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Estimation of Two-Phase Petroleum Reservoir Properties by Regularization

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An algorithm is developed, based on the theory of regularization and on spline approximation, to estimate the absolute permeability in two-phase petroleum reservoirs from noisy well pressure data. The regularization feature of the algorithm converts the ill-posed estimation problem to a well-posed one. The algorithm, which employs the partial conjugate gradient method of Nazareth as its core minimization technique, automatically chooses the regularization parameter based on the non-regularized estimation. It is shown that regularized estimation is more stable and insensitive to the choice of initial guess as compared to non-regularized conventional estimation. © 1987 Academic Press, Inc.

1. INTRODUCTION

The spatial distribution of the properties of petroleum reservoirs cannot be measured directly; rather they must be inferred from matching the observed reservoir behavior to that predicted by a mathematical model. A reservoir that can be modeled as containing a single phase, e.g., oil, leads to a single linear PDE of heat conduction type for the pressure. Although the single-phase reservoir is clearly the first step in addressing reservoir parameter estimation problems, from the point of view of practical application, one really must consider two- (oil and water) and three- (gas, oil, and water) phase reservoirs. In this paper we present a comprehensive study of the estimation of two-phase petroleum reservoir properties.

The estimation of reservoir properties such as permeability and porosity based on measurements of pressure and production data at wells is an ill-posed problem, as it is neither unique nor continuously dependent on the measured data. Considerable effort has been devoted recently to attempting to develop well-posed algorithms for estimating petroleum reservoir properties. The critical problems in generating an effective algorithm for reservoir parameter estimation are twofold: (1) The original problem must be defined in a manner that alleviates the ill-posed nature of the problem; and (2) An efficient computational algorithm must be developed for solving the large, constrained, nonlinear minimization problem that results.

With respect to the inherent ill-posedness of the reservoir parameter estimation

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problem, Kravaris and Seinfeld [10, 11] have shown that the concept of regularization can be extended to the estimation of spatially varying parameters in partial differential equations of parabolic type, and Lee *et al.* [12] applied the approach to estimating parameters in single-phase (oil) reservoirs. The regularization idea, first advanced by Tikhonov [19], has been widely used in the solution of ill-posed integral equations, but had not heretofore been developed for the estimation of parameters in partial differential equations. In short, regularization of a problem refers to solving a related problem, called the regularized problem, whose solution is more "regular" (in a certain sense) than the solution of the original problem and approximate (in a certain sense) the solution of the original problem. More precisely, regularization of an ill-posed problem refers to solving a well-posed problem, whose solution gives a physically meaningful answer to the original ill-posed problem. The regularization formulation of parameter estimation measures the "non-smoothness" of the estimated parameter as a norm of the parameter in an appropriate Hilbert space. No prior information about the parameter is required other than a general idea of the degree of smoothness desired in the estimated field. The only unspecified parameter is that reflecting the relative weight given to the smoothness norm versus the usual least-squares objective function.

In the present context, the regularized problem is to find the parameters that minimize a performance index, called the smoothing functional, J_{SM}, that consists of the weighted sum of the conventional least-squares discrepancy term, J_{LS}, and a term that penalizes non-smoothness of the parameters, called the stabilizing functional, J_{ST}. Thus

$$J_{SM} = J_{LS} + \beta J_{ST}, \tag{1}$$

where β is the weighting coefficient, called the regularization parameter, chosen to reflect the degree of importance ascribed to J_{ST}.

The second major problem posed above is that of generating an efficient computational algorithm. Because the properties in an inhomogeneous reservoir vary with location, conceptually an infinite number of parameters are required for a full description of the reservoir. From a computational point of view, a reservoir model contains only a finite number of parameters, corresponding to each grid block or element in the spatial domain. In field scale simulations, it is not unusual for the reservoir domain to consist of the order of 10,000 grid cells, and consequently 20,000 or more parameters may need to be estimated simultaneously.

Banks and co-workers [2–5] and Kravaris and Seinfeld [11] have shown that an effective way to represent the spatial variation of unknown parameters in PDE's is by spline approximation. Then the parameter estimation problem reduces to determining the coefficients in the spline approximation. An important computational question concerns the choice of the spline parameter grid relative to the grid employed for the numerical solution of the governing PDEs.

This paper is a comprehensive study of the estimation of parameters in two-phase (oil–water) petroleum reservoirs. The numerical aspects of the problem will be considered in detail including (1) the choice of the stabilizing functional, (2) the choice of the regularization parameter, (3) the choice of the spline grid, and (4) the development of a computationally efficient algorithm.

2. Mathematical Model of Two-Phase Petroleum Reservoir

We consider a two-phase water–oil reservoir which has a sufficiently large areal extent so that we can assume that the pressure change and hence flow in the vertical direction is negligible compared to flow in the other two directions [1]. If the water and oil phases are immiscible, then the equations of mass conservation for water and oil phases are given by

$$R_{\mathrm{w}} \equiv -\frac{\partial}{\partial t}(\rho_{\mathrm{w}} \phi S_{\mathrm{w}}) - \nabla \cdot (\rho_{\mathrm{w}} \mathbf{v}_{\mathrm{w}}) + \sum_{\kappa=1}^{N_{\mathrm{w}}} \rho_{\mathrm{w}} q_{\mathrm{w}_{\kappa}} \frac{\delta(x-x_{\kappa})\,\delta(y-y_{\kappa})}{h} = 0 \tag{2.a}$$

$$R_{\mathrm{o}} \equiv -\frac{\partial}{\partial t}(\rho_{\mathrm{o}} \phi S_{\mathrm{o}}) - \nabla \cdot (\rho_{\mathrm{o}} \mathbf{v}_{\mathrm{o}}) + \sum_{\kappa=1}^{N_{\omega}} \rho_{\mathrm{o}} q_{\mathrm{o}_{\kappa}} \frac{\delta(x-x_{\kappa})\,\delta(y-y_{\kappa})}{h} = 0 \tag{2.b}$$

for $(x, y) \in \Omega \subset \Re^2$ and for $0 < t < T$ and the linear velocities of the two fluid phases are represented by Darcy's law for flow in porous media

$$\mathbf{v}_{\mathrm{w}} = -\frac{k k_{\mathrm{rw}}}{\mu_{\mathrm{w}}} \nabla p \tag{3.a}$$

$$\mathbf{v}_{\mathrm{o}} = -\frac{k k_{\mathrm{ro}}}{\mu_{\mathrm{o}}} \nabla p, \tag{3.b}$$

where

$$S_{\mathrm{w}} + S_{\mathrm{o}} = 1. \tag{4}$$

The initial conditions are

$$p(x, y, 0) = p_0 \tag{5}$$

$$S_{\mathrm{w}}(x, y, 0) = S_{\mathrm{iw}} \tag{6}$$

for $(x, y) \in \Omega$ and the no flux boundary condition

$$\mathbf{n} \cdot \nabla p = 0 \tag{7}$$

is assumed to hold for $(x, y) \in \partial\Omega$ and for $0 < t < T$. The relative permeabilities of water and oil phases are functions of saturation, relatively general forms of which, and those employed here, are

$$k_{rw}(S_w) = a_w \left(\frac{S_w - S_{iw}}{1 - S_{ro} - S_{iw}} \right)^{b_w} \tag{8.a}$$

$$k_{ro}(S_w) = a_o \left(\frac{1 - S_{ro} - S_w}{1 - S_{ro} - S_{iw}} \right)^{b_o}, \tag{8.b}$$

respectively, where the coefficients a_w, a_o, b_w, and b_o are constants independent of location.

3. Definition of the Parameter Estimation Problem

The reservoir parameter estimation problem can be considered as solving an inverse problem involving the nonlinear operator equation

$$K\alpha = u_\delta, \tag{9}$$

where α is the unknown reservoir parameter, u_δ is the noisy pressure and production data measured at the observation wells, and the operator K is the reservoir model.

