

The Total Compressibility Condition and Resolution of Local Nonlinearities in an Implicit Black-Oil Model with Capillary Effects

Dedicated to the memory of John J. Wheeler

MAŁGORZATA PESZYŃSKA

*Department of Mathematics, Oregon State University, Corvallis, OR 97331-4605, U.S.A.;
E-mail: mpezsz@math.oregonstate.edu*

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Abstract. An implicit black-oil model with capillary effects is studied. Various primary unknowns which include one of the phase pressures are considered, and qualitative and quantitative consequences of a choice are discussed. In particular, a total compressibility condition is defined and a local nonlinear problem is studied. A numerical method to solve the local problem is discussed.

Key words: black-oil model, multiphase multicomponent flow, implicit formulation, total compressibility, capillary pressure, nonlinear local solver, primary unknowns.

1. Introduction

Computational modeling of multiphase flow and transport in porous reservoirs is of great importance to the economy and environment, as it is essential to optimize production of natural energy resources and to predict and control contamination risks and remediation efforts. In this paper, we focus on a the *black-oil* model which has been known in reservoir engineering since 1970s (Peaceman, 1977; Watts, 1986; McCain, 1990; Killough, 1995). The motivation for this work arose originally from a benchmark problem with large capillary pressure Killough (1995) simulated with the computational black-oil model from IPARS reservoir simulation framework (Integrated Parallel Accurate Reservoir Simulator) (Wheeler, 2000; Lu, 2000; Lu *et al.*, 2001) and from studies of an optimal choice of primary unknowns in such a model.

The black-oil model is a functional subset of a comprehensive *compositional model*; the latter is very complex and even with today's computational power it can still rarely be used for simulations over large computational

domains. The black-oil model approximates its functionality while it is capable of accounting for significant variations in the amount of gas and in its pressures. Fully implicit formulations of a black-oil model are solved for three unknowns per cell only: such a lean and substantial structure makes it an attractive element in coupled flow, seismic, and geomechanics simulations (Aziz and Settari, 1979; Minkoff *et al.*, 2003, 2004) as well as in multidomain couplings (Peszyńska *et al.*, 2002; Lu *et al.*, 2002; Wheeler and Peszyńska, 2002; Peszyńska, 2003).

In such coupled systems it is not uncommon for the current initial or boundary condition of an individual model to fall outside a set of *physical* values, that is, those that can represent physical quantities and pressures observable in a porous medium. This can be caused by, and in turn can cause a convergence failure or near-failure of another part of the coupling, or an inherent inconsistency in the formulation of a part or of the whole of the coupled system. Related is the issue of robustness and consistency of individual models, for example, the presence of mass errors inherent in time-lagged or time-split formulations (Trangenstein and Bell, 1989; Coats, 1999; Chen *et al.*, 2004). It turns out that fully implicit models, albeit complex, are the best candidates for robust and stable “black box” elements of coupled systems. It is then desirable to find explicit conditions defining the admissible inputs and correct outputs of such models and to improve their efficiency, if possible.

In this paper, we investigate the choice of *primary unknowns* Υ in an implicit formulation of a black-oil model with capillary effects in saturated and unsaturated conditions written as

$$F(\Upsilon) = \mathbf{0}. \quad (1)$$

The set of three independent *primary unknowns* in Υ includes usually at least one *pressure unknown* P and several *saturation or concentration unknowns*. We investigate how certain choices of unknowns in Υ influence the structure of the model and its numerical implementation.

In particular, we define the coefficients of *total compressibility* \bar{c}_t and *total mobility* $\bar{\lambda}_t$ and study the structure of the pressure equation in the case when

$$\bar{c}_t \geq 0, \quad \bar{\lambda}_t > 0. \quad (2)$$

We then derive explicit conditions on the data sufficient for (2) which can be used to verify internal consistency of the data of the model as well as the physical meaningfulness of the current guesses for Υ . They are independent of how we choose P in Υ .

Next, we consider practical consequences of the choice of Υ and in particular, the ease with which model variables can be computed from Υ . Some such calculations are explicit, others may be implicit. In some instances the map $\Upsilon \mapsto S_w$, where S_w is water saturation, is implicit; S_w is found numerically as a solution of a *local nonlinear problem* parametrized by Υ denoted by

$$f(\Upsilon; S_w) = 0. \quad (3)$$

Below we show how to construct a robust and efficient solver for (3) whose cost is similar to that of an explicit evaluation; this study is supported by our analysis of f and by numerical evidence.

