MATHEMATICAL MODELS FOR OIL RESERVOIR SIMULATION

KNUT-ANDREAS LIE AND BRADLEY T. MALLISON

Petroleum resources are found within sedimentary rocks that have a sufficient interconnected void space to store and transmit fluids. The actual flow of liquid and gas phases occurs on a micrometer scale in the void space between rock grains. On the other hand, the hydrocarbon is typically carried in rock zones that are a few tens of meters thick but extend several kilometers in the lateral directions. The rock formations are typically heterogeneous at all length scales in between and phenomena at all length scales can have a profound impact on flow, making flow in subsurface reservoirs a true multiscale problem.

Observing dynamic fluid behavior and measuring the pertinent parameters of a subsurface reservoir is difficult. Predicting reservoir performance therefore has a large degree of uncertainty attached. Simulation studies are usually performed to quantify this uncertainty. Reservoir simulation is the means by which one uses a numerical model of the geological and petrophysical characteristics of a hydrocarbon reservoir to analyze and predict fluid behavior in the reservoir over time. In its basic form, a reservoir simulation model consists of three parts: (i) a geological model in the form of a volumetric grid with cell/face properties that describes the given porous rock formation; (ii) a flow model that describes how fluids flow in a porous medium, typically given as a set of partial differential equations expressing conservation of mass or volumes together with appropriate closure relations; and (iii) a well model that describes the flow in and out of the reservoir, including a model for flow within the well bore and any coupling to flow control devices or surface facilities.

Reservoir simulation is used for two main purposes: (i) to optimize development plans for new fields; and (ii) assist with operational and investment decisions.. In particular, simulation is used in inverse modeling to integrate static and dynamic (production) data. The role and need for simulation depends greatly depend on the geological setting, the production environment (onshore versus offshore), and field maturity.

1. Geological model

The first part of the reservoir model is a mathematical description of the reservoir and its petrophysical properties. Herein, we will focus on macroscale models that rely on a continuum hypothesis and the existence of *representative elementary volumes* (REV), see Figure 1. This concept is based on the idea that petrophysical flow properties are constant on some ranges of scale, and REVs, if they exist, mark transitions between scales of heterogeneity, and present natural length scales for modeling.

Two petrophysical properties are fundamental in all models: the rock *porosity*, ϕ, is a dimensionless quantity that denotes the void volume fraction of the medium available to be filled by fluids. Porosity depends on the fluid pressure if the rock is compressible. The *permeability*, K, is a measure of the rock's ability to transmit a single fluid at certain conditions.
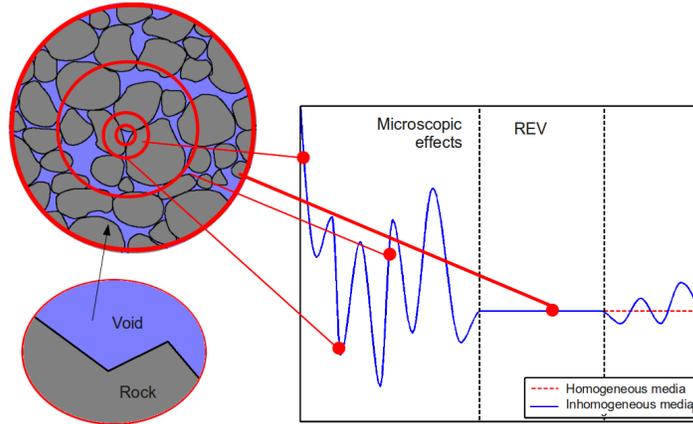
FIGURE 1. A representative elementary volume is the smallest volume over which a measurement can be made and be representative of the whole, here illustrated for porosity.

Although its SI-unit is m^2, permeability is commonly represented in units Darcy[1]. Permeability is often positively and strongly correlated to porosity, but because the orientation and interconnection of pores are essential to flow, it is seldom a direct function of porosity. In general, K is a tensor and we say that the medium is isotropic (as opposed to anisotropic) if K can be represented as a scalar function. Moreover, due to transitions between different rock types, the permeability may vary rapidly over several orders of magnitude, local variations in the range 1 mD to 10 D are not unusual in a typical field.