In a multi-phase petroleum reservoir, the parameter α being estimated can in theory be the absolute permeability (k), porosity (ϕ), or coefficients appearing in the expressions for the relative permeabilities (k_{rw} and k_{ro}). In general, the porosity is better known from log and well data than is the absolute permeability, and the functional form of relative permeabilities are frequently given as shown in Eq. (8), so that the unknowns are the coefficients in the relative permeability expressions (a_w or a_o, b_w, and b_o) which are independent of location. In the present work we focus on the estimation of absolute permeability assuming the porosity and relative permeabilities are known so that the reservoir model K includes the reservoir model equations, Eqs. (2)–(8), known parameters (ϕ, k_{rw}, and k_{ro}), and the numerical solution scheme. This inverse problem is often referred to in the petroleum literature as "history matching" since the parameter is to be estimated from the measured transient history of pressure and production data at wells distributed over the reservoir domain.

Often there is no solution α that satisfies Eq. (9) exactly nor is the operator K directly invertible. Thus the inverse problem is stated as one of minimizing the error in approximating Eq. (9). As we have noted, the parameter is usually replaced by a finite (but usually large) number of new parameters by finite difference [8, 17] or spline approximation [2–5].

Conventional least-squares estimation seeks the parameter that minimizes the discrepancy between pressure and production data,

$$J_{LS} = \| K\alpha - u_\delta \|^2. \tag{10}$$

The performance function J_{LS} is generally non-convex, minimized over a large number of variables, and insensitive to changes in the parameters. As a consequence, the parameter estimates are (1) dependent on the given initial guess, (2) highly oscillatory and dependent on the grid system chosen for numerical solution, and (3) not continuously dependent on the measured data. Thus the inverse problem is "ill-posed" in the sense that the estimation of the parameters is neither unique nor stable.

Regularization of an ill-posed parameter estimation problem leads to penalizing the undesired features (non-smoothness) of the parameter estimates. In regularization the stabilizing functional represents non-smoothness of the parameter,

$$J_{\mathrm{ST}} = \| L\alpha \|^2_{H^{(L)}(\Omega)}, \tag{11}$$

where L is either identity or a differential operator and $H^{(L)}(\Omega)$ is an appropriate Sobolev space. The total performance index is then the smoothing functional given in Eq. (1) which now becomes

$$J_{\mathrm{SM}} = \| K\alpha - u_\delta \|^2 + \beta \, \| L\alpha \|^2_{H^{(L)}(\Omega)}, \tag{12}$$

where the regularization parameter, β, measures the relative weight of the penalty on the non-smoothness compared to the discrepancy in matching data.

Tikhonov's stabilizing functional [18, 19] is defined as the Sobolev norm of the unknown parameter. When we use spline approximation with cubic B-spline functions for representing the unknown parameter, $\alpha(x, y)$, Tikhonov's stabilizing functional is given by $\| \alpha \|^2_{H^3(\Omega)}$, where the Sobolev space $H^3(\Omega)$ is the set of functions that are square-integrable over Ω and have square-integrable derivatives up to order 3 [11, 12]. More precisely this stabilizing functional is given by

$$J_{\mathrm{ST}} = \sum_{m=0}^{3} \zeta_m J_{\mathrm{ST}}^{(m)} \tag{13}$$

where $J_{\mathrm{ST}}^{(m)}$, $m = 0, \ldots, 3$, represents mth order derivative terms given by

$$J_{\mathrm{ST}}^{(m)} = \iint_\Omega \sum_{\nu=0}^{m} \binom{m}{\nu} \left(\frac{\partial^m \alpha(\xi, \eta)}{\partial \xi^\nu \, \partial \eta^{m-\nu}} \right)^2 d\xi \, d\eta \tag{14}$$

with dimensionless space variables $\xi = x/\Delta x$ and $\eta = y/\Delta y$, and the coefficients ζ_m, $m = 0, 1, 2$, and 3, satisfy (1) $\zeta_m > 0$ for $m = 0, \ldots, 3$ [18]; or (2) $\zeta_m \geqslant 0$ for $m = 0, 1$, and 2 and $\zeta_3 > 0$ [19].

In practical applications of the theory of regularization, as Trummer [20] has pointed out, Tikhonov's stabilizing functional can lead to underestimation of the parameter value itself owing to the term $J_{\mathrm{ST}}^{(0)}$ in Eq. (13), which is the usual Euclidean norm of the parameter. Locker and Prenter [13] suggested regularization with a differential operator defined by $\| Lk \|^2_{H^{(L)}(\Omega)}$ for the linear least-squares problem so that the stabilizing functional is the norm of derivatives of the parameter in the Sobolev space. When the operator L in Eq. (11) is equal to the two-dimensional gradient ∇, Locker and Prenter's stabilizing functional becomes

$$J_{\mathrm{ST}} = \sum_{m=1}^{3} \zeta_m J_{\mathrm{ST}}^{(m)}, \tag{15}$$

where $J_{\mathrm{ST}}^{(m)}$, $m = 1,..., 3$, is the same as above and the coefficients ζ_m, $m = 1,..., 3$, satisfy $\zeta_1 > 0$, $\zeta_2 \geqslant 0$, and $\zeta_3 > 0$ so that it does not include the Euclidean norm of the parameter.

The choice of values of ζ_m in Eqs. (13) and (15) is arbitrary except for the inequality conditions given above. One possible choice of ζ_m's is based on the length scales used for the finite difference approximation of the PDEs, Δx and Δy. We will subsequently use $\zeta_1 = \zeta_2 = \zeta_3 = 1$ in Eqs. (13) and (15), while the choice of ζ_0 will be examined in the computational results.

A traditional question in the use of regularization to solve ill-posed problems is the choice of the regularization parameter β. Clearly $\beta = 0$ corresponds to the non-regularized problem, while $\beta \to \infty$ would lead to a physically unrealistic solution. Miller [14] suggested a way of determining the regularization parameter β from the ratio of an upper bound of J_{LS} values evaluated from the measured data (say $\overline{J_{\mathrm{LS}}}$) to a upper bound of J_{ST} (say $\overline{J_{\mathrm{ST}}}$). In this study, assuming that neither $\overline{J_{\mathrm{LS}}}$ nor $\overline{J_{\mathrm{ST}}}$ is available a priori, we will develop "a rule of thumb" to determine Miller's choice of β within our framework of regularization and spline approximation. Extensive numerical tests show that, for the solutions of non-regularized ($\beta = 0$) and regularized ($\beta > 0$) problems when the spline approximation is used for both cases,

(a) J_{LS} does not vary significantly for a wide range of $\beta \geqslant 0$ and the values of J_{LS} are close to the observation error in magnitude.

(b) J_{ST} generally decreases as β increases and J_{ST} at $\beta = 0$ in somewhat larger than the values of J_{ST} evaluated for the true profile.

This observation suggests that the value $J_{\mathrm{LS}}/J_{\mathrm{ST}}$ calculated from the non-regularized ($\beta = 0$) estimation can be used as an approximation of the optimal regularization parameter. We will discuss later in this paper how this idea can be implemented in the estimation algorithm.

One might define a "quasi-optimal" value of the regularization parameter as a $\beta > 0$ such that parameter estimates are minimally sensitive to the (logarithmic) change of β, i.e., $J_{\mathrm{ST}}(\beta(\partial\alpha/\partial\beta))$ is a minimum [19]. The numerical algorithm to find such a quasi-optimal β requires repeated solution of the regularized problem for different β's. Although we will later examine the effect on the estimates of the value of β, we will not use this particular strategy.

The intuitive idea of Generalized Cross Validation (GCV) is to find a β at which the parameter estimate gives the best prediction of unobserved data values. For that purpose, a GCV function is defined and minimized over $\beta > 0$ [9]. To apply this idea to reservoir parameter estimation one needs the parametric sensitivity of pressure and production data, the calculation of which is specifically avoided in our estimation algorithm for computational efficiency. Thus, we will not consider the selection of β by GCV.