The plan of the paper is as follows. In Section 2, we recall the black-oil model and give examples of Υ . In Section 3, we discuss the *total compressibility condition* for the black-oil model in unsaturated and saturated conditions with capillary effects; these results extend (Watts, 1986; Chavent and Jaffre, 1986; Trangenstein and Bell, 1989; Coats, 1999; Chen, 2000). In Section 4, we analyze f , discuss a local nonlinear numerical solver, and provide criteria that verify whether values of Υ are physically meaningful. The results are illustrated by numerical experiments.

2. The Black-oil Model

Here we briefly recall the black-oil model of flow. Generally, we follow (Bear, 1972; Peaceman, 1977; Lake, 1989; McCain, 1990). We consider a porous reservoir Ω and the coefficients of porosity $\phi(x)$ and permeability $K(x)$, $x \in \Omega$ as defined in Bear (1972) and recall that their values may not be independent of one-another; moreover, they are, in general, correlated to the specific area and tortuosity coefficients of the porous medium. Finally, these coefficients depend in general on the pressure and temperature in the medium; such effects however for lack of space will not be discussed in this paper.

Our focus in this paper is on the fluids which fill the void (pore) space of Ω . The fluids can exist in different phases, can be made of different components, and are classified according to their composition and pressure–volume–temperature (PVT, phase behavior) properties. We consider three phases: aqueous, oleic and gaseous, denoted by subscripts w, o, g, respectively. We also consider three components: the water component denoted by subscript W, and various hydrocarbon components. In the black-oils it is known that more than 20 mole percent components are heavy; these are lumped in the (heavy) *oil* pseudo-component denoted by O; the other (light) *gas* pseudo-component is denoted by G. These components can remain in one phase only or can be partitioned between many phases depending on PVT conditions; general phase behavior of arbitrary fluids is possible using a full *equation of state* (EOS) (McCain, 1990; Coats *et al.*, 1995). Generally one assumes a local equilibrium between light and heavy components expressed quantitatively by a pressure-dependent *gas–oil ratio*.

Phases. Phases are characterized by several quantitative properties. Phase saturations (volume fractions), relative permeabilities, pressures, viscosities, densities, and reference densities, are denoted by S_m , k_m , P_m , μ_m , ρ_m , ρ_{mr} , respectively. Phase mobilities are $\lambda_m = k_m/\mu_m$. If a phase m is *absent* then

$S_m = 0$. In general, for each phase m we have $0 \leq S_m \leq 1, \forall m$. The phase saturations satisfy the *volume constraint*:

$$S_w + S_o + S_g = 1. \quad (4)$$

In this paper, we are concerned with *water-wet* reservoirs, that is, reservoirs in which the water phase w is always present so that $S_w > S_{w,r}$, where $S_{w,r} > 0$ denotes the *residual* water saturation. In consequence, other phases cannot occupy more than the fraction $1 - S_{w,r}$ of pore space:

$$0 \leq S_m < 1 - S_{w,r}, \quad m = o, g, \quad 0 \leq S_o + S_g < 1 - S_{w,r}. \quad (5)$$

Phase velocities are given by the multiphase (Muskat) extension of Darcy's law for the volumetric phase velocity \vec{V}_m

$$\vec{V}_m = -\frac{K k_m}{\mu_m} (\nabla P_m - \rho_m g \nabla D) = -K \lambda_m (\nabla P_m - \rho_m g \nabla D), \quad (6)$$

where g denotes the gravity constant and $D(x), x \in \Omega$ the depth.

We recall that phase relative permeabilities $k_m = k_m(S_m)$ increase with their phase saturations S_m ; for a more general situation (Chavent and Jaffre, 1986).

The interface between phases is due to capillary forces: we have

$$P_o - P_w := P_{ow}^c(S_w), \quad (7)$$

$$P_g - P_o := P_{go}^c(1 - S_g) = P_{go}^c(S_w + S_o). \quad (8)$$

Typical properties of capillary pressure in water-wet reservoirs are given in (A1). Multiple *rock types* and dependence on other phase saturations are discussed in Lake (1989), Helmig (1997) and Chavent and Jaffre (1986).