This description of a reservoir and its petrophysical parameters is usually developed through a complex workflow that involves a multitude of data sources that span a large variety of spatial (and temporal) scales, from knowledge of the geologic history of the surrounding basin, via seismic and electromagnetic surveys and study of geological analogues (rock outcrops), to rock samples extracted from exploration and production wells. All this information is accumulated and presented as input to the reservoir simulation in the form of a geo-cellular model (volumetric grid) that describes the geometry of the reservoir rock. Each grid cell is assumed to be an REV and provides the petrophysical properties that are needed as input to the simulation model, primarily porosity and permeability. Hence, the grid is closely attached to the parameter description and cannot be easily adjusted to provide a certain numerical accuracy as it can in many other fluid dynamics applications.

Although rectilinear and curvilinear grids are sometimes used for reservoir simulation, they are seldom sufficient to accurately describe the volumetric structures of a reservoir. Instead, the industry standard is to use so-called stratigraphic grids that are designed to reflect that reservoirs are usually formed through deposition of sediments and consist of stacks of sedimentary beds with different mixtures of solid particles of varying sizes that extend in the lateral direction. Because of differences in deposition and compaction, the thickness and inclination of each bed will vary in the lateral directions. Parts of the beds may have been weathered down or completely eroded away, and the layered structure of the beds may have been disrupted due to geological activity, introducing fractures and faults. For the purpose

---

[1]The precise definition of 1 Darcy ($\approx 0.987 \cdot 10^{-12}$ m^2) involves transmission of a fluid with viscosity 1 cp through a homogeneous rock at a speed of 1 cm/s by a pressure gradient of 1 atm/cm.

Volumetric extrusion of areal Voronoi grid.

Eroded sedimentary layers in a bed model.

A corner-point reservoir model.

Cross-section of corner-point grid with five faults.
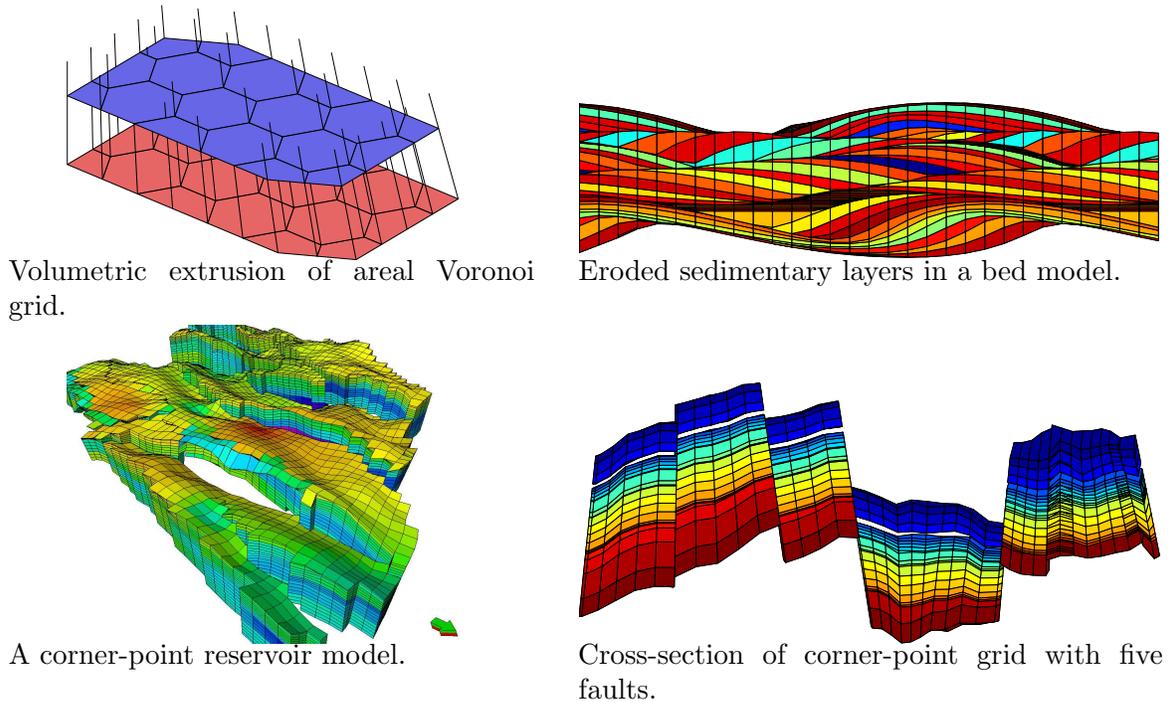
FIGURE 2. Examples of stratigraphic grids.