4. Spline Approximation of Unknown Parameters

A general approach to representing the spatial variation of the unknown parameters is through the use of bicubic spline functions, in which the parameter $\alpha(x, y)$ is represented as

$$\alpha(x, y) = \sum_{l_y=1}^{N_{ys}} \sum_{l_x=1}^{N_{xs}} b_x(l_x, x)\, W_{l_x, l_y} b_y(l_y, y), \tag{16}$$

where

$$b_x(l_x, x) = \chi^{*4}\left(4 - l_x + \frac{x}{\Delta x_s}\right), \qquad l_x = 1, 2,..., N_{xs} \tag{17}$$

$$b_y(l_y, y) = \chi^{*4}\left(4 - l_y + \frac{y}{\Delta y_s}\right), \qquad l_y = 1, 2,..., N_{ys}, \tag{18}$$

and where $\chi^{*4}(\cdot)$ is the cubic B-spline function. Δx_s and Δy_s are the grid distance of the spline grid along x- and y-directions, respectively. With this approximation, $\alpha(x, y)$ is replaced by the set of unknown coefficients, W_{l_x, l_y}, $l_x = 1, 2,..., N_{xs}$ and $l_y = 1, 2,..., N_{ys}$.

The grid used for spline representation of the unknown properties need not necessarily coincide with that on which the actual reservoir model is solved. In general, the number of coefficients for spline representation should not exceed either the number of grid cells for the PDE or the number of available data. If too few coefficients are employed for the spline approximation, the functional derivative of J_{LS} with respect to the absolute permeability given by Eq. (B7) in Appendix B cannot be properly represented by the derivative of J_{LS} with respect to the spline coefficients during the minimization of J_{SM}, and this may slow the rate of convergence. Hence, we will employ a spline grid system as dense as that for the reservoir PDEs with a minimizing algorithm that is suitable for a system with large dimensionality.

5. Numerical Algorithm

The problem we now seek to solve is to minimize the augmented objective funciton J_{SM} with respect to the spline coeifficients W_{l_x, l_y}, $l_x = 1, 2,..., N_{xs}$ and $l_y = 1, 2,..., N_{ys}$, subject to Eqs. (2)–(8). To obtain an algorithm to solve this problem two steps are required. First, we must compute the gradient of J_{SM} with respect to each W_{l_x, l_y}, and second, that gradient is then used in a numerical minimization method to minimize J_{SM}. The calculation of these gradients represents the most time consuming part of updating the parameter iterates. In a problem as large as the current one these derivatives must be able to be calculated directly. Seinfeld and co-workers [6, 8, 21] and Chavent, *et al* [7] have developed algorithms for estimating parameters in PDEs based on optimal control theory so that the algorithm requires only first order functional derivatives of the performance functional with respect to the parameter to be estimated and this approach is used here. To compute the functional derivative of J_{LS} with respect to the absolute permeability, first solve the reservoir PDEs with given initial conditions at $t=0$, then, as shown in Appendix B, solve the adjoint system equations, Eqs. (B3), (B4), backward with terminal constraints given by Eqs. (B5), (B6). At the end of each time step during the solution of adjoint system equations, compute $\partial J_{LS}/\partial k_i$, $i=1,\ldots,N$, by Eq. (B7).

For most multivariate minimization problems, from the point of view of computational efficiency, methods that require second order derivatives of the performance function are not recommended. As a result, various methods have been developed that utilize only first order derivatives, among which are conjugate gradient, quasi-Newton, and partial conjugate gradient methods. The conjugate gradient algorithm requires an exact line search to compute the length of each descent direction vector. Quasi-Newton methods use the inverse Hessian matrix to compute the descent vector, which requires a substantial amount of memory, although it does not require an exact line search. In general, quasi-Newton methods are preferred for relatively small problems, and conjugate gradient methods for large problems [16]. On the other hand, partial conjugate gradient methods use about the same amount of memory as does the conjugate gradient method without requiring an exact line search, and show good performance over a range of problem sizes. In this study the partial conjugate gradient method of Nazareth [15] is used as the core minimization technique.

An important question concerns starting the algorithm. Convergence difficulties are sometimes experienced when the initial guesses of the parameters are far from their actual values. To attempt to alleviate this problem and to generate an algorithm that is as "automatic" as possible, we begin the estimation by determining the unknown parameter as uniform over the entire region. Thus, to start, we estimate a single value of k for the entire region that minimizes J_{LS}. This value then serves as a starting point for the full estimation algorithm. The rationale behind this strategy is that convergence problems should not be encountered in estimating a single parameter. The single value, while not accurate in its spatial detail, nevertheless serves as a good starting point for the full algorithm

Based on the foregoing discussion we suggest the following algorithm:

Step 1. In the absence of *a priori* information on the unknown parameters, find the flat initial guess of the parameter, *i.e.*, whose values are the same over the whole spatial domain, that minimizes J_{LS}.

Step 2. Using the initial guess of the parameter determined from Step 1, find the spatially varying parameter that minimizes J_{LS} and compute the values of J_{LS} and J_{ST}.

Step 3. Using the parameter profile and the values of J_{LS} and J_{ST} determined in Step 2, let $\beta = J_{LS}/J_{ST}$ and find the spatially varying parameter that minimizes J_{SM}.

6. Computational Examples

The remainder of this work is devoted to the numerical evaluation of the algorithm on the estimation of absolute permeability in a two-phase, two-dimensional reservoir, as described by Eqs. (2)–(8). We want to evaluate the algorithm on a well-defined test problem for which the "true" absolute permeability distribution is known *a priori.* For this reason, we will specify the true parameter values, generate the pressure data by solving the reservoir model with these values, and then try to recover the true parameter values by using the estimation algorithm.

The specification of the reservoir is given in Table I, and its shape and well locations are shown in Fig. 1. The production rate at each of two production wells (denoted by "P") is 3×10^{-3} m^3/s, and the injection rate at each of six injection wells (denoted by "I") is 10^{-3} m^3/s. The data were chosen so that the system is representative of actual reservoirs. To generate noisy measured pressure data at the observation wells we solve the reservoir PDEs for the presumed true absolute per-

TABLE I

Specification of Reservoir Shown in Fig. 1

	Water	Oil
(1) Fluid properties		
Compressibility (Pa^{-1})	1.94×10^{-9}	0.97×10^{-9}
Viscosity (Pa · s)	10^{-3}	3×10^{-3}
Relative permeability	$a_w = 0.9$	$a_o = 1.0$
	$b_w = 2.5$	$b_o = 2.0$
	$S_{iw} = 0.1$	$S_{ro} = 0.2$
Well flow rate		
$q_\kappa < 0$ for production wells	$q_{w_\kappa} = \dfrac{\lambda_w}{\lambda_w + \lambda_o} q_\kappa$	$q_{o_\kappa} = q_\kappa - q_{w_\kappa}$
$q_\kappa > 0$ for injection wells	$q_{w_\kappa} = q_\kappa$	$q_{o_\kappa} = 0$
(2) Rock and reservoir properties		
Compressibility (Pa^{-1})	2.91×10^{-9}	
Porosity	$\phi_{SC} = 0.2 - 0.05 \sin(2\pi x/x_L) \sin(\pi y/y_L)$	
Initial pressure (Pa)	1.52×10^7	
Reservoir dimension (m^3)	$1500 \times 1000 \times 10$	

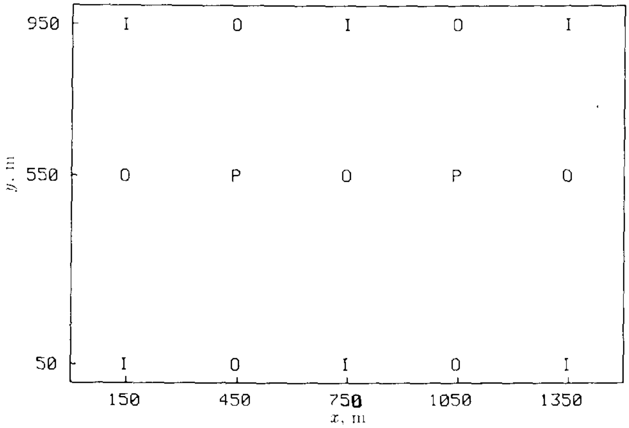

FIG. 1. Shape of reservoir and location of wells. (I) Injection and observation well, (P) production and observation well, (O) Observation well.

meability profile and add a set of uniformly distributed pseudo-random numbers (which are generated by the IMSL subroutine GGNML on a VAX 11/780).