(A1). Define $\mathcal{A}_S := (S_{w,r}, 1]$ and assume that $P_{ow}^c, P_{go}^c, P_{ow}^{c'} \leq 0, P_{go}^{c'} \leq 0$, for $S \in \mathcal{A}_S$, and $P_{go}^c(S_{w,r}^+) = +\infty, P_{ow}^c(S_{w,r}^+) = +\infty$. Assume also $P_{ow}^c(1) \geq 0, P_{go}^c(1) \geq 0$.

Components. The mass conservation equation for each component is

$$\frac{\partial}{\partial t}(\phi N_M) + \nabla \cdot \vec{U}_M = q_M, \quad x \in \Omega, \quad (9)$$

where q_M denotes the component's source or sink terms due to injection and production wells. The components M can exist in different phases m ; this is described by mass fractions η_{Mm} . Here we consider the "standard" black-oil model (Peaceman, 1977; Watts, 1986; Lake, 1989; Trangenstein and Bell, 1989) and assume $\eta_{ww} = 1$ so the water component can be identified with the aqueous phase. Also, we assume $\eta_{Gg} = 1, \eta_{Oo} > 0$. It follows that $\eta_{Oo} + \eta_{Go} = 1$: the gas component G is partitioned between the oleic o and gaseous g phases; the components O, G make up the oil phase o, but the gaseous phase g, if it exists, is made only of component G.

The *concentrations* of components are $N_W = S_w(\varrho_w/\varrho_{wr})$, $N_O = \eta_{Oo}S_o(\varrho_o/\varrho_{or})$, $N_G = \eta_{Go}(S_o\varrho_o/\varrho_{gr}) + S_g(\varrho_g/\varrho_{gr})$, where ϱ_{mr} is the reference density of that phase $m = m(M)$ which is naturally associated with the given component M , that is, w with W, o with O, g with G. We use the *phase formation volume factors* $B_m = \varrho_{mr}/\eta_{Mm}\varrho_m$, $m = m(M)$, with $B_m = \varrho_{mr}/\varrho_m$ for $m = w, g$. Also, we use the *component gas/oil ratio* $R_o = \eta_{Go}\varrho_{or}/\eta_{Oo}\varrho_{gr}$. Thus $N_W = (S_w/B_w)$, $N_O = (S_o/B_o)$, $N_G = (S_oR_o/B_o) + (S_g/B_g) = N_OR_o + (S_g/B_g)$. The flux of a component M is $\vec{U}_M = \sum_m \eta_{Mm} \vec{V}_m \varrho_m / \varrho_m(M) \mathbf{r}$; we can write $\vec{U}_M = \vec{V}_m / B_m$, $M = W, O, m = m(M)$, and $\vec{U}_G = \vec{V}_o R_o / B_o + \vec{V}_g / B_g$.

In summary, the black-oil model is given by (4), (7), (8) and (9), along with appropriate definitions. It can be written as a square system (1) whose size is determined by the Gibbs' rule: the number of unknowns in Υ and the number of equations in (1) is three.

To complete the model, we assume either the no-flow boundary conditions or that the values of primary unknowns $\Upsilon(x, t)|_{x \in \partial\Omega}$ are specified. Also, initial values $\Upsilon(x, t)|_{t=0}$, $x \in \Omega$ must be given. Conditions on whether these boundary and initial data are physical will be discussed in the sequel.

2.1. PHASE BEHAVIOR

Recall the definition of compressibilities as $c_m = -(B'_m/B_m)$. In the slightly compressible case we have $c_m \equiv \text{const}$. In general, for the uni-component phases $c_w, c_g \geq 0$; typically $c_g \gg c_w$, where c_g is a highly varying decreasing function of pressure. In general, B_g and B_w are given as reservoir data.

Next consider the oleic phase $m = o$ which is composed of two hydrocarbon components O and G: we have three distinct cases, summarized in Table I. We note that data on B_o in unsaturated conditions where the oleic phase behaves like a liquid (McCain, 1990) is rarely available; a physically meaningful formula defining B_o must match the data B_{do} and B_{so} in their respective dead-oil and saturated limits. Here we use a linear formula proposed in Lu (2000).

Typical properties of the rock-fluid data are given in (A2).