of reservoir simulation, fractures can be considered as cracks or breakage in the rock, across which the layers in the rock have not been displaced. Faults are fractures with displacement.

A stratigraphic grid can be built by extruding 2D tessellations of geological layers in the vertical direction or along inclined lines that follow major fault surfaces. The most popular format, so-called corner-point grids, consists of a set of hexahedral cells that align so that the cells can be numbered using a logical ijk index. Each cell has eight logical corner points that are specified as pairs of depth-coordinates defined on four straight or curved pillars. One or more corner-points may coincide, giving degenerate cells, and cells that are logical neighbors need not have matching faces, which gives rise to unstructured connections. Increased areal flexibility is obtained using PEBI grids, which are based upon extrusion of areal Voronoi grids. Stratigraphic grids will usually have high aspect ratios and geometries that deviate far from regular hexahedra; this poses challenges for both discretization methods and (non)linear solvers. Further challenges are encountered as fully unstructured grids are becoming more popular.

2. FLOW MODELS

The second part of a reservoir model is a mathematical model that describes the fluid flow. In the following, we will describe the most common models for isothermal flow. For brevity, we do not discuss thermal and coupled geomechanical-fluid models even though these are sometimes necessary to represent first-order effects.

Single-phase flow. The flow of a single fluid with density ρ through a porous medium is described using the fundamental property of conservation of mass:

$$\frac{\partial(\rho\phi)}{\partial t} + \nabla \cdot (\rho\vec{v}) = q. \tag{1}$$

Here, $\vec{v}$ is the superficial velocity and q denotes a fluid source/sink term used to model wells. The velocity is related to the fluid pressure p through an empirical relation named after the french engineer Henri Darcy:

$$\vec{v} = -\frac{K}{\mu}\left(\nabla p - \rho\vec{g}\right), \tag{2}$$

where K is the permeability, μ the fluid viscosity, and $\vec{g}$ the gravity vector. Introducing rock and fluid compressibilities, $c_r = \phi^{-1}d\phi/dp$ and $c_f = \rho^{-1}d\rho/dp$, (1) and (2) can be combined to a parabolic equation for the fluid pressure

$$\phi\rho\left(c_r + c_f\right)\frac{\partial p}{\partial t} - \nabla \cdot \left(\rho\frac{K}{\mu}\left(\nabla p - \rho\vec{g}\right)\right) = q. \tag{3}$$

In the special case of incompressible rock and fluid, (3) simplifies to a Poisson equation with variable coefficients, $-\nabla \cdot (K\nabla\Phi) = q\mu/\rho$, for the fluid potential $\Phi = p - \rho|\vec{g}|z$.

Two-phase flow. The void space in a reservoir will generally be filled by both hydrocarbons and (salt) water. In addition, water is frequently injected to improve hydrocarbon recovery. If the fluids are immiscible[2] and separated by a sharp interface, they are referred to as phases. A two-phase system is commonly divided into a wetting and a non-wetting phase, given by the contact angle between the solid surface and the fluid-fluid interface on the microscale (acute angle implies wetting phase). On the macroscale, the fluids are assumed to be present at the same location, and the volume fraction occupied by each phase is called the *saturation* of that phase; for a two-phase system the saturation of the wetting and non-wetting phases therefore sum to unity, $S_n + S_w = 1$.

