THE IMPACT OF UNCERTAIN CENTRIFUGE CAPILLARY PRESSURE ON RESERVOIR SIMULATION*

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Abstract. The capillary pressure in a reservoir determines the saturation distribution, and hence the total in situ volumes of fluids (oil/water/gas). The accurate knowledge of the capillary pressure distribution is one of the primary factors that may be decisive in the reliable estimation of hydrocarbon reserves.

The centrifuge procedure provides laboratory data, which can be inverted to derive capillary pressure curves in laboratory conditions. The derived laboratory capillary pressure curves are then scaled up for full-field simulation of petroleum reservoirs.

The inversion procedure is uncertain and gives nonunique capillary pressure curves. The standard industrial practice, however, has been to derive a single capillary pressure curve, and ignoring the uncertainty. Since the capillary pressure is uncertain, estimates of important reservoir parameters dependent on capillary pressure distribution are uncertain.

This paper shows how the uncertainty in centrifuge capillary pressure can be quantified. It also shows how this uncertainty propagates through the scale-up process and impacts on the estimate of the oil recovery potential. We illustrate using a simple, two-phase (oil/water) synthetic reservoir model.

Key words. uncertainty, Volterra, linear integral equation, inverse, ill-posed, stochastic algorithm, Voronoi cells, measured data, synthetic data, capillary pressure, centrifuge

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1. Introduction. Due to capillary forces, when two fluids are put into contact in an evacuated porous medium, one will be spontaneously imbibed in preference to the other. The spontaneously imbibed medium is referred to as the wetting fluid and the other the nonwetting fluid. The capillary pressure in a porous medium is defined as the differential pressure that exists between two fluid phases at their interfaces when they are distributed under static equilibrium within the porous material [33].

For a porous medium, which is partially saturated with two fluids, if we denote the pressure in the wetting and nonwetting phases, respectively, by P_w and P_{nw} , then by definition, the capillary pressure P_c is given by

$$(1.1) \quad P_c(S_w) = P_{nw} - P_w.$$

That is, the pressure excess in the nonwetting fluid, $P_c(S_w)$, is the capillary pressure, and this quantity is a function of the wetting phase saturation S_w . By definition S_w is the proportion of the total pore volume of the core occupied by the fluid. Equation (1.1) is the defining equation for capillary pressure in a porous medium. For a given porous medium, the normal assumption is that there exists a one-to-one relationship between the capillary pressure value and the wetting phase saturation. The relationship is often expressed through a curve relating the two parameters. This curve is referred to as a capillary pressure curve or function. The capillary pressure is

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one of the most important parameters controlling reservoir performance, determining, among others, initial saturation and distribution of fluids and the degree of ultimate reservoir recoveries; see [12] and [6].

In the exploitation of petroleum reservoirs, knowledge of the capillary pressure distribution is utilized in the estimation of initial saturation of fluids in the reservoir, and hence the total amount of hydrocarbon initially in place. Further, making quantitative assessment of possible exploitation strategies (e.g., displacing the oil in the reservoir by water) requires a simulation of the reservoir behavior. The set of partial differential equations describing flow in porous media, however, contains the capillary pressure function. Hence the accurate determination of this function is imperative in the modeling of petroleum oil reservoirs.

As it is impractical to take direct measurements of the reservoir, a series of techniques have been developed for the laboratory determination of the capillary pressure functions, using small porous media samples (typically, cylindrical cores, 1.5 inches in diameter and 2–3 inches in length). Distinctly, two main measurement procedures are identifiable, namely, displacement and dynamic methods. Displacement methods are based on the establishment of successive states of hydrostatic equilibrium, while dynamic methods are based on the establishment of successive states of steady or near steady flow of a pair composed of a wetting and a nonwetting fluid. The most common procedures for measuring capillary pressure curves are based on dynamic methods, of which the porous plate [47], mercury injection [34], and the centrifuge [24] are examples. See [13] for a discussion of the relative strengths of these methods. This paper will concentrate on the centrifuge method as a procedure for deriving capillary pressure functions.

Since its inception in 1945, the centrifuge technique has become quite popular in the oil industry for several reasons. Among others, it offers residual saturation in the core plug after centrifugation in the same range as expected in the underground reservoir after a water flooding. Further, the technique is quite rapid and relatively inexpensive. The drawback with the centrifuge technique, however, has been the interpretation of the results. The interpretation technique has been the subject of controversy ever since Hassler and Brunner published their article 57 years ago [24].

The determination of capillary pressure functions from centrifuge laboratory data is an inverse and ill-posed problem, and involves a Volterra integral equation of the first kind. Hence the problem has a nonunique solution [44], [45], and slight perturbations in the laboratory data give disproportionate responses in the solutions derived. Earlier proposed interpretation techniques have not paid sufficient attention to the nature of the problem, and the fundamental principles upon which the methodologies are based are not without criticism.

Most of the earlier methods had aimed at determining discrete solutions to the problem, thus neglecting the functional relationship that exists between the saturation and the capillary pressure. Several solutions based on this approach abound in the literature; see [15], [24], [25], [26], [28], [29], [35], [36], [42], and [46]. Most recent methodologies have aimed at deriving continuous functions from the data [31], [27].

Based on the mathematical methodology by which the capillary pressure function is derived, we can distinguish between explicit and implicit methods. Explicit approaches involve solving for the capillary pressure function explicitly by relating a given capillary pressure value to a measured average saturation of the core. Implicit methods, on the other hand, involve a parameterization of the sought capillary pressure function and solving for the parameters using optimization algorithms [5], [27].

Irrespective of the methodology employed, the assumption has been that there exists a single, correct capillary pressure function, which can be derived on the basis of the experimental data.