(A2) Assume that $B_w, B_g, B_{do}, B_{so}, R_s$ are continuous and piecewise differentiable on \mathbb{R}_0^+ . In addition,

$$B_w : B'_w \leq 0, \quad B_w(0) = 1 \geq B_w > 0, \quad (10)$$

$$B_{do} : B'_{do} \leq 0, \quad B_{do}(0) = 1 \geq B_{do} > 0, \quad (11)$$

$$B_{so} : B'_{so} > 0, \quad B_{so}(0) = 1, \quad (12)$$

$$R_s : R'_s > 0, \quad \lim_{P \rightarrow +\infty} R_s(P) = +\infty, \quad (13)$$

$$B_g : B'_g \leq 0, \quad (14)$$

Table I. Summary of oil/gas PVT definitions

Case	Pressure	Gas/oil ratio R_o	Oil formation volume factor B_o	S_g
<i>Dead-oil</i>	any	$N_G = 0, R_o = 0$	$B_o = B_{do}$	$S_g = 0$
<i>Unsaturated</i>	$P \leq P^*(R_o)$	$0 < R_o \leq R_s(P),$ $R_o = N_G/N_O$	$B_o = B_{do} + R_o/R_s$ $[B_{so}(P^*) - B_{do}(P^*)]$	$S_g = 0$
<i>Saturated</i>	$P > P^*$	$\frac{N_G}{N_O} > R_s(P)$	$B_o = B_{so}$	$S_g > 0$

The following functions are given as rock-fluid data: *dead-oil formation volume factor* $B_{do} := B_o|_{N_G=0}$, the *saturated gas/oil ratio* R_s , or its inverse $P^*(R_o)$ with $P^*(R_o)$ called the *saturation (bubble) pressure*, and the *saturated oil formation volume factor* B_{so} .

Remark 1. From (12) and (11) we see that $B_{so}(P) \geq B_{do}(P)$ for any pressure P and that whenever $N_G > 0$, we have $B_{so}(P) > B_{do}(P)$. It follows that if $R_o < R_s$ is fixed, then $B'_o(P) \leq B'_{do}(P) \leq 0$. Also, if $N_G > 0$, then we have $B'_o < B'_{do} \leq 0$. In other words, the compressibility $c_o|_{R_o < R_s}$ of “live” oil with dissolved gas in unsaturated conditions, which behaves like a liquid, is larger than the one of “dead-oil”. At the same time, $c_o|_{0 < R_o < R_s}$ is always positive because $B'_o(P) \leq -R'_s < 0$. Also, by (11) and (13) $B_o^{\min} := \lim_{P \rightarrow \infty} B_o(P) \geq 0$.

It remains to point out that R_o, B_o are nondifferentiable at the phase transition point $P = P^*$ where $N_G/N_O = R_s(P)$. In addition, the piecewise representations of the *rock-fluid* data are not differentiable either. In other words, both the data and phase properties make F in (1) only piecewise smooth. These facts introduce mild additional numerical difficulties when solving (1) numerically.

Two more assumptions are formulated on the data that will be needed in the sequel. These can be used to verify internal consistency of data and unknowns of the model.

(A3) $B'_{so} - B_g R'_s \leq 0$ (see Coats, 1999),

(A4) $1 + N_O B'_{so} P'_{go^c} \geq 0$.

2.2. PRIMARY UNKNOWNNS

The results presented in this paper are essentially independent of the spatial discretization and are valid for a fully implicit in time temporal discretization with backward Euler implicit time-stepping. Hence, in what follows we identify the continuous problem (1) with its fully discrete form; details on the latter can be found in Lu *et al.* (2002).

The system (1) is solved by Newton iteration, where in each Newton step $n=0, 1, 2, \dots$ we solve

$$DF^n \Delta \Upsilon^n = -F^n, \quad \Upsilon^{n+1} = \Upsilon^n + \Delta \Upsilon^n, \quad (15)$$

with $F^n = F(\Upsilon^n)$, $DF^n = DF(\Upsilon^n)$. The initial guess Υ^0 is determined by extrapolation from previous time steps; the nonlinear (1) and linear (15) iterations terminate when some stopping criteria are satisfied. This is a standard setting, see Lu (2000) and Lu *et al.* (2001, 2002) for details and Kelly (1995) Lacroix *et al.* (2003) for information on the solvers.

The choice of unknowns Υ in (1) is motivated by several criteria. First, Υ must describe the state of reservoir without ambiguity and must have an easy physical interpretation. Second, all quantities in (1) and (15) should be easy to compute from Υ . Third, the conditioning and pre-conditioning of the Jacobian DF must be considered, in particular, in the presence of various types of injection and production wells and in degenerate conditions.