In the absence of phase transitions, the saturations change when one phase displaces the other. During the displacement, the ability of one phase to move is affected by the interaction with the other phase at the pore scale. In the macroscopic model, this effect is represented by the relative permeability $k_{r\alpha}$ $(\alpha = w, n)$, which is a dimensionless scaling factor that depends on the saturation and modifies the absolute permeability to account for the rock's reduced ability to transmit each fluid in the presence of the other. The multiphase extension of Darcy's law reads

$$\vec{v}_\alpha = -\frac{Kk_{r\alpha}}{\mu_\alpha}\left(\nabla p_\alpha - \rho_\alpha\vec{g}\right), \tag{4}$$

which together with the mass conservation of each phase

$$\frac{\partial(\rho_\alpha S_\alpha \phi)}{\partial t} + \nabla \cdot (\rho_\alpha\vec{v}_\alpha) = q_\alpha \tag{5}$$

forms the basic equations. Because of interfacial tension, the pressure in the two phases will differ. The pressure difference is called capillary pressure $p_{cnw} = p_n - p_w$ and is usually assumed to be a function of saturation on macroscale.

---

[2]A phase is a physically distinctive form of solid, liquid, or gaseous states of ordinary matter. Two phases are said to be *miscible* if they mix in all proportions to form a homogeneous solution. Conversely, two phases are *immiscible* if they, in some proportion, do not form a solution.

To better reveal the nature of the mathematical model, it is common to reformulate (4) and (5) as a flow equation for fluid pressure and transport equations for saturations. A straightforward manipulation leads to a system for one phase pressure and one saturation in which the capillary pressure appears explicitly. The resulting equations are nonlinear and strongly coupled. To reduce the coupling, one can introduce a global pressure $p = p_n - p_c$, where the complementary pressure contains saturation-dependent terms and is defined as $\nabla p_c = f_w \nabla p_{cnw}$. The dimensionless fractional-flow function $f_w = \lambda_w/(\lambda_w + \lambda_n)$ measures the fraction of the total flow that contains the wetting phase and is defined from the phase mobilities $\lambda_\alpha = k_{r\alpha}/\mu_\alpha$. In the incompressible and immiscible case, (4) and (5) can now be written in the so-called fractional form which consists of an elliptic pressure equation

$$(6) \qquad \nabla \cdot \vec{v} = q, \qquad \vec{v} = -K(\lambda_n + \lambda_w)\nabla p + K(\lambda_w \rho_w + \lambda_n \rho_n)\vec{g},$$

for the pressure and the total velocity $\vec{v} = \vec{v}_n + \vec{v}_w$ and a parabolic saturation equation

$$(7) \qquad \phi \frac{\partial S_w}{\partial t} + \nabla \cdot f_w(S_w)\big[\vec{v} + K\lambda_n(\rho_w - \rho_n)\vec{g} + K\lambda_n \nabla p_{cnw}\big] = \frac{q_w}{\rho_w}$$

for the saturation S_w of the wetting phase. The capillary pressure can often be neglected on a sufficiently large scale, in which case (7) becomes hyperbolic.

To solve the system (6) and (7) numerically, it common to use a sequential solution procedure. First, (6) is solved to determine the pressure and velocity, which are then held fixed while advancing the saturation a time step Δt, and so on.

