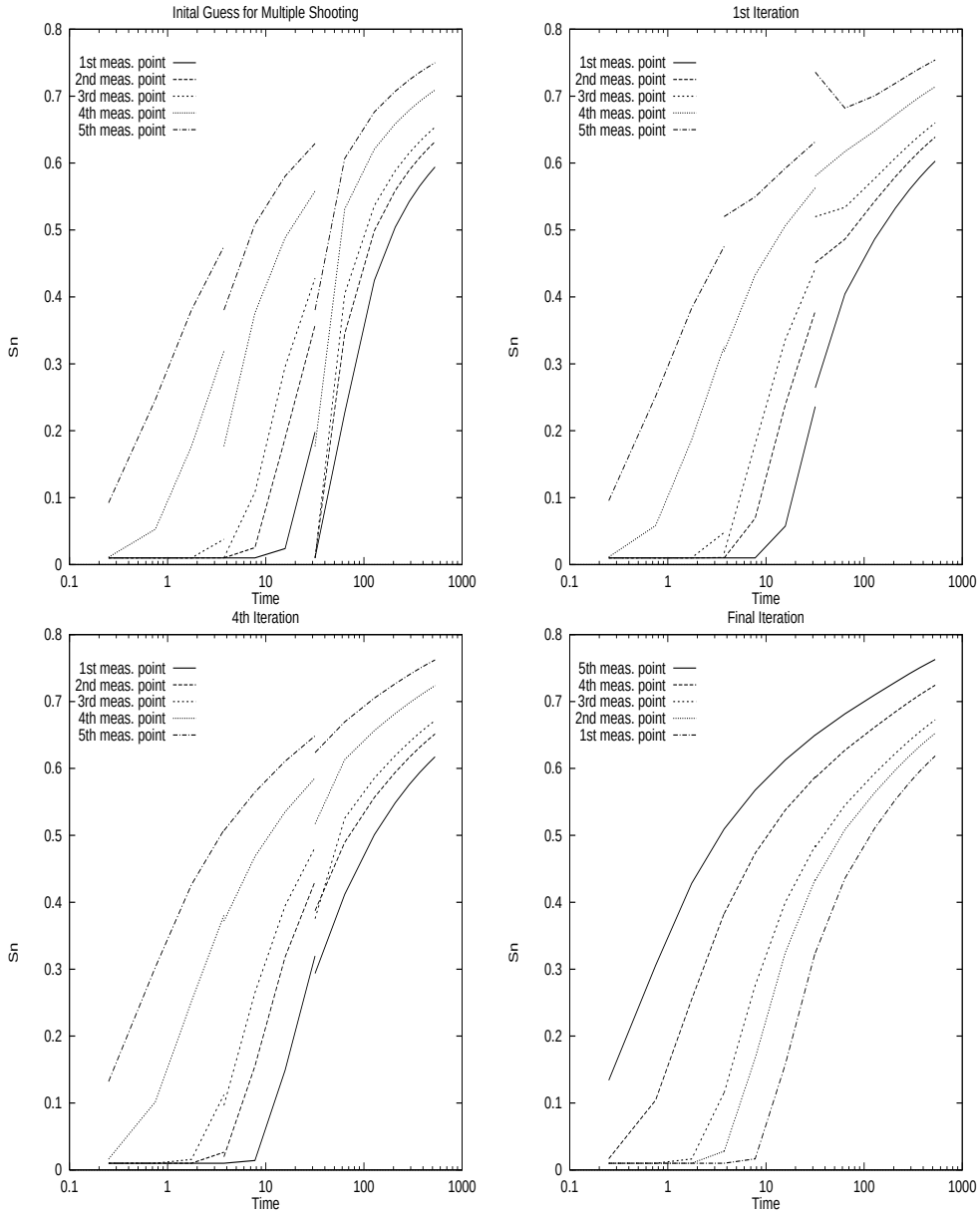

Figure 3: *Saturation of non-wetting phase at different iteration*

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