A survey conducted by the SCA (Society of Core Analysts) [18] on methodologies for determining capillary pressure functions showed that given a set of experimental data, one can derive as many capillary pressure functions as there are methodologies available. The experimental data set for this survey was generated from eight different mathematical models for the capillary pressure function. The data set consisted of discrete pairs of capillary pressure and average water saturation of the core. “White noise” was added to the data to make it as realistic as possible. The respondents were then required to generate capillary pressure functions, using the supplied data set. The quality of the results were judged on the basis of how close a derived function was to the truth, i.e., the analytical function. The two results judged to be most accurate were those by [15] and [27]. These methodologies incorporated a stabilization parameter (smoothing term in [15] and Tikhonov in [27]) into the solution. In practice, however, the truth is unknown and the task of judging the accuracy of a derived capillary pressure function is nontrivial.

In petroleum engineering, the ultimate use of the derived capillary pressure curves is in reservoir simulation of the capillary relationship between oil and water. The centrifuge experiment, however, provides data for deriving the capillary function between water and gas. The water/gas capillary function is then scaled to derive the oil/water function, which is used in simulation. The uncertainty in the water/gas function therefore leads to uncertainty in the oil/water capillary function. The issue of how this uncertainty in centrifuge data propagates, and how it impacts on reservoir simulation, has never been addressed.

The aim of this paper is to show how uncertainty in the centrifuge capillary pressure can be quantified. It shows how this uncertainty impacts on the estimation of some important, global reservoir properties. We use a synthetic capillary pressure model to generate error-free data, to which we added white noise to generate laboratory data. We present the impact of the uncertainty in the laboratory data on the estimation of the initial oil in place and the oil recovery potential during water flooding. We demonstrate using a two-phase (oil/water) reservoir model.

This paper is organized in the following way. The next section presents the background to the problem, including the experimental setup. Section 3 presents the parameterization of the sought function and shows how the problem leads to the task of solving a constrained system of linear equations. Section 4 presents a brief description of the stochastic algorithm for solving the system of equations and describes our uncertainty quantification procedure. Section 5 discusses how the model parameter uncertainties are calculated and the scale-up process for capillary pressure functions from laboratory to reservoir conditions. Section 6 describes our validation approach. We show how the synthetic centrifuge data is generated from an analytical function and describe the synthetic reservoir model. Finally, we present and discuss results obtained using the synthetic model.

2. Background. In a centrifuge experiment, a core sample is initially saturated with one phase (the wetting and denser phase), usually water. The core is put into a core holder and surrounded by the lighter, nonwetting fluid, which is usually air. The core holder is spun horizontally at a series of consecutively higher angular velocities in the centrifuge. A schematic diagram of the centrifuge setup is shown in Figure 2.1.

FIG. 2.1. Schematic diagram of centrifuge system.

During centrifugation, the nonwetting phase enters the core at the end located at inner centrifuge radius, r_i , and the wetting phase exits the core at outer radius, r_e . The cumulative volume of fluid displaced from the core, v_k^{exp} , at each equilibrium ω_k (i.e., when no more fluid is displaced) can be measured, often manually (by eye), utilizing stroboscopic light and a graded fluid container.

At equilibrium, for an angular velocity ω , the pressure in phase j at a radius $r : r_i \leq r \leq r_e$ is given by

$$P_j(r, \omega) = \rho_j \omega^2 (r_e^2 - r^2) / 2.$$

By assumption, the capillary pressure P_c is zero at $r = r_e$; see [24]. If we define the difference in density between the fluids by $\Delta\rho$, then $\Delta\rho = \rho_{nw} - \rho_w$, and we derive

$$(2.1) \quad P_c(r, \omega) = \Delta\rho \omega^2 (r_e^2 - r^2) / 2,$$

$\Downarrow$

$$(2.2) \quad P_c(r_i, \omega_k) = \Delta\rho \omega_k^2 (r_e^2 - r_i^2) / 2 = P_k.$$

Using the observed data, the average saturation of the core is calculated as

$$(2.3) \quad \bar{S}_k = 1 - v_k^{exp} / v_p,$$

where v_p refers to the pore volume, i.e., the volume of the core that is open to fluid occupation. This parameter is usually predetermined experimentally.

The experimental procedure therefore provides discrete data in the form of the average saturation of the core sample at increasing capillary pressure values, $(P_k, \bar{S}_k)$.

2.1. Sources of uncertainty. The main sources of uncertainty in the centrifuge capillary pressure function have been well established in the literature. These can be attributed to simplifying assumptions in the mathematical modeling of the experimental procedure and in the data errors. Some of the sources of the modeling errors are listed below, and include the assumption of

1. zero capillary pressure at the outlet;
2. zero vertical gravitational acceleration;
3. one-dimensional distribution of the centrifugal field within the core;
4. the inadequate account for the effects of horizontal centrifugal field;
5. the omission of core sample heterogeneity effects on the flow mechanism.

For points 2, 4, and 5 above, see [7], [8], [9], [16], and [17]. Assumption 1 is fundamental to the Hassler–Brunner model. In recent years, attempts have been made

to correct for the impact of some of the above assumptions (notably assumptions 2–4) on the accuracy of the derived functions. However, a consistent and unifying approach does not exist. As shown by the results of the SCA survey [18], model errors are also an integral part of the problem formulation.