Multiphase, multicomponent flow. Extending the equations describing two-phase flow to immiscible flow of more than two phases is straightforward mathematically, but defining parameters such as relative permeability becomes more challenging. In addition, each phase will consist of more than one chemical species, which are typically grouped into fluid components. Because fluid components may transfer between phases (and change composition), the basic conservation laws are expressed for each component ℓ

$$(8) \qquad \frac{\partial}{\partial t}\Big(\phi \sum_\alpha c_\alpha^\ell \rho_\alpha S_\alpha\Big) + \nabla \cdot \Big(\sum_\alpha c_\alpha^\ell \rho_\alpha \vec{v}_\alpha\Big) = \sum_\alpha c_\alpha^\ell q_\alpha,$$

Here, c_α^ℓ denotes the mass fraction of component ℓ in phase α, ρ_α is the density of phase α, $\vec{v}_\alpha$ is phase velocity, and q_α is phase source. As above, the velocities are modeled using the multiphase extension of Darcy's law (4). The system consisting of (8) and (4) is just the starting point of modeling and must be further manipulated and supplied with closure relations (PVT models, phase equilibrium conditions, etc) for specific fluid systems. Different choices for closure relationships are appropriate for different reservoirs and different recovery mechanisms and lead to different levels of model complexity.

The black-oil model. The flow model that is used most within reservoir simulation is the black-oil model. The model uses a simple PVT description in which the hydrocarbon chemical species are lumped together to form two components at surface conditions: a heavy hydrocarbon component called "oil" and a light hydrocarbon component called "gas", for which the chemical composition remains constant for all times. At reservoir conditions, the gas component may be partially or completely dissolved in the oil phase, forming one or two phases (liquid and vapor) that do not dissolve in the water phase. In more general models, oil can be dissolved in the gas phase, the hydrocarbon components are allowed to be dissolved in

the water (aqueous) phase, and the water component may be dissolved in the two hydrocarbon phases.

The black-oil model is often formulated as conservation of volumes at standard conditions rather than conservation of component masses [10] by introducing formation volume factors $B_\alpha = V_\alpha/V_{\alpha s}$ (V_α and $V_{\alpha s}$ are volumes occupied by a bulk of component α at reservoir and surface conditions) and a gas solubility factor $R_{so} = V_{gs}/V_{os}$, which is the volume of gas, measured at standard conditions, dissolved at reservoir conditions in a unit of stock-tank oil (at surface conditions). The resulting conservation laws read

$$\frac{\partial}{\partial t}\left(\frac{\phi\rho_s^\alpha}{B_\alpha}S_\ell\right) + \nabla\cdot\left(\frac{\rho_s^\alpha}{B_\alpha}\vec{v}_\ell\right) = q^\alpha, \quad \alpha = o, w$$

(9)

$$\frac{\partial}{\partial t}\left(\frac{\phi\rho_s^g}{B_g}S_g + \frac{\phi R_{so}\rho_s^g}{B_o}S_\ell\right) + \nabla\cdot\left(\frac{\rho_s^g}{B_g}\vec{v}_g + \frac{R_{so}\rho_s^g}{B_o}\vec{v}_\ell\right) = q^g.$$

Commercial simulators typically use a fully implicit discretization to solve the nonlinear system (9). However, there are also several sequential methods that vary in the choice of primary unknowns and the manipulations, linearization, temporal and spatial discretization, and the order in which these operations are applied to derive a set of discrete equations. As an example, the IMPES (implicit pressure, explicit saturation) method starts by a temporal discretization of the balance equations (9) and then eliminates the volume factors to derive a pressure equation that is solved implicitly to obtain pressure and fluxes. These are then used to update the volumes (or saturations) in an explicit time step. Improved stability can be obtained by a sequential implicit method [12] that also treats the saturation equation implicitly.

3. Well models

In its simplest form, a well is a vertical, open hole through which fluid can flow in and out of the reservoir. More advanced wells are cemented and then perforated along specific intervals along a path that may stretch kilometers along the reservoir in the horizontal direction. Production wells are designed to extract hydrocarbons, whereas injection wells can be used for disposal of produced water/gas, to maintain reservoir pressure, or to displace hydrocarbons towards production wells. The injection and production of fluids is controlled through surface facilities, but wells may also contain (advanced) down-hole control devices.