The ill-posed nature of parameter estimation problems often leads to irregular estimated surfaces. In order to demonstrate this ill-conditioning, we will use the inclined plane shown in Fig. 2a as the true absolute permeability profile. We will also test the ability to recover a k surface of complicated geometry such as that shown in Fig. 2b. Since the k profile shown in Fig. 2a yields $J_{ST}^{(2)} = J_{ST}^{(3)} = 0$ and that

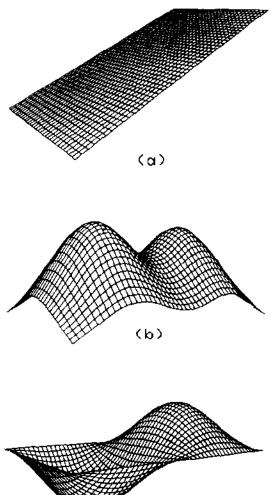

FIG. 2. Assumed absolute permeability profiles. (a) $k = 0.2 + 0.2x/x_L$, (b) $k = 0.2 + 0.2e^{-(4x/x_L-1)^2-(2y/y_L-1)^2} + 0.2e^{-(4x/x_L-3)^2-(2y/y_L-1)^2}$, (c) $k = 0.3 - 0.1\sin(2\pi x/x_L)\sin(\pi y/y_L)$.

shown in Fig. 2b is inadequate to test ill-conditioned estimation in the middle of the domain, we use yet a third k surface, shown in Fig. 2c, for which $J_{ST}^{(2)}$ and $J_{ST}^{(3)}$ have nonzero finite values and for which irregular behavior of the estimates can be visualized over the whole reservoir domain.

Throughout the numerical example, we use Locker and Prenter's [13] stabilizing functional with differential operator ($L \equiv \nabla$ and $\zeta_1 = \zeta_2 = \zeta_3 = 1$), the regularization parameter based on J_{LS}/J_{ST} calculated from the non-regularized estimation, and a 15×10 grid system for spline approximation, unless specified otherwise, with a PDE grid system of 15×10. Since absolute permeability can be estimated from pressure data alone [6], we use only pressure data in this study. The smoothing functional is minimized until the maximum value of the derivative of J_{SM} with respect to the spline coefficients is less than 1/1000th of that for the flat initial guess of k. All computations were carried out on a CRAY X-MP/48.

6.1. Effect of Initial Guess

Since the uniqueness of the solution of the parameter estimation problem is not guaranteed and there may exist unidentifiable regions based on the configuration of measurements and the time period over which the data are available, convergence of the algorithm may depend on the given initial guess.

The assumed true absolute permeability profile shown in Fig. 2a,

$$k(x, y) = 0.2 + 0.2 \frac{x}{x_L}, \tag{19}$$

was estimated using 300 noisy pressure data from 15 wells (20 data from each well) measured over the period $0 \leqslant t \leqslant 1.3$ yr. (The conversion unit of the absolute permeability, used in Eq. (19) and thereafter, is the darcy ($= 1.013 \times 10^{12}$ m^2). For consistency of units, k in Eq. (3) is in units of square meters.) The flat k value described

TABLE II

Effect of Initial Guess on the Estimation of k Given by Eq. (19)

Initial guess of k	β (darcies^{-2})	J_{SM}	J_{LS}	J_{ST}	$J_{ST}^{(0)}$	$J_{ST}^{(1)}$	$J_{ST}^{(2)}$	$J_{ST}^{(3)}$	CPU time (s)[a]
(a) 0.29	0	0.997	0.997	0.443	13.7	0.088	0.105	0.250	21.9
(b) $0.1 + 0.4x/x_L$	0	1.000	1.000	0.531	14.7	0.170	0.117	0.243	27.7
(c) Converged solution of (a)	2.3	1.077	1.003	0.032	13.8	0.022	0.007	0.003	36.4
(d) Converged solution of (b)	2.3	1.067	0.999	0.030	13.9	0.023	0.004	0.003	35.4
True k		1.160[b]	1.099	0.027	14.0	0.027	0	0	

[a] CRAY X-MP/48.
[b] For $\beta = 2.3$ darcies^{-2}.

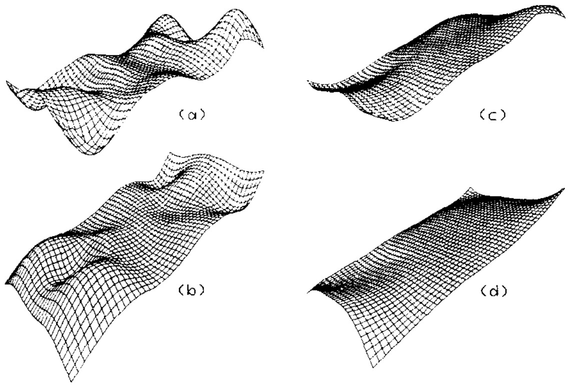

FIG. 3. Effect of initial guess on the estimation of k given by Eq. (19) for $\beta=0$ (non-regularized) and $\beta=2.3$ darcies^{-2}. (a) Initial guess of $k=0.29$, (b) initial guess of $k=0.1+0.4x/x_L$, (c) initial guess of k from (a), (d) initial guess of k from (b).

in Step 1 of our algorithm that minimizes J_{LS} is 0.29 darcy and the J_{LS} value at this value of k is 28.8 times as large as the J_{LS} value calculated from the observation error. For an initial guess of $k(x, y)=0.29$ darcy and $k(x, y)=0.1+0.4x/x_L$ darcies the smoothing functional was minimized for $\beta=0$ (the suggested β's based on our algorithm are 2.25 and 1.88 darcies^{-2}, respectively) and again minimized for $\beta=2.3$ darcies^{-2} starting from the result of the non-regularized estimation. Table II shows the results of the estimation, and Fig. 3 shows the parameter estimates. Figure 3 shows multiple solutions for non-regularized estimation, whereas for regularized estimation the regions of multiple solution exist only near the boundaries of $x=0$ and $x=x_L$ where flows of both oil and water are too small to provide meaningful data.

6.2. *Effect of Spline Grid*

To study the effect of the choice of spline grid, we consider 15×10, 12×9, 9×7, and 6×5 spline grid systems where the grid cells are square for the last three cases. In all cases the PDE grid remains as 15×10. The assumed true profile of absolute permeability shown in Fig. 2b,

$$k(x, y)=0.2+0.2\exp\left(-\left(4\frac{x}{x_L}-1\right)^2-\left(2\frac{y}{y_L}-1\right)^2\right)$$
$$+0.2\exp\left(-\left(4\frac{x}{x_L}-3\right)^2-\left(2\frac{x}{y_L}-1\right)^2\right), \qquad (20)$$

was estimated. The flat initial guess of $k=0.31$ darcy results from Step 1. We then carry out the estimation for $\beta=0$ and $\beta=1.7$ darcies^{-2} starting from the converged

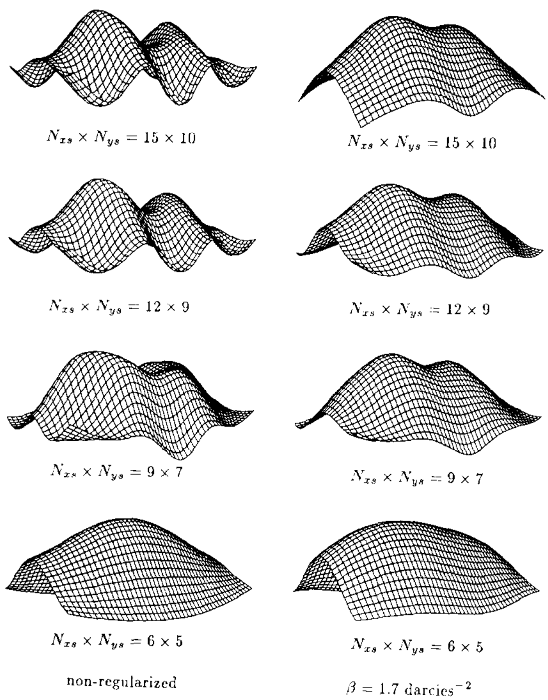

FIG. 4. Effect of spline grid on the estimation of k given by Eq. (20) for $\beta = 0$ (non-regularized) and $\beta = 1.7$ darcies^{-2}.