2.2. Deriving the continuous model equation. We relate $(P_k, \bar{S}_k)$ to the point saturation $S(r)$ through the following analysis. The average saturation of the porous medium from the outlet end to any point in the core is defined as

$$(2.4) \quad \bar{S}(r) = \frac{\int_r^{r_e} S(r) dr}{\int_r^{r_e} dr} = \frac{1}{r_e - r} \int_r^{r_e} S(r) dr.$$

To simplify expressions, we substitute $x = P_c(r_i, \omega)$, $t = P_c(r, \omega)$, and $f = r_i/r_e$. Combining (2.1) and (2.4), and performing a change of variables, we arrive at

$$(2.5) \quad \int_0^x K(x, t) S(t) dt = \bar{S}(x),$$

where

$$(2.6) \quad K(x, t) = [(1 + f)/2] \left[1/\sqrt{x(x - tf_2)} \right], \\ f_2 = 1 - f^2, \quad 0 \leq f \leq 1, \quad 0 \leq x \leq T.$$

Equation (2.5) relates the point saturation along the length of the core, the average saturation in the core, and the capillary pressure at the inlet. This is the Hassler–Brunner (H&B) equation. It is a Volterra integral equation of the first kind with an exactly known kernel $(K(x, t))$ and a right-hand side represented by experimental data. The kernel contains geometrical information about the experimental setup. In (2.5) above, T is the maximum experimental value of x .

Even though $\bar{S}(x)$ has been obtained in the form of discrete data, the sought function $S(t)$ is assumed to be continuous. Solving (2.5) involves inverting a linear smoothing operator. However, this operator has no bounded inverse, and the inversion is unstable. The problem fails to satisfy Hadamard’s condition for the well-posedness of a problem [22]. It is therefore an inverse and ill-posed problem.

3. Deriving the system of linear equations. We can express $\bar{S} = \bar{S}^{tr} + \epsilon$, where $\bar{S}^{tr}$ represents the true functional value, and ϵ is the (unobserved) error in the data $\bar{S} = \{\bar{S}(x_j)\}_{j=1}^n$. The functions S and $\bar{S}$ are assumed to be continuous and differentiable functions of x ; see [3], [4], [12], [33], and [43].

Suppose we select m basis functions $N_1, \dots, N_m$ and approximate the sought solution $S(t)$ by $\tilde{S}(t)$; then we can write

$$(3.1) \quad \sum_{j=1}^m c_j N_j(t) \approx S(t),$$

where the coefficients c_j are determined from the relation

$$(3.2) \quad \sum_{j=1}^m c_j \beta_j(x) = \bar{S}(x),$$

and β_j is an integral over the basis functions, i.e.,

$$(3.3) \quad \int_0^x K(x, t) N_j(t) dt = \beta_j(x).$$

We follow the same approach as in [27] and [43] and choose quadratic spline basis functions in our parameterization. Each of the basis functions can be expressed as a quadratic polynomial

$$(3.4) \quad N_j(t) = a_{l,j}t^2 + b_{l,j}t + c_{l,j},$$

where $a_{l,j}$, $b_{l,j}$, and $c_{l,j}$ are all constants, and l denotes the internodal interval for which the constants apply to spline number j . The parameterization reduces the continuous integral problem to a system of linear equations of the form

$$(3.5) \quad A\mathbf{c} = \mathbf{b},$$

where

$$(3.6) \quad A_{i,j} = \beta_j(x_i),$$

$$(3.7) \quad \mathbf{b}_i = \bar{S}(x_i),$$

$$(3.8) \quad \mathbf{c}_j = c_j.$$

To evaluate the elements of A in (3.5), we need the integrals

$$(3.9) \quad M(r, a, b) = \int_a^b K(x, t) t^r dt, \quad 0 \leq a \leq b \leq x \leq T.$$

In the case $r = 0$, we derive

$$(3.10) \quad M(0, a, b) = [(1 + f)(b - a)] / [\sqrt{x}(\sqrt{x - af_2} + \sqrt{x - bf_2})].$$

When r is a positive integer, we make a change of variables

$$(3.11) \quad t = (x^2 - u) / xf_2$$

and arrive at

$$(3.12) \quad M(r, a, b) = [(1 + f)/(xf_2)^{r+1}] \int_{x^2 - xbf_2}^{x^2 - xaf_2} (x^2 - u)^r / \sqrt{u} du.$$

Expanding the last factor of the integrand in powers of u , we derive

$$(3.13) \quad \begin{aligned} M(r, a, b) &= [(1 + f)/(xf_2)^{r+1}] \int_{x^2 - xbf_2}^{x^2 - xaf_2} \sum_{k=0}^r \binom{r}{k} (-1)^k x^{2r-2k} u^{k-1/2} du \\ &= [(1 + f)/(xf_2)^{r+1}] \sum_{k=0}^r \binom{r}{k} (-1)^k x^{2r-2k} (1/(2k+1)) c_k, \end{aligned}$$

$$(3.14) \quad c_k = \int_{x^2 - xbf_2}^{x^2 - xaf_2} u^{k-1/2} du.$$

Equation (3.14) can be evaluated exactly and is stable if the difference $a - b$ is relatively large. However, we can derive an exact expression for it, which is stable

when a and b are close to each other and the difference $(b - a)$ is known with relatively good accuracy. We find

$$\begin{aligned}
 (k + 1/2)c_k &= (x^2 - axf_2)^{k+1/2} - (x^2 - bxf_2)^{k+1/2} \\
 &= [(x^2 - axf_2)^{2k+1} - (x^2 - bxf_2)^{2k+1}] / [(x^2 - axf_2)^{k+1/2} + (x^2 - bxf_2)^{k+1/2}] \\
 &= [(b - a)xf_2] / [(x^2 - axf_2)^{k+1/2} + (x^2 - bxf_2)^{k+1/2}] \sum_{j=0}^{2k} (x^2 - axf_2)^{2k-j} (x^2 - bxf_2)^j.
 \end{aligned}
 \tag{3.15}$$

The ill-posedness of the continuous problem in equation (2.5) translates into the ill-conditioning of the matrix A in (3.5). Hence A is not directly invertible; see [43] for a detailed discussion. The solution of the system of equations will therefore depend very much on the condition of A . The condition number of A , however, depends on the experimental data and on the degree of parameterization of the capillary pressure function; see [43].