The main purpose of a well model is to accurately represent the flow in the wellbore and provide equations that can be used to compute injection or production rates when the flowing bottom hole pressure is known, or compute the pressure for a given well rate. When the flow equations presented above are discretized using a volumetric grid, the wellbore pressure will be significantly different from the average pressure in the perforated grid blocks. The diameter of the wellbore is small compared to the size of the blocks, which implies that large pressure gradients appear in a small region inside the perforated blocks. Modeling injection and production of fluids using point sources gives singularities in the flow field and is seldom used in practice. Instead, one uses an analytical or semi-analytical solution of the form $-q = WI(p_b - p_{wb})$ to relate the wellbore pressure p_{wb} to the numerically computed pressure p_b inside the perforated blocks. Here, the well index WI accounts for the geometric characteristics of the well and the properties of the surrounding rock.

The first, and still most used model was developed by Peaceman [8]. Assuming steady-state radial flow and a 7-point finite-difference discretization, the well index for an isotropic

medium with permeability K represented on a Cartesian grid with cell $\Delta x \times \Delta y \times \Delta z$ reads,

$$(10) \qquad WI = \frac{2\pi K \Delta z}{\ln(r_0/r_w)}, \qquad r_0 = 0.14(\Delta x^2 + \Delta y^2)^{\frac{1}{2}}.$$

Here, r_w is the radius of the well and r_0 is the effective block radius at which the steady-state pressure equals the computed block pressure. The Peaceman model has later been extended to multiphase flows, anisotropic media, horizontal wells, non-square grids, and other discretization schemes, as well as to incorporate gravity effects, changes in near-well permeability (skin), and non-Darcy effects. More advanced models also describe the flow inside the wellbore and how this flow is coupled to surface control and processing facilities.

4. Bridging scales (upscaling)

Describing all pertinent flow processes with a single model is impossible. Flow simulation is therefore divided according to physical scales and performed on a hierarchy of models: flow in core samples (cm scale), bed models (meter scale), sector models, and field models (km scale). These models must be calibrated against static and dynamic data of very different spatial (and temporal) resolution: thin sections, core samples, well logs, geological outcrops, seismic surveys, well tests, production data, core flooding and other laboratory experiments, etc. Moreover, use of geostatistical methods tends to produce geo-cellular models having significantly more detail than conventional reservoir simulation tools can handle. For all these reasons, upscaling is inevitable to perform model reduction and transfer parameters and effective properties up in the model hierarchy. A proper coarse-scale reservoir model should ideally capture the impact of heterogeneous structures at all scales that are not resolved by the coarse grid used for flow simulation.

The simplest type of upscaling is single-phase upscaling: assuming incompressible flow modeled by $-\nabla \cdot K \nabla p = q$, we seek an effective K^* inside each coarse grid block B such that $K^* \int_B \nabla p \, dx = \int_B K(x) \nabla p \, dx$. Upscaling methods range from simple averaging techniques to sophisticated methods that employ a combination of local and global computations [5].

Power averaging techniques, $K^* = \left(\frac{1}{|B|} \int_B K(x)^r \, dx \right)^{1/r}$, $-1 \le r \le 1$, give correct upscaling in special cases[3], but tend to perform poorly in practice since the averages do not reflect the structure or orientation of the heterogeneous structures.

In flow-based upscaling, one solves a set of homogeneous pressure equations, $-\nabla \cdot K \nabla p = 0$, for each grid block with prescribed boundary conditions that induce a desired flow pattern. Methods differ in the way boundary conditions are prescribed. A popular choice is to consecutively impose a pressure drop in each coordinate direction, giving three flow rates for each grid block, from which an effective diagonal permeability tensor can be computed. Another popular option is to impose periodic boundary conditions. Alternatively, one may look at the discretized flow equation, $v_{ij} = T_{ij}(p_i - p_j)$, where v_{ij} denotes the flux from block B_i to B_j, and upscale the *transmissibility* T_{ij} directly by solving a flow problem in $B_i \cup B_j$.