TABLE III

Effect of Spline Grid on the Estimation of k Given by Eq. (20)

$N_{xs} \times N_{ys}$	β (darcies^{-2})	J_{SM}	J_{LS}	J_{ST}	$J_{ST}^{(0)}$	$J_{ST}^{(1)}$	$J_{ST}^{(2)}$	$J_{ST}^{(3)}$	CPU time (s)[a]
15 × 10	0	0.927	0.927	0.548	16.0	0.144	0.151	0.253	14.0
12 × 9	0	0.933	0.933	0.370	16.1	0.133	0.108	0.128	12.8
9 × 7	0	0.911	0.911	0.407	16.3	0.169	0.106	0.132	28.3
6 × 5	0	0.982	0.982	0.197	16.4	0.153	0.031	0.013	18.2
15 × 10	1.7	1.221	0.954	0.157	16.1	0.118	0.025	0.014	31.3
12 × 9	1.7	1.229	0.957	0.160	16.1	0.113	0.029	0.017	21.2
9 × 7	1.7	1.253	0.954	0.176	16.0	0.126	0.032	0.018	13.9
6 × 5	1.7	1.276	0.980	0.174	16.3	0.140	0.024	0.009	31.5
True k		1.438[b]	1.070	0.217	15.8	0.162	0.036	0.019	

[a] CRAY X-MP/48.
[b] For $\beta = 1.7$ darcies^{-2}.

solution of the $\beta=0$ case. Figure 4 shows the parameter estimates for the cases given in Table III. Based on the non-regularized estimation, our algorithm suggests β's as 1.7, 2.5, 2.2, and 5.0 darcies^{-2} for the spline grid systems given above. Non-regularized estimates shows ill-conditioning near the boundaries for the $N_{xs} \times N_{ys} = 15 \times 10$ and 12×9 cases, but the regularized estimates are insensitive to the choice of spline grid except for the 6×5 spline grid, for which the parameter estimates are incorrect no matter whether regularization is applied or not. (See Table III.) CPU times in Table III show that reducing the number of spline coefficients, $N_{xs} \times N_{ys}$, does not increase the rate of convergence. Thus a grid system on the order of that used to solve the PDEs can be employed for the parameter estimation by regularization without introducing the ill-conditioning that is prevalent in non-regularized algorithms. The regularization parameter depends on the spline grid system, such that a finer grid system generally yields a smaller value of β.

6.3. *Effect of Stabilizing Functional*

The main difference between Tikhonov's and Locker and Prenter's stabilizing functionals is the value of the weighting coefficient ζ_0. We will test the cases $\zeta_0 = 1$, 0.3, 0.1, and 0 and $\zeta_1 = \zeta_2 = \zeta_3 = 1$ for the true k shown in Fig. 2c,

$$k(x, y) = 0.3 - 0.1 \sin\left(\frac{2\pi x}{x_L}\right) \sin\left(\frac{\pi y}{y_L}\right). \tag{21}$$

In this case it is advantageous to have a large amount of data so that effects of the number of data are absent. Consequently, we use 1500 noisy pressure data measured over a period $0 \leqslant t \leqslant 6.3$ yr (100 data at each of the 15 wells). Step 1 produces the flat initial guess of $k = 0.28$ darcy. The regularization parameter is then chosen based on our algorithm using $\zeta_0 = 0$, which is 2.1 darcies^{-2}. Table IV shows that the larger ζ_0 leads to a mismatch of data (J_{LS}), an underestimate of the parameter ($J_{ST}^{(0)}$), and ill-conditioning of parameter estimates ($J_{ST}^{(2)}$ and $J_{ST}^{(3)}$). It can be deduced from this example that, with Tikhonov's stabilizing functional, increas-

TABLE IV

Effect of Stabilizing Functional on the Estimation of k Given by Eq. (21)

ζ_0	β (darcies^{-2})	J_{SM}	J_{LS}	J_{ST}	$J_{ST}^{(0)}$	$J_{ST}^{(1)}$	$J_{ST}^{(2)}$	$J_{ST}^{(3)}$	CPU time (s)[a]
	0	0.952	0.952		13.6	0.102	0.100	0.247	150.5
1	2.1	26.69	2.877	11.21	10.8	0.169	0.129	0.158	124.3
0.3	2.1	9.563	1.237	3.920	12.5	0.088	0.041	0.038	79.6
0.1	2.1	4.078	1.006	1.447	13.4	0.075	0.023	0.012	66.4
0	2.1	1.187	0.963	0.105	13.8	0.075	0.020	0.010	81.1
True k			0.973		13.9	0.106	0.030	0.008	

[a] CRAY X-MP/48.

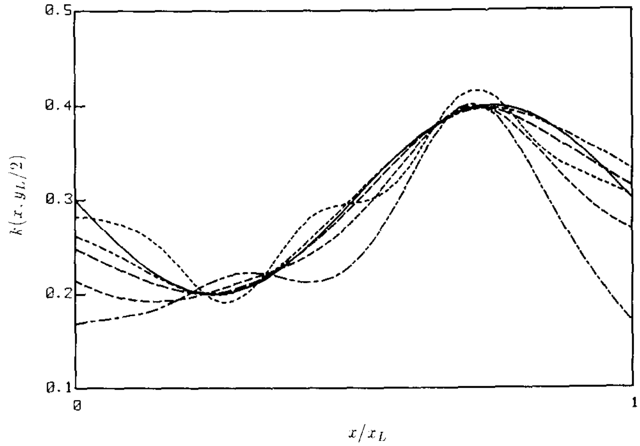

FIG. 5. Effect of stabilizing functional on the estimation of k given by Eq. (21). (——) true k, (---) $\beta=0$, (—-—) $\zeta_0=1$ and $\beta=2.1$ darcies^{-2}, (---) $\zeta_0=0.3$ and $\beta=2.1$ darcies^{-2}, (———) $\zeta_0=0.1$ and $\beta=2.1$ darcies^{-2}, (---) $\zeta_0=0$ and $\beta=2.1$ darcies^{-2}.

ing β will amplify the mismatch of data and the underestimate of the parameter; while decreasing β increases ill-conditioning of the estimates. One possible way to improve the parameter estimates is by decreasing ζ_0, the limiting case of which is use of a stabilizing functional with the differential operator given by Eq. (15). Figure 5 shows how the estimates vary as ζ_0 changes.

6.4. *Effect of Regularization Parameter*

We now wish to study the effect of the value of the regularization parameter β on the estimation. To do so we employ the true k given by Eq. (21), and return to the

TABLE V

Effect of Regularization Parameter on the Estimation of k Given by Eq. (21)

β (darcies^{-2})	J_{SM}	J_{LS}	J_{ST}	$J_{ST}^{(0)}$	$J_{ST}^{(1)}$	$J_{ST}^{(2)}$	$J_{ST}^{(3)}$	CPU time (s)[a]
0	0.924	0.924	0.630	13.6	0.118	0.139	0.372	33.7
0.091	0.946	0.925	0.231	13.7	0.106	0.059	0.066	21.7
0.183	0.967	0.929	0.207	13.7	0.098	0.054	0.055	13.4
0.367	0.993	0.932	0.166	13.7	0.096	0.040	0.030	16.0
0.734	1.062	0.937	0.170	13.7	0.091	0.043	0.036	8.4
1.468[b]	1.105	0.950	0.106	13.8	0.075	0.020	0.010	34.2
2.935	1.248	0.973	0.094	13.8	0.067	0.018	0.009	29.2
5.870	1.499	1.023	0.081	13.7	0.058	0.015	0.007	31.5
11.74	1.931	1.126	0.069	13.6	0.045	0.013	0.006	62.8
True k		1.041	0.144	13.9	0.106	0.030	0.008	

[a] CRAY X-MP/48.
[b] β based on the proposed algorithm.