It is customary to include in Υ some pressure variable(s) and some of the concentration- or saturation-based variables. In fact, in implicit models the inclusion of *at least one* pressure unknown in Υ is necessary in order for the reservoir pressure to be known. The use of more than one of the phase pressures is undesirable because it creates a large pressure block, requires resolution of capillary relationships which is ill-posed close to degenerate conditions, and may cause unphysical numerical countercurrent phase flows.

The pressure unknown P can be one of phase pressures $P_m, m=w, o, g$ or one of *global-* or *pseudo-*pressures as in (Chavent and Jaffre, 1986; Chen, 2000); the latter are convenient in analysis but cumbersome in implementation of implicit models. In this paper we choose the former; here one should choose this phase $m=w, o, g$ which has the most likelihood of being continuous in the reservoir and throughout the simulation time: this criterion eliminates P_g . Next, when water movement is deemed relatively insignificant, P_o can be selected (ecl, 1998; Chen, 2000). However, the oleic phase may be discontinuous in water-wet reservoirs as well as in aquifer parts of reservoirs such as in (Killough, 1995); there, P_w should be used.

The remaining two unknowns in Υ are the concentrations or saturations; the former are preferable in mass conservative implicit formulations in compressible conditions. The hydrocarbon concentrations N_O, N_G , or their ratio N_G/N_O *must* be used in order to describe unsaturated conditions unambiguously; in addition, the use of N_W provides less information than either of N_G, N_O .

It is logical therefore to consider only $\Upsilon = (P, N_O, N_G)$ where P is either P_w or P_o . In the remainder of this paper we investigate these two choices in view of (i) and (ii). A comprehensive comparison including (iii) is regrettably beyond our scope.

3. The Total Compressibility Condition

The structure of multiphase flow models is revealed through the transformation of the original system (9) to a system composed of one *pressure equation* and two *saturation-like* equations. Typically, it is found that, based on some conditions, the pressure equation has a (degenerate) parabolic–elliptic (diffusion-like) character and that the saturation-like equations have a (degenerate) parabolic–hyperbolic (transport-like) character.

Here we investigate the former; it is derived from (9) in the form

$$\phi \bar{c}_t \frac{\partial P}{\partial t} = \nabla \cdot (K \bar{\lambda}_t \nabla P) + \bar{q}_t, \quad (16)$$

where \bar{c}_t is a “compressibility-like” term and $\bar{\lambda}_t$ is a “mobility-like” term. Both $\bar{c}_t, \bar{\lambda}_t$ depend nonlinearly on the data and on Υ ; therefore, the character of (16) may change locally. The term \bar{q}_t contains lower order derivatives and source terms which do not influence the structure of (16) but preserve the coupling between (16) and other equations.

By change of variable from P to $v = \int_0^P \bar{\lambda}_t(q) dq$ (Kirchoff transformation), one can consider, in place of (16), the abstract problem

$$\phi \bar{c}_t \bar{\lambda}_t^{-1} \frac{\partial v}{\partial t} = \nabla \cdot (K \nabla v) + \bar{q}_t. \quad (17)$$

If (2) holds, then the structure of (17) is nonlinear degenerate parabolic; see the analysis in Showalter (1997) and the applied point of view in (Coats, 1999). Since, by physical reasoning, this is the expected behavior of the pressure equation, (2) can be used for verification of internal consistency of the data of a model.

We now proceed to find sufficient conditions that guarantee (2) for the full model with nonzero capillary pressure in both unsaturated and saturated conditions in which the primary pressure unknown is one of the phase pressures. We note that in a similar discussion in Watts (1986), Trangenstein and Bell (1989), Coats (1999); the capillary pressures are ignored; in Chavent and Jaffre (1986) and Chen (2000) only the global pressure is considered; in Chen (2000) only the saturated case is considered and in Chavent and Jaffre (1986) the water phase is deemed immobile or absent. In this paper, we demonstrate that conditions (A1)–(A4) are sufficient for (2) and in turn that they guarantee the expected behavior of the pressure equation for all considered choices of primary unknowns.