The classical approach to solving (3.5) involves finding a single solution which solves

$$\min_{\mathbf{c} \in \mathcal{R}^m} \|\mathbf{A}\mathbf{c} - \mathbf{b}\|_\ell
 \tag{3.16}$$

in an ℓ -norm (usually $\ell = 2$). This usually involves the use of gradient-type optimization algorithms. In this paper, our approach is to determine a family of solutions.

We argue that since the sought capillary pressure function is nonunique, a reasonable approach is to generate multiple capillary pressure functions, which possess the property of being able to reproduce the experimental data by forward modeling. Generating multiple capillary pressure functions involves solving for all possible values of the vector $\mathbf{c}$, which satisfy the model equation $\mathbf{A}\mathbf{c} \approx \mathbf{b}$. We recall that $\mathbf{b}$ represents the vector of observed (experimental) data. Mathematically, we seek to find a set $\mathcal{C}$ consisting of an ensemble of solutions and defined by (3.17) below.

$$\mathcal{C} = \{\mathbf{C} \mid \forall \mathbf{c} \in \mathbf{C}, \mathbf{A}\mathbf{c} \approx \mathbf{b}\}.
 \tag{3.17}$$

This ensemble of solutions can then be used to generate an uncertainty envelope for the sought capillary pressure function. The accuracy of a particular capillary pressure function can then be judged on the basis of whether it lies within the generated uncertainty envelope. We measure the closeness of $\mathbf{A}\mathbf{c}$ to $\mathbf{b}$ in ℓ_2 -norm, and we employ a stochastic algorithm in deriving the family of solutions.

3.1. Checking the degree of parameterization. As mentioned above, the fact that the integral operator does not have a bounded inverse means that the condition numbers of its finite-dimensional approximations grow with the quality of approximation. That is, the ill-posedness of the continuous integral problem translates into the ill-conditioning of the system of equations $\mathbf{A}\mathbf{c} = \mathbf{b}$. Thus for an extremely high degree of parameterization, where the discrete problem highly approximates the continuous problem, the condition of A will be expected to be poor. Our approach is to simply project the problem unto a low-dimensional space ($n \geq m$) and ensure that for the chosen degree of parameterization, a square integrable solution exists. The analysis follows.

If $A \in \mathcal{R}^{n \times m}$ such that $n \geq m$, then the SVD (singular value decomposition) of A is a decomposition of the form

$$(3.18) \quad A = W \Sigma V^T = \sum_{i=1}^n \mathbf{w}_i \sigma_i \mathbf{v}_i^T,$$

where W and V are unitary matrices, and $\Sigma = \text{diag}(\sigma_1, \sigma_2, \dots, \sigma_m)$ is such that the singular values of A , $\{\sigma_r\}_{r=1}^m$, satisfy $\sigma_1 \geq \sigma_2 \cdots \sigma_m \geq 0$. By substituting the SVD expression into $A\mathbf{c} = \mathbf{b}$, we obtain

$$(3.19) \quad A\mathbf{c} = \sum_{i=1}^n \mathbf{w}_i \sigma_i (\mathbf{v}_i^T \mathbf{c}).$$

$\mathbf{b}$ can be resolved along the n left singular vectors, i.e., $\mathbf{b} = \sum b_i w_i$. Thus we obtain

$$(3.20) \quad \|\mathbf{b} - A\mathbf{c}\|^2 = \sum_{i=1}^m (b_i - \sigma_i c_i)^2 + \sum_{i=m+1}^n b_i^2,$$

where the last equation employs the orthonormality of the vectors w_k and the Pythagorean theorem. To minimize $\|\mathbf{b} - A\mathbf{c}\|^2$, we can adjust c_i such that its optimal value $\hat{c}_i$ satisfies $\hat{c}_i = b_i/\sigma_i$, $i = 1, \dots, m$. Hence we obtain

$$(3.21) \quad \hat{\mathbf{c}} = \sum_{i=1}^m (b_i/\sigma_i) \mathbf{v}_i = \sum_{i=1}^m (\mathbf{w}_i^T \mathbf{b}/\sigma_i) \mathbf{v}_i.$$

The immediate and obvious consequence of (3.21) is that for a square integrable solution of the original integral equation to exist, the value of $\Psi = |\mathbf{w}_i^T \mathbf{b}|$ must on average decay to zero faster than the σ_i . This is referred to as the discrete Picard condition [23]. Our approach has been to arbitrarily choose a degree of parameterization, i.e., m , and check that the discrete Picard condition is satisfied. This could be viewed as a means of preregularization of the problem. Issues of determining an optimal degree of parameterization will not be addressed in this paper.

3.2. Introducing solution space constraints. Solving (3.5) in the classical sense results in oscillatory, nonphysical solutions; see [43] and [30]. A restriction on the solution space is therefore required in order to generate physically plausible solutions. For this particular problem, it is known from the physics of the problem that the sought function is monotonically decreasing function of x ; see [3], [12], and [33]. Hence we can restrict the solution space by imposing monotonicity constraints on the solutions. Using quadratic splines, a sufficient and necessary condition for monotonicity [40] is an ordering of the spline coefficients according to

$$(3.22) \quad 1 \geq c_1 \geq c_2 \geq c_3 \geq \cdots \geq c_m \geq 0.$$

We can incorporate this information into a sampling procedure in the following way. We first sample $c_1 \sim [0 \ 1]$. Next, we introduce a set of parameters λ_i and sample $\lambda_i \sim [0 \ 1]$. Then if we write

$$(3.23) \quad c_j = c_1 \prod_{i=2}^j \lambda_{i-1}, \quad 2 \leq j \leq m,$$

we obtain c 's which satisfy (3.22).