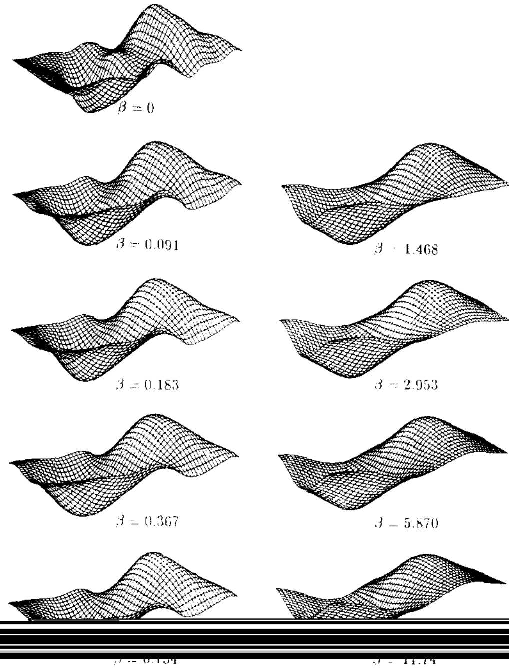

FIG. 6. Effect of regularization parameter on the estimation of k given by Eq. (21) (in darcies^{-2}).

case of 300 data over the period of 1.3 yr. The results are summarized in Table V. The value of β based on the non-regularized estimation is 1.468 darcies^{-2}. Other values of β were chosen so that they form a geometric sequence increasing and decreasing by factors of 2 around this value. If $\beta < 0.091$ darcies^{-2}, the minimization of J_{SM}, which is started from the result of the non-regularized estimation, is completed in one iteration since the regularization component (βJ_{ST}) is negligible compared to J_{LS}. If $\beta > 11.74$ darcies^{-2}, the values of J_{LS} become very large, and the algorithm experiences convergence difficulties. For $\beta = 0.734$ darcies^{-2}, the algorithm converges faster than any of the other cases. On the whole, J_{LS} increases and J_{ST} and its component terms (except $J_{ST}^{(0)}$) decrease as β increases. Figure 6 shows the effect of the values of β on the estimated surface. We note that at the value of β based on our algorithm, neither is the regularization effect negligible nor is there significant data mismatch, and the estimated surface shown in Fig. 6 approximates the true surface shown in Fig. 2c.

6.5. *Stability of Regularized Solution*

The most important feature of regularization is the stability of the solution so that small perturbations in measured data (random measurement error in the pressure data) imply small perturbations in the parameter estimates. To explore the stability of the parameter estimates, we use the absolute permeability given by

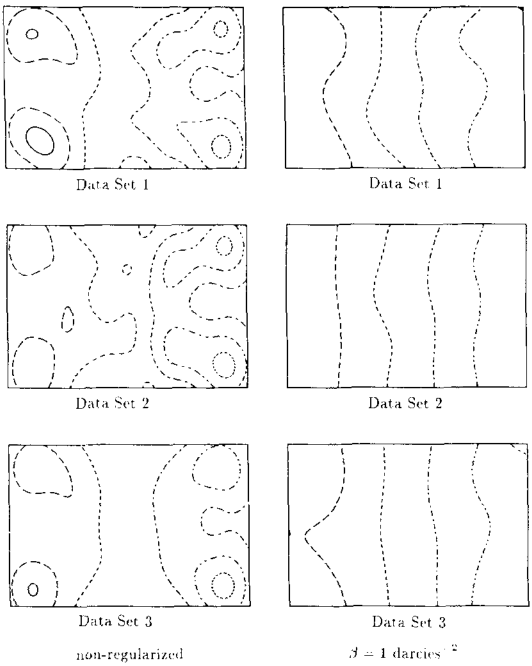

FIG. 7. Stability of solution for the estimation of k given by Eq. (19). Contour values are (——) $k = 0.2$ darcies, (–––) $k = 0.24$ darcies, (---) $k = 0.28$ darcies, (–––) $k = 0.32$ darcies, (––––) $k = 0.36$ darcies, (---) $k = 0.4$ darcies.

TABLE VI

Stability of Solution for the Estimation of k Given by Eq. (19)

Data set	β (darcies^{-2})	J_{SM}	J_{LS}	J_{ST}	$J_{ST}^{(0)}$	$J_{ST}^{(1)}$	$J_{ST}^{(2)}$	$J_{ST}^{(3)}$	CPU time (s)[a]
1	0	0.913	0.913[b]	0.664	13.9	0.127	0.157	0.380	36.5
2	0	0.922	0.922[c]	0.922	13.8	0.132	0.202	0.588	35.7
3	0	0.997	0.997[d]	0.442	13.7	0.088	0.105	0.250	22.0
1	1.0	0.988	0.935[b]	0.053	14.0	0.030	0.012	0.010	35.4
2	1.0	0.983	0.942[c]	0.041	13.9	0.024	0.006	0.015	37.6
3	1.0	1.032	0.997[d]	0.035	13.9	0.021	0.005	0.007	37.8
True k				0.027	14.0	0.027	0	0	

[a] CRAY X-MP/48.
[b] J_{LS} for true k is 1.070.
[c] J_{LS} for true k is 1.041.
[d] J_{LS} for true k is 1.099.

Eq. (19) and three different simulated noisy pressure sequences scaled so that the root mean square observation error is about 0.3×10^5 Pa. Figure 7 shows that the non-regularized estimates are unstable over the entire reservoir domain while the regularized estimates exhibit instability only in the regions near the boundaries ($x = 0$ and $x = x_L$) of the reservoir where the flow is negligible. Table VI shows the performance data for the three different data sets. Note that the differences between the values of J_{ST} and its terms (except $J_{ST}^{(0)}$) for the different data sets are reduced by a factor of 10 as a consequence of regularization.

7. Conclusions

The purpose of this study has been to develop an algorithm for parameter estimation by regularization and spline approximation for two-phase petroleum reservoirs.

The algorithm is divided into three steps. Step 1 seeks a flat initial guess of the parameter. This step avoids convergence difficulties that may arise in estimating spatially varying parameters from a poor initial guess. Usually this step converges within a few (4–6) iterative solutions of the reservoir and adjoint equations. Step 2 is devoted to nonregularized ($\beta = 0$) conventional least-squares estimation by spline approximation. The spline grid system is chosen so that the number of spline coefficients is the same as the number of grid cells for the solution of reservoir PDEs unless the number of observed data is less than the number of unknown coefficients. The parameter estimates from this step are usually ill-conditioned and dependent on the choice of the spline grid. This step usually requires 20–40 iterative solutions of the reservoir and adjoint equations to reduce the gradient value of the performance index to 1/1000th of its starting value. In this step, approximate values of the upper bounds of J_{LS} and J_{ST} are then estimated. In Step 3, parameter estimation by regularization and spline approximation is carried out to obtain the final solution. In this step, the regularization parameter is selected as the ratio of J_{LS} to J_{ST} determined in Step 2, and Locker and Prenter's stabilizing functional is used. The algorithm generally converges after 20–40 iterative solutions of the reservoir and adjoint equations.

For non-regularized estimation, the parameter estimates are sensitive to the choice of the spline grid, whereas for regularized estimation, the results are found to be insensitive to the choice of the spline grid (unless it is too coarse to properly represent the spatial variation). Since the value of the regularization parameter is dependent on the dimension of the spline grid, it is recommended that one use a grid system for spline approximation such that the number of spline coefficients is approximately equal to the smaller of the number of PDE grid cells or the number of observation data. Locker and Prenter's stabilizing functional with gradient operator was found to be superior to Tikhonov's stabilizing functional from the point of view of numerical performance.

The algorithm does not require any *a priori* information on the parameter to be estimated except that the parameter can be properly represented by a spline approximation. The parameter estimates based on the algorithm are shown to be superior to conventional non-regularized least-squares estimation in the sense of stability to the observation error and initial guess dependency.