What is the best average in a specific case depends both on the heterogeneity and the flow process (flow direction, boundary conditions, etc). More sophisticated methods therefore use extended local domains to lessen the impact of the boundary conditions, or rely on bootstrapping methods that combine the solution of local and (generic or the full) global flow problems. Moreover, single-phase upscaling alone is often not sufficient to capture large-scale

---

[3]The arithmetic average ($r = 1$) is correct for flow parallel to isotropic, layered media, whereas the harmonic average ($r = -1$) is correct for flow perpendicular to isotropic, layered media.

heterogeneity effects in a multi-phase system. The macroscopic effect of relative permeabilities and capillary pressures are captured in terms of *pseudo functions*, i.e., effective functions that are used in coarse-scale transport equations to model unresolved subscale effects.

Recently, research on simulation is moving in the direction of so-called multiscale methods [6] in which the solution of local flow problems is embedded in coarse-scale approximation spaces consisting of a set of multiscale basis functions which have fine-scale subresolution that is consistent with the local properties of the differential operator(s). The multiscale basis functions can be coupled through a global coarse-scale formulation to produce flow solutions that are conservative both on the coarse and the fine scale. Performing a single multiscale flow solve will typically be as expensive as performing flow-based upscaling or computing a single fine-scale flow solution. However, for subsequent updates to the flow field, multiscale methods offer a significant gain in computational efficiency by systematically reusing computations from the previous flow solves (i.e., reusing the basis functions).

References

[1] K. Aziz and A. Settari. *Petroleum Reservoir Simulation.* Elsevier Applied Science Publishers, London and New York, 1979.

[2] J. Bear. *Dynamics of Fluids in Porous Media.* Environmental Science Series. American Elsevier Publishing Company, 1972.

[3] G. Chavent and J. Jaffre. *Mathematical Models and Finite Elements for Reservoir Simulation.* North Holland, 1986.

[4] Z. Chen, G. Huan, and Y. Ma. *Computational Methods for Multiphase Flows in Porous Media*, volume 2 of *Computational Science & Engineering.* Society for Industrial and Applied Mathematics, 2006.

[5] L. J. Durlofsky. Upscaling of geocellular models for reservoir flow simulation: A review of recent progress. In *7th International Forum on Reservoir Simulation*, pages 23–27, 2003.

[6] Y. Efendiev and T. Y. Hou. *Multiscale Finite Element Methods*, volume 4 of *Surveys and Tutorials in the Applied Mathematical Sciences.* Springer Verlag, 2009.

[7] R. Helmig. *Multiphase Flow and Transport Processes in the Subsurface: A Contribution to the Modeling of Hydrosystems.* Springer-Verlag, Berlin, Heidelberg, 1997.

[8] D. W. Peaceman. Interpretation of well-block pressures in numerical reservoir simulation with nonsquare grid blocks and anisotropic permeability. *SPE J.*, 23(3):531–543, 1983. doi: 10.2118/10528-PA. SPE 10528-PA.

[9] D. W. Peaceman. *Fundamentals of Numerical Reservoir Simulation.* Elsevier Science Inc., New York, NY, USA, 1991.

[10] J. A. Trangenstein and J. B. Bell. Mathematical structure of the black-oil model for petroleum reservoir simulation. *SIAM J. Appl. Math.*, 49(3):749–783, 1989. ISSN 0036-1399.

[11] J. A. Trangenstein and J. B. Bell. Mathematical structure of compositional reservoir simulation. *SIAM J. Sci. Statist. Comput.*, 10(5):817–845, 1989. ISSN 0196-5204.

[12] J. W. Watts. A compositional formulation of the pressure and saturation equations. *SPE J.*, 1(3):243–252, 1986.

(K.-A. Lie) SINTEF ICT, Department of Applied Mathematics,
P.O. Box 124 Blindern, N-0314 Oslo, Norway
E-mail address: Knut-Andreas.Lie@sintef.no, http://folk.uio.no/kalie

(B. T. Mallison) Chevron Energy Technology Company,
6001 Bollinger Canyon Rd, D2104, San Ramon, CA, USA
E-mail address: btmb@chevron.com