It has been established (see [43] and [44]) that acceptable solutions from $\mathcal{C}$ should be convex functions. Hence we impose convexity constraints to eliminate conceivable yet nonphysical solutions. From (3.4), we derive convexity constraints in the following way:

$$(3.24) \quad [N_j(t)]_{tt} = 2a_{l,j}.$$

Our second derivative matrix then takes the form

$$L_{l,j} = \begin{cases} 2a_{l,j}, & j = l(1)l + 2, \\ 0 & \text{otherwise.} \end{cases}$$

Define $\mathbf{0}$ as the null vector; then convexity of the solution requires that

$$(3.25) \quad L\mathbf{c} \geq \mathbf{0}.$$

We use the Neighborhood Approximation (NA) algorithm, which is a stochastic algorithm, to generate the family of solutions.

4. The NA algorithm. The NA algorithm is a stochastic algorithm which was originally developed by Sambridge [37], [38] for solving a nonlinear inverse problem in seismology. The algorithm first identifies regions in the parameter space which give good match to the observed or measured data. It then preferentially samples the parameter space in a guided way and generates new models in the good-fit regions. It uses Voronoi cells to represent the parameter space.

4.1. Voronoi cells and the neighborhood algorithm. We begin with an introductory discussion on Voronoi cells; see [2] and [32].

DEFINITION 4.1. Let ψ denote a set of n points in the plane. For two distinct points $y_1, y_2 \in \psi$, the dominance of y_1 over y_2 , $\text{dom}(y_1, y_2)$, is defined as

$$(4.1) \quad \text{dom}(y_1, y_2) = \{y \in R^2 \mid \delta(y, y_1) \leq \delta(y, y_2)\}$$

for δ denoting the Euclidean distance function.

From Definition 4.1 above, $\text{dom}(y_1, y_2)$ is a closed half plane bounded by the perpendicular bisector (*separator*) of y_1 and y_2 .

DEFINITION 4.2. The region of a point $y_1 \in \psi$ is the portion of the plane lying in all of the dominances of y_1 over the remaining points in ψ , i.e.,

$$(4.2) \quad \text{reg}(y_1) = \bigcap_{y_2 \in \psi - \{y_1\}} \text{dom}(y_1, y_2).$$

The regions are thus convex polygons constructed from $n - 1$ half planes. Each point on an edge of a region is equidistant from exactly two points, and each vertex is equidistant from at least three. Thus the regions are joined edge to edge and vertex to vertex, i.e., a polygonal partition of the plane. This partition is called the *Voronoi diagram*, $V(\psi)$, of the finite point-set ψ . Figure 4.1 shows an update of Voronoi cells in two dimensions for 100, 200, and 300 points in the plane. The figure shows some of the properties of the Voronoi cells; e.g., the sizes (area) of the cells are proportional to the density of the points in that region, and the cells are nonoverlapping. Specifically, observe the development of region $ABCD$ in Figure 4.1 as more cells are added to the Voronoi diagram. Each Voronoi polygon can be regarded as a closed set where each cell is simply the nearest neighbor region about the generator point.

FIG. 4.1. Updating Voronoi diagram in two dimensions.

FIG. 4.2. NA Gibbs sampler.

This NA property of Voronoi diagrams provides a simple way of performing non-smooth interpolation of an irregular distribution of points in multidimensional space. Thus if one represents sought model parameters by a Voronoi diagram, the problem of generating multiple model realizations translates into one of sampling a multidimensional parameter space defined by the Voronoi cells. By exploiting the interpolatory properties of Voronoi cells, new models can be generated and concentrated in specific regions of parameter space, using a prescribed rule. This is the principle behind the neighborhood sampling algorithm [38]; see also [37] for a more general discussion.

The NA algorithm generates multiple models iteratively in parameter space in the following way. First, an initial set of n_s models is randomly generated. In the second step, the n_r best models among the most recently generated n_s models are determined. The n_r models are chosen on the basis of how well their forward solutions match the measured data by defining a misfit function, which we discuss shortly. Finally, new n_s models are generated by uniform random walk in the Voronoi cell of each of the n_r chosen models. Thus at each iteration, n_r cells are resampled, and in each Voronoi cell, n_s/n_r models are generated. The ratio n_s/n_r controls the performance of the algorithm.

Generating new n_s/n_r cells within a Voronoi cell is accomplished by a Gibbs sampler [20]. Figure 4.2 shows a two-dimensional example. To generate a new model in cell A, we set the conditional probability density function outside Voronoi cell A to be zero. A new x -axis component, x_{aa} , is obtained by a uniform random perturbation from point x_a . This perturbation is restricted to (x_1, x_2) . From (x_{aa}, y_a) , we generate a new y -axis component by a uniform random perturbation, restricted to (y_1, y_2) , to

arrive at (x_{aa}, y_{aa}) . This approach extends directly to multidimensional space. For a chosen model, at each step the i th component of the model parameter is replaced with a uniform random perturbation restricted to the boundaries of the Voronoi cell representing the model. This can be viewed as a series of one-dimensional updates. Thus for an m -dimensional space problem, one generates m random walks, one per axis, resulting in an m -dimensional convex polygon. See [38] for details.

The philosophy behind the algorithm is that the misfit of each of the previous models is representative of the region of its neighborhood, defined by its Voronoi cell. Therefore at each iteration, new samples are concentrated in the neighborhoods surrounding the better data-fitting models [38]. Thus the algorithm exploits information obtained in all previous models to selectively sample parameter space regions which give better fit to the observed data. This approach also overcomes one of the principal weaknesses of stochastic algorithms, namely, slow convergence.