APPENDIX A: Finite Difference Reservoir Equations

The basic model consists of two coupled nonlinear PDEs for pressure p and water saturation S_w. It is customary to discretize them using finite difference approximations to yield a set of nonlinear algebraic equations. We solve these equations sequentially at each time step, i.e., solve the equations for pressure first, then for water saturation, and repeat these procedures until the solution converges [1].

In order to solve the reservoir PDEs, Eqs. (2), (3), and (7) are discretized to give implicit time finite difference approximation by

$$\begin{aligned} R^n_{w_i} \equiv & -Q_t \frac{\phi_{SC_i}}{B^{n-1}_{f_i}} (c_w + c_f)\, S^n_{w_i}(p^n_i - p^{n-1}_i) - Q_t \frac{\phi_{SC_i}}{B^{n-1}_{f_i}} (S^n_{w_i} - S^{n-1}_{w_i}) \\ & - \sum_{j \in \mathbf{J}_i} Q_{i,j} \lambda^n_{w_{i,j}} (p^n_i - p^n_j) + \sum_{\kappa=1}^{N_w} q^n_{w_\kappa} \frac{\delta_{i,i_\kappa}}{h} \\ = & \; 0 \end{aligned} \tag{A1}$$

$$\begin{aligned} R^n_{o_i} \equiv & -Q_t \frac{\phi_{SC_i}}{B^{n-1}_{f_i}} (c_o + c_f)(1 - S^n_{w_i})(p^n_i - p^{n-1}_i) + Q_t \frac{\phi_{SC_i}}{B^{n-1}_{f_i}} (S^n_{w_i} - S^{n-1}_{w_i}) \\ & - \sum_{j \in \mathbf{J}_i} Q_{i,j} \lambda^n_{o_{i,j}} (p^n_i - p^n_j) + \sum_{\kappa=1}^{N_w} q^n_{o_\kappa} \frac{\delta_{i,i_\kappa}}{h} \\ = & \; 0 \end{aligned} \tag{A2}$$

for $n = 1,..., N_t$ and $i \in \mathbf{N}$ defined by

$$\begin{aligned} \mathbf{N} \equiv & \{ i \mid i = i_x + N_x(i_y - 1),\ i_x = 1,..., N_x,\ i_y = 1,..., N_y \} \\ = & \{1,..., N\}, \end{aligned} \tag{A3}$$

where $N = N_x N_y$ and i_x and i_y denote PDE grid blocks along x- and y-directions, respectively, and the index set $\mathbf{J}_i$ defined for each $i \in \mathbf{N}$ by

$$\mathbf{J}_i = \{ j \mid j = i - N_x, i - 1, i + 1, i + N_x \} \cap \mathbf{N} \tag{A4}$$

is introduced for simplicity, with initial conditions

$$p^0_i = p_0 \tag{A5}$$

$$S^0_{w_i} = S_{iw}. \tag{A6}$$

In Eqs. (A1) and (A2) the mobilities $\lambda^n_{w_{i,j}}$ and $\lambda^n_{o_{i,j}}$, $i = 1,\ldots, N$, are given by

$$\lambda^n_{w_{i,j}} = \frac{k_{i,j} k^n_{rw_{i,j}}}{\mu_w} \tag{A7}$$

$$\lambda^n_{o_{i,j}} = \frac{k_{i,j} k^n_{ro_{i,j}}}{\mu_o}, \tag{A8}$$

where the algebraic average is used for the absolute permeability

$$k_{i,j} = \frac{k_i + k_j}{2} \tag{A9}$$

and upstream weighting is used for the relative permeabilities for the stability of numerical integration given by

$$\begin{aligned} k^n_{rw_{i,j}} &= k_{rw}(S^n_{w_i}) \quad \text{and} \quad k^n_{ro_{i,j}} = k_{ro}(S^n_{w_i}) \quad \text{if} \quad p^n_i \geqslant p^n_j \\ k^n_{rw_{i,j}} &= k_{rw}(S^n_{w_j}) \quad \text{and} \quad k^n_{ro_{i,j}} = k_{ro}(S^n_{w_j}) \quad \text{otherwise.} \end{aligned} \tag{A10}$$

The porosity distribution at pressure p_{SC}, denoted by ϕ_{SC}, is known where SC denotes "standard condition." Compressibility effects are included by using the so-called formation volume factor of rock B_f,

$$B_f(p) = e^{c_f(p_{SC} - p)}, \tag{A11}$$

where in evaluating B_f an explicit time difference scheme is used in the finite difference approximation.

First order variations of Eqs. (A1), (A2) with respect to S_w are given by

$$\begin{aligned} \delta R^n_{w_i} \equiv & - Q_i \frac{\phi_{SC_i}}{B^{n-1}_{f_i}} (c_w + c_f)\, \delta S^n_{w_i} (p^n_i - p^{n-1}_i) - Q_i \frac{\phi_{SC_i}}{B^{n-1}_{f_i}} \delta S^n_{w_i} \\ & - \sum_{j \in \mathbf{J}_i} Q_{i,j} \left(\frac{\partial \lambda^n_{w_{i,j}}}{\partial S^n_{w_i}} \delta S^n_{w_i} + \frac{\partial \lambda^n_{w_{i,j}}}{\partial S^n_{w_j}} \delta S^n_{w_j} \right) (p^n_i - p^n_j) \\ & + \sum_{\kappa=1}^{N_w} \frac{dq^n_{w_\kappa}}{dS^n_{w_i}} \delta S^n_{w_i} \frac{\delta_{i,i_\kappa}}{h} \end{aligned} \tag{A12}$$

$$\begin{aligned} \delta R^n_{o_i} \equiv & + Q_i \frac{\phi_{SC_i}}{B^{n-1}_{f_i}} (c_o + c_f)\, \delta S^n_{w_i} (p^n_i - p^{n-1}_i) + Q_i \frac{\phi_{SC_i}}{B^{n-1}_{f_i}} \delta S^n_{w_i} \\ & - \sum_{j \in \mathbf{J}_i} Q_{i,j} \left(\frac{\partial \lambda^n_{o_{i,j}}}{\partial S^n_{w_i}} \delta S^n_{w_i} + \frac{\partial \lambda^n_{o_{i,j}}}{\partial S^n_{w_j}} \delta S^n_{w_j} \right) (p^n_i - p^n_j) \\ & + \sum_{\kappa=1}^{N_w} \frac{dq^n_{o_\kappa}}{dS^n_{w_i}} \delta S^n_{w_i} \frac{\delta_{i,i_\kappa}}{h} \end{aligned} \tag{A13}$$

to solve the finite difference equations for S_w.

At time step $t_n = n\Delta t$, $n = 1,\dots, N_t$, take initial guesses of $p_i^n = p_i^{n-1}$ and $S_{w_i}^n = S_{w_i}^{n-1}$ for $i = 1,\dots, N$ and solve

$$R_{w_i}^n + R_{o_i}^n = 0 \tag{A14}$$

for p_i^n, $i = 1,\dots, N$, where R_w's and R_o's are given in Eqs. (A1) and (A2), respectively. Equation (A14) does not include time derivative terms of S_w, and is a linear pentadiagonal system with respect to p so that it is easily solved by the Iterative Alternate Direction Implicit (IADI) method.

Second, solve

$$\frac{(c_o + c_f)(1 - S_{w_i}^n)}{c_{t_i}^n} R_{w_i}^n - \frac{(c_w + c_f)\, S_{w_i}^n}{c_{t_i}^n} R_{o_i}^n = 0 \tag{A15}$$

for $S_{w_i}^n$, $i = 1,\dots, N$, by Newton's method since Eq. (A15) is nonlinear with respect to S_w. Equation (A15) does not include time derivative terms of p and the total compressibility, $c_{t_i}^n$, is given by

$$c_{t_i}^n = (c_w + c_f)\, S_{w_i}^n + (c_o + c_f)(1 - S_{w_i}^n). \tag{A16}$$

Taylor series expansion of Eq. (A15) up to first order gives

$$\frac{(c_o + c_f)(1 - S_{w_i}^n)}{c_{t_i}^n} (R_{w_i}^n + \delta R_{w_i}^n) - \frac{(c_w + c_f)\, S_{w_i}^n}{c_{t_i}^n} (R_{o_i}^n + \delta R_{o_i}^n) = 0 \tag{A17}$$

for $i = 1,\dots, N$, where the first order variation terms, δR_w's and δR_o's, are given in Eqs. (A12) and (A13), respectively. Equation (A17) is a linear pentadiagonal system with respect to δS_w and is solved for $\delta S_{w_i}^n$, $i = 1,\dots, N$, by the IADI method.