4.2. Quantifying model misfit. In the least square sense, the measure of misfit, Γ , is given by (4.3). We are assuming uncorrelated white noise, and hence the covariance matrix C is defined by (4.4).

$$(4.3) \quad \Gamma = \langle \Delta \bar{\mathbf{S}} | C^{-1} | \Delta \bar{\mathbf{S}} \rangle,$$

$$(4.4) \quad C_{i,j}^{-1} = \delta_{ij} / \chi^2,$$

where χ is the standard deviation, and δ_{ij} is the Kronecker-delta function. $\Delta \bar{\mathbf{S}}$ is the difference between the measured $\bar{\mathbf{S}}^{meas}$ and the model $\bar{\mathbf{S}}^{model}$, values of $\bar{\mathbf{S}}$, i.e.,

$$(4.5) \quad \Delta \bar{\mathbf{S}} = \bar{\mathbf{S}}^{model} - \bar{\mathbf{S}}^{meas}.$$

For each of the models M_j generated, the degree of likelihood, p , that the observed data $\mathcal{O}$ is obtainable given the model is defined as

$$(4.6) \quad p(\mathcal{O} | M_j) \sim e^{-0.5\Gamma}.$$

The refinement criterion for the NA sampling algorithm is based on the rank of the misfit. The misfit ζ is defined as $-\log$ of the likelihood. Thus

$$(4.7) \quad \zeta = -\log p(\mathcal{O} | M_j) = -0.5\Gamma.$$

4.3. Bayes theorem. Given a model, M , in model space, we express our prior knowledge about this model in a probabilistic framework by defining a prior probability density function $p(M)$. In the absence of any prior information about the individual models, the use of a noninformative or uniform prior is a justifiable paradigm [41] since there is no basis for prioritizing one model over the other.

A comparison of the model output with the measured data creates a basis for the modification of our prior beliefs. This comparison allows for the quantification of the likelihood that the observed data is explainable by the model for which the likelihood $p(\mathcal{O} | M)$ holds. Bayes theorem allows an update of prior beliefs by calculating a posterior probability, $p(M | \mathcal{O})$, using the likelihood. This posterior function is defined by

$$(4.8) \quad p(M | \mathcal{O}) = p(\mathcal{O} | M)p(M) / \int p(M | \mathcal{O})p(M)dM.$$

One of the challenges in applying the Bayes theorem lies in evaluating the normalizing term $\int p(M | \mathcal{O})p(M)dM$. Even for problems of very low dimension, the solution

FIG. 4.3. The NA-Bayes Gibbs sampler.

is nontrivial. Markov chain Monte Carlo (MCMC) methods [21] provide a means of evaluating the posterior probability distribution, which involves calculating ratio of probabilities. The attraction with this approach is that it eliminates the need to calculate the normalizing constant. The NA algorithm, used in a Bayesian framework, uses an MCMC algorithm to generate new models in model space whose distribution approximates that of the input ensemble. We present a brief analysis of the NA algorithm in a Bayesian framework. Refer to [39] for details.

4.4. NA-Bayes algorithm. By sampling from the posterior distribution, one aims at reconstructing the posterior probability density (PPD) from a finite ensemble of models. Thus using the finite number of models, the aim is to generate a new ensemble of models whose distribution asymptotically tends to the distribution of the original ensemble. This is effectively an interpolation problem in multidimensional space. The computation becomes unwieldy for higher than two dimensions [39]. The NA-Bayes approach is to use Voronoi cells in constructing the multidimensional interpolant. The principle is to replace the true posterior probability density function with its neighborhood approximation. Specifically,

$$(4.9) \quad p(M) \approx p_{NA}(M),$$

where $p_{NA}(M)$ is the Neighborhood Approximation of the posterior probability distribution $p(M)$ for model M . This is at the heart of the algorithm.

The attraction with this approach is that the scale lengths of variation in the interpolated (misfit) surface are directly tied to the spacing of the samples in the ensemble. Further, since by construction $p_{NA}(M)$ has a uniform probability inside each cell, the influence of each model is spread uniformly across each cell, rather than concentrated at a point.

To resample from the posterior distribution, the NA-Bayes algorithm uses a Gibbs sampler [20], [39]. Figure 4.3 shows a two-dimensional schematic diagram of the resampling process. The algorithm for generating new models can be summarized as follows. From model $M(x_a, y_a)$, in cell A, we start a random walk along the x -axis. From x_a , we propose a new position $x_i^p = x_{aa}$, generated from a uniform random deviate, and constrained to lie between the endpoints of the parameter axis. We note

that these endpoints are defined by the range within which we sample. Next, we draw a second deviate r on the unit interval $(0, 1)$ and make a decision to either accept or reject x_i^p according to

$$\begin{cases} r \leq p_{NA}(x_i^p|x_{-i})/p_{NA}(x_i^{max}|x_{-i}), & \text{accept,} \\ \text{otherwise,} & \text{reject.} \end{cases}$$

x_{-i} denotes the fixed value of the other component of the model M , i.e., y_a . We define $p_{NA}(x_i^p|x_{-i})$ as the conditional probability density function of $p_{NA}(M)$ along the x -axis, and $p_{NA}(x_i^{max}|x_{-i})$ is the maximum value of the conditional along the same axis. At each step, one element of M is updated, and the iteration is complete when both dimensions have been cycled through once and a complete new model is generated [39]. We recall that using the neighborhood approximation property of the Voronoi cells, p_{NA} is constant within each cell. Hence generating the conditionals $p_{NA}(M)$ amounts to the task of finding the intercept of the x -axis with the cells' boundaries, i.e., x_1 , x_2 , and x_3 . Note that the random walk can enter any of the Voronoi cells, and the probability of this occurring is determined by the product of the posterior probability density and the width of the intersection of the axis with the cell.

This approach is extendable to multidimensional space, and the theory is that after several iterations, the random walk will produce model space samples whose distribution asymptotically tends towards the target distribution [39] and [19].

5. Model parameter uncertainties. A property of interest derivable from the posterior probability distribution is the uncertainty in the individual model parameters, i.e., the one-dimensional probability distribution P_{1D} . The one-dimensional marginal of a parameter c_i is defined as the integral of the posterior probability over the remaining dimensions of the parameter space [39], i.e.,

$$(5.1) \quad P_{1D}(c_i) = \int \cdots \int p(M) \prod_{\substack{k=1 \\ k \neq i}}^m dc_k.$$

Equation (5.1) provides information about the uncertainty of a single parameter with all possible variations of the other parameters taken into account. The NA-Bayesian algorithm uses a multidimensional Monte Carlo integration over the model space to obtain an estimate for (5.1). The algorithm uses the approximation in (4.9) to evaluate the Bayesian integrals in (5.1). This involves generating a new set of Monte Carlo integration points. These new points are then used to evaluate the Bayesian integrals. See [39] for a detailed description and mathematical analysis.

5.1. Uncertainty propagation: Oil/water capillary pressure functions.

The analysis above generates water/gas capillary pressure functions. However, for petroleum reservoirs, the phases of interest are oil and water. The normal practice is therefore to convert the derived water/gas capillary functions to oil/water curves, which are then used in petroleum reservoir simulation. The conversion to an oil/water capillary pressure curve is as follows (see [1]). First, we denote the contact angle between air and water and between oil and water, respectively, by σ_{wg} , and σ_{ow} .

The oil/water capillary pressure x^{ow} is then a scalar multiple of the water/gas capillary pressure x^{wg} , and given by (see [1] and [6])

$$(5.2) \quad x^{ow} = \sigma_{ow} \cdot x^{wg} / \sigma_{wg}.$$

The contact angles σ_{wg} and σ_{ow} are theoretically known to be temperature dependent. In general, petroleum reservoir processes are nonisothermal. However, the uncertainties in the values of the contact angles are negligible compared to the overall uncertainties in the capillary pressure values.

6. Validation.

6.1. The centrifuge data. We chose a true (analytical) function $S \equiv S(x, \tau, S_c, \theta)$, where τ , S_c , and θ are fixed model parameters. S is explicitly defined by

$$S(x) = \begin{cases} (x/\tau)^{-\theta}(1 - S_c) + S_c, & x > \tau, \\ 1, & x \leq \tau. \end{cases}$$

We then substituted S into (2.5) and solved for the right-hand side, $\bar{S}$. A typical centrifuge experiment gives a maximum of 15 experimental pairs of data. Hence we chose 15 discrete points x_j and generated a set of data $\bar{S}(x_j)$. “White noise” was then added to the generated data in order to create experimental data, according to the expressions

$$(x_j^{meas}, \bar{S}_j^{meas}) \equiv \left\{ (x_j^{tr}(1 + \epsilon_{x,j}), \bar{S}_j^{tr}(1 + \epsilon_{\bar{S},j})), \quad j = 1, \dots, 15. \right\}.$$

$\epsilon_{x,j}$ and $\epsilon_{\bar{S},j}$ are drawn from normal distributions with zero mean and unit standard deviation, and the superscripts *tr* and *meas* refer to true and measured values, respectively. We note that this testing approach is particularly attractive in the method verification phase, as our estimation results can be compared with the true (analytical) function.

This paper presents results using the above definition of S for the true function. Table 6.1 below lists the parameters used.

TABLE 6.1
Model parameters.

τ	S_c	θ	$\epsilon_{\bar{S},j}$	$\epsilon_{x,j}$	f	T	σ_{wg}	σ_{ow}
0.05	0.20	1.00	0.00	0.02	0.79	1.5	0.070	0.022

6.2. Reservoir simulation model. The original fine grid is a geostatistical model. It is represented in a three-dimensional domain $[(x, y), z] \in \mathcal{R}^2 \times \mathcal{R}$, being $[1200 \times 2200 \times 170]$ feet³, and discretized into $[60 \times 220 \times 85]$ cells. The model consists of two distinct geological formations. The top 70 feet (35 layers) represents the Tarbert formation, and the bottom 100 feet (50 layers) represents the Upper Ness. The model, which consists of part of a Brent geological sequence, was originally generated for use in the PUNQ project [14]. For a full description of the model as well as details of the fluid properties, see [11].

We generated a coarser grid model consisting of $5 \times 11 \times 10$ grid cells, using single phase upscaling of the fine grid [10]. There are 4 producers in the four corners of the model ($P1 - P4$) and a central injector (I1). All wells are vertical and penetrate up to the eighth layer of the vertical column.

Figure 6.1(a) shows the top layer of the coarse grid and the position of the wells, while Figure 6.1(b) shows an x - z plane of the model. The z plane in Figure 6.1(b) is exaggerated by a factor of 5.

 FIG. 6.1. *Simulation model.*

7. Results and discussions. By sampling a five-dimensional parameter space defined by Voronoi cells, we generated 600 models, which give monotonic capillary pressure functions. This requirement is based on the physics of the problem. Figure 7.1(a) shows all the models, with the true solution in red. However, we imposed an extra constraint by requiring that the acceptable capillary pressure curves be both monotone and convex. Figure 7.1(b) shows the result of imposing both monotonic and convexity constraints on the solution, which resulted in the rejection of 97 of the 600 models.

Figure 7.1(c) shows a plot of all the model misfits (o) and models satisfying both monotonicity and convexity constraints (+). The plot shows how the algorithm evolves to better fit regions in the parameter space. We also observe that in practice, it suffices with about 500 models. We observe that a large number of our rejected models belong to the high misfit region of the model space. The model with the least misfit, i.e., the maximum likelihood (ML) model derivation of the sought function is, plotted in Figure 7.1(d). The true analytical function has been plotted on the same graph, and we observe that the maximum likelihood model is highly accurate in deriving the true solution.