Then we compare the current iterate of p_i^n and $S_{w_i}^n$, $i = 1,\dots, N$, with the previous ones, and repeat solving Eqs. (A14)–(A17) until convergence.

APPENDIX B: Functional Derivative of J_{LS}

We present the finite difference version of the first order necessary condition for a minimum of the least-squares discrepancy function defined by

$$J_{LS} = \frac{1}{N_t N_o} \sum_{n=1}^{N_t} \sum_{\nu=1}^{N_o} \left(W_p (p(x_\nu, y_\nu, t_n) - (p^{obs})_\nu^n)^2 + W_F (F_{wo}(x_\nu, y_\nu, t_n) - (F_{wo}^{obs})_\nu^n)^2\right), \tag{B1}$$

where $(p^{obs})_\nu^n$ and $(F_{wo}^{obs})_\nu^n$ are the pressure and water-to-oil ratio ($\equiv S_w/S_o$) data measured from the νth observation well located at (x_ν, y_ν), $\nu = 1,\dots, N_o$, at time

t_n, $n = 1, \ldots, N_t$. The corresponding Hamiltonian of the conventional least-squares problem is

$$\widetilde{J_{\mathrm{LS}}} = J_{\mathrm{LS}} + \sum_{n=1}^{N_t} \sum_{i=1}^{N} (\psi^n_{\mathrm{w}_i} R^n_{\mathrm{w}_i} + \psi^n_{\mathrm{o}_i} R^n_{\mathrm{o}_i}). \tag{B2}$$

Collecting terms that include δp^n_i yields

$$\begin{aligned} R^n_{\mathrm{p}_i} \equiv\; & Q_t \frac{\phi_{\mathrm{SC}_i}}{B^n_{\mathrm{f}_i}} ((c_\mathrm{w} + c_\mathrm{f}) S^{n+1}_{\mathrm{w}_i} \psi^{n+1}_{\mathrm{w}_i} + (c_\mathrm{o} + c_\mathrm{f})(1 - S^{n+1}_{\mathrm{w}_i}) \psi^{n+1}_{\mathrm{o}_i}) \\ & - Q_t \frac{\phi_{\mathrm{SC}_i}}{B^{n-1}_{\mathrm{f}_i}} ((c_\mathrm{w} + c_\mathrm{f}) S^n_{\mathrm{w}_i} \psi^n_{\mathrm{w}_i} + (c_\mathrm{o} + c_\mathrm{f})(1 - S^n_{\mathrm{w}_i}) \psi^n_{\mathrm{o}_i}) \\ & - \sum_{j \in \mathbf{J}_i} Q_{i,j} (\lambda^n_{\mathrm{w}_{i,j}} (\psi^n_{\mathrm{w}_i} - \psi^n_{\mathrm{w}_j}) + \lambda^n_{\mathrm{o}_{i,j}} (\psi^n_{\mathrm{o}_i} - \psi^n_{\mathrm{o}_j})) \\ & + 2W_\mathrm{p} \sum_{\nu=1}^{N_\mathrm{o}} (p^n_i - (p^{\mathrm{obs}})^n_\nu)\, \delta_{i,i_\nu} \\ =\; & 0 \end{aligned} \tag{B3}$$

and terms that include $\delta S^n_{\mathrm{w}_i}$ yields

$$\begin{aligned} R^n_{\mathrm{s}_i} \equiv\; & Q_t \left(\frac{\phi_{\mathrm{SC}_i}}{B^n_{\mathrm{f}_i}} (\psi^{n+1}_{\mathrm{w}_i} - \psi^{n+1}_{\mathrm{o}_i}) - \frac{\phi_{\mathrm{SC}_i}}{B^{n-1}_{\mathrm{f}_i}} (\psi^n_{\mathrm{w}_i} - \psi^n_{\mathrm{o}_i}) \right) \\ & - ((c_\mathrm{w} + c_\mathrm{f}) \psi^n_{\mathrm{w}_i} - (c_\mathrm{o} + c_\mathrm{f}) \psi^n_{\mathrm{o}_i}) Q_t \frac{\phi_{\mathrm{SC}_i}}{B^{n-1}_{\mathrm{f}_i}} (p^n_i - p^{n-1}_i) \\ & - \sum_{j \in \mathbf{J}_i} Q_{i,j} \left(\frac{\partial \lambda^n_{\mathrm{w}_{i,j}}}{\partial S^n_{\mathrm{w}_i}} (\psi^n_{\mathrm{w}_i} - \psi^n_{\mathrm{w}_j}) + \frac{\partial \lambda^n_{\mathrm{o}_{i,j}}}{\partial S^n_{\mathrm{w}_i}} (\psi^n_{\mathrm{o}_i} - \psi^n_{\mathrm{o}_j}) \right) (p^n_i - p^n_j) \\ & + 2W_\mathrm{F} \frac{dF^n_{\mathrm{wo}_i}}{dS^n_{\mathrm{w}_i}} \sum_{\nu=1}^{N_\mathrm{o}} ((F_\mathrm{wo})^n_i - (F^{\mathrm{obs}}_\mathrm{wo})^n_\nu)\, \delta_{i,i_\nu} + (\psi^n_{\mathrm{w}_i} - \psi^n_{\mathrm{o}_i}) \sum_{\kappa=1}^{N_\mathrm{w}} \frac{dq^n_{\mathrm{w}_\kappa}}{dS^n_{\mathrm{w}_i}} \frac{\delta_{i,i_\kappa}}{h} \\ =\; & 0 \end{aligned} \tag{B4}$$

for $i \in \mathbf{N}$ and $n = N_t, N_t - 1, \ldots, 2, 1$, with terminal constraints

$$\psi^{N_t+1}_{\mathrm{w}_i} = 0 \tag{B5}$$

$$\psi^{N_t+1}_{\mathrm{o}_i} = 0 \tag{B6}$$

for $i \in \mathbf{N}$. The functional derivative of J_{LS} with respect to k_i, $i \in \mathbf{N}$, is given by

$$\frac{\partial J_{\mathrm{LS}}}{\partial k_i} = -\frac{1}{2} \sum_{n=1}^{N_t} \sum_{j \in \mathbf{J}_i} Q_{i,j} \left(\frac{k^n_{\mathrm{rw}_{i,j}}}{\mu_\mathrm{w}} (\psi^n_{\mathrm{w}_i} - \psi^n_{\mathrm{w}_j}) + \frac{k^n_{\mathrm{ro}_{i,j}}}{\mu_\mathrm{o}} (\psi^n_{\mathrm{o}_i} - \psi^n_{\mathrm{o}_j}) \right) (p^n_i - p^n_j). \tag{B7}$$

The adjoint system equations are solved sequentially, i.e., Eq. (B3) is solved for a new variable ψ_p defined by

$$\psi^n_{p_i} \equiv \frac{(c_w + c_f)\, S^n_{w_i}}{c^n_{t_i}} \psi^n_{w_i} + \frac{(c_o + c_f)(1 - S^n_{w_i})}{c^n_{t_i}} \psi^n_{o_i} \tag{B8}$$

and Eq. (B4) for ψ_s defined by

$$\psi^n_{s_i} \equiv \psi^n_{w_i} - \psi^n_{o_i}, \tag{B9}$$

where the IADI method is employed for the solution of each equation, repeating this procedure until the solution converges. From $\partial L_{LS}/\partial k_i$, $i = 1,\ldots, N$, and the derivative of J_{ST} with respect to the spline coefficients we can compute the derivative of J_{SM} with respect to each spline coefficient [12].

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