One of the criteria for judging the accuracy of derived functions using gradient-type algorithms is to compare the solution $\mathbf{b}_{opt}$ of the forward problem $\mathbf{b}_{opt} = \mathbf{A}\mathbf{c}_{opt}$ with the original “experimental data,” i.e., $\mathbf{b}$. Here $\mathbf{c}_{opt}$ is the optimized model parameters.

Figure 7.1(e) shows such a plot for our maximum likelihood model and the original experimental data. It should be noted that all the acceptable models are able to reproduce the input data to some acceptable tolerance. Hence on the basis of this criterion, there is no cause for rejecting any of these models, even though we observe some degree of variability in the derived functions. The issue therefore is how to account for this variability in the solution.

We contend that since the observed data is uncertain, the problem is statistical. Hence our approach to the inverse problem has been first to ensure that we generate a family of functions, which are representative of the distribution of the solution. Next, we use this family to define an uncertainty envelope for the solution. This is

FIG. 7.1. *Sampling results.*

a different focus compared to the quest of finding accurate algorithms, which at best gives one of several solutions, without a guarantee of accuracy, because the truth is unknown.

Our approach to defining an uncertainty envelope involved running several long chains of the MCMC algorithm on the misfit surface and performing a Bayes update

of the probabilities. We monitored the frequency of visits to each Voronoi cell during the random walk. Thus we were able to calculate the relative probability p_j of each model M_j in an ensemble of size n_m , based on the frequency λ_j , using

$$(7.1) \quad p_j = \lambda_j / \sum_{k=1}^{n_m} \lambda_k.$$

Assuming Gaussian statistics, we calculated the first and second moments of the sought function from

$$(7.2) \quad \langle u(x) \rangle_1 = \sum_k p_j u_k(x),$$

$$(7.3) \quad \langle u(x) \rangle_2 = \sum_k p_j u_k^2(x) - [\langle u(x) \rangle_1]^2.$$

Using these parameters, we calculated the 10th and 90th percentiles, P_{10} and P_{90} , respectively, of $S(x)$.

Figure 7.1(f) shows plots of the P_{10} and P_{90} profiles, together with the true analytical solution, the maximum likelihood function (ML), and the mean solution. We observe that the error bounds predicted by the algorithm rightly envelope both the true analytical and the maximum likelihood solutions.

Figures 7.2(a)–7.2(e) show the one-dimensional probability marginals for parameters 1–5, i.e., the spline coefficients. These were generated by several long chains of the MCMC random walks, a total of 5×10^5 steps. The one-dimensional marginals are projections of the multidimensional distribution onto two-dimensional space. The values in the brackets indicate the maximum likelihood model values of each parameter. With the exception of the first model parameter c_1 , the parameters exhibit a skewed-normal distribution, with the modal values close to the values for the maximum likelihood model.

As mentioned earlier, our aim is to transform the problem to a low-dimensional space and ensure that for a chosen degree of parameterization, a square integrable solution of the problem exists. This is achieved by checking that the discrete Picard condition is satisfied. Figure 7.2(f) shows the Picard plot for the model. We realize that from $\kappa = 5$, Ψ appears to decay faster than σ . Hence the discrete Picard condition for the model solutions is satisfied.

Using (5.2), we derived scaled capillary pressure functions for the reservoir model. We generated oil/water capillary functions using the P_{10} , P_{90} maximum likelihood, mean, and the true analytical functions. Thus in total we run five simulation models for a period of 4000 days. The models are identical in all aspects except for the definition of the capillary pressure functions.

For each of the models, the volume of water existing in equilibrium with oil in each pore of the porous media is determined by the capillary forces, defined by the oil/water capillary function. Hence one of the parameters, which are certain to be affected by the uncertainty in our capillary function, is the volume of the fluids in place. For each of the models, therefore, we monitored the total amount of pore volume filled by oil with time. Figure 7.3(a) shows the plot for the projected volume of oil in place, measured in barrels, for all five models. Whereas the maximum likelihood model performance is highly accurate, this plot shows that the uncertainty in the centrifuge data leads to 8.4% overestimation and 15.2% underestimation of the initial oil in place in the reservoir.

FIG. 7.2. One-dimensional marginal probability distribution and Picard results.

Another parameter of interest is a measure of uncertainty in the oil recovery efficiency. Here, oil recovery efficiency E_o is defined as a function of time by

$$(7.4) \quad E_o(t) = (V_o(t=0) - V_o(t)) / (V_o(t=0)),$$

where $V_o(t)$ refers to the volume of oil in the reservoir at time t . Figure 7.3(b) shows

FIG. 7.3. Reservoir simulation results.

the plot for E_o , and we observe a large degree of variability with time in the recovery efficiency. Since this is an oil/water model, the proportion of water present in the reservoir (referred to as the water saturation) is tied in with the amount of oil taken out of the model. Figure 7.3(c) shows a plot of the water saturation with time of the model. The plot shows that our uncertainty envelop rightly encapsulates the truth and the maximum likelihood model behavior.

A balance of forces requires a fall in the average pressure with time of the reservoir, as it is depleted of oil and water. An accurate knowledge of this parameter is imperative in determining a sustainable oil production rate from the reservoir. Figure 7.3(d) shows the uncertainty in the average pressure of the model due to uncertainty in the centrifuge data.

8. Conclusions. We have demonstrated a methodology for generating multiple capillary pressure functions using the NA algorithm. Using the algorithm in a Bayesian framework, we have shown how the uncertainty in oil/water capillary functions can be quantified.

This paper has shown that small-scale uncertainties propagate during scale-up procedures and have an impact on important reservoir parameters such as volume of in situ oil, recovery efficiencies, and average reservoir pressures. We have shown how the uncertainties in these parameters can be quantified.

We have demonstrated our methodology on a two-phase (oil/water) synthetic reservoir model. Our results show that our uncertainty envelopes rightly encapsulate the truth, and that our maximum likelihood model performance is highly accurate.

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