3.1. DERIVATION OF THE PRESSURE EQUATION

Here we derive (16). We multiply each of (9) for $M = W, O$ by B_m with $m = m(M)$ and manipulate terms to get

$$\begin{aligned} \frac{\partial}{\partial t}(\phi S_m) + \phi S_m \left(\frac{-1}{B_m} \frac{\partial B_m}{\partial t} \right) \\ = B_m \left(-\nabla \cdot \vec{U}_M + q_M \right), \quad M = W, O, \quad m = m(M). \end{aligned} \quad (18)$$

For $M = G$ we multiply (9) by B_g from which we subtract (9) written for $M = O$ multiplied by $B_g R_s$, and we get

$$\begin{aligned} \frac{\partial}{\partial t}(\phi S_g) + \phi S_g \left(\frac{-1}{B_g} \frac{\partial B_g}{\partial t} \right) + \phi \left(\frac{S_o B_g}{B_{s_o}} \frac{\partial R_s}{\partial t} \right) \\ = B_g \left(-\nabla \cdot \vec{U}_G + q_G \right) - B_g R_s \left(-\nabla \cdot \vec{U}_O + q_O \right). \end{aligned} \quad (19)$$

Now we exploit (4) to eliminate the term $\sum_m \frac{\partial}{\partial t}(\phi S_m) = 0$; as a result, (16) with appropriately defined $\bar{c}_t, \bar{\lambda}_t, \bar{q}_t$ is derived. We consider separately the unsaturated and saturated cases.

Unsaturated case. Here $S_g = 0$; we add (18) for $M = W, O$, substitute $\partial B_m / \partial t = B'_m (\partial P_m / \partial P) (\partial P / \partial t)$, and use the definition of phase compressibilities. We define

$$\bar{c}_t|_{S_g=0} := \sum_m S_m \left(-\frac{B'_m}{B_m} \right) \frac{\partial P_m}{\partial P} = \sum_m S_m c_m \frac{\partial P_m}{\partial P}, \quad (20)$$

$$\bar{\lambda}_t := \sum_m \lambda_m \frac{\partial P_m}{\partial P}, \quad (21)$$

$$\bar{q}_t := \sum_M q_M B_m - c_m \nabla P_m \cdot (\lambda_m K \nabla P_m), \quad m = m(M), \quad (22)$$

to get the desired pressure equation (16).

Saturated case. Here $S_g > 0$; we add both of (18) and (19), use $B_o = B_{s_o}, R_o = R_s$ to get

$$\begin{aligned} \phi S_w \left(\frac{-1}{B_w} \frac{\partial B_w}{\partial t} \right) + \phi S_o \left(\frac{-1}{B_{s_o}} \frac{\partial B_o}{\partial t} + \frac{B_g}{B_{s_o}} \frac{\partial R_s}{\partial t} \right) + \phi S_g \left(\frac{-1}{B_g} \frac{\partial B_g}{\partial t} \right) \\ = -B_w \left(\nabla \cdot \vec{U}_W \right) - (B_{s_o} - B_g R_s) \left(\nabla \cdot \vec{U}_O \right) - B_g \left(\nabla \cdot \vec{U}_G \right) \\ + B_w q_W + (B_{s_o} - B_g R_s) q_O + B_g q_G \end{aligned}$$

Now substitute

$$\frac{\partial B_m}{\partial t} = B'_m \frac{\partial P_m}{\partial P} \frac{\partial P}{\partial t},$$

use $R_s = R_s(P_o)$ and define

$$\bar{c}_t|_{S_g > 0} := -\frac{S_w}{B_w} B'_w \frac{\partial P_w}{\partial P} - \frac{S_o}{B_{so}} (B'_{so} - B_g R'_s) \frac{\partial P_o}{\partial P} - \frac{S_g}{B_g} B'_g \frac{\partial P_g}{\partial P}. \tag{23}$$

Equivalently, we have

$$\bar{c}_t|_{S_g > 0} = -N_w B'_w \frac{\partial P_w}{\partial P} - N_o (B'_{so} - B_g R'_s) \frac{\partial P_o}{\partial P} - (N_g - N_o R_s) B'_g \frac{\partial P_g}{\partial P}.$$

Also, $\bar{\lambda}_t$ can be defined in a manner analogous to (21).

If P is the common *reservoir pressure* with no capillary effects included, then $\partial P_m / \partial P = 1$ for any phase m and (23) reduces to the expressions in (Watts, 1986; Coats, 1999). In that case, by (10) and (14), $c_w \geq 0, c_g \geq 0$ and we see that for $\bar{c}_t|_{S_g > 0, P_{ow}^c \equiv 0 \equiv P_{go}^c} \geq 0$ it is sufficient and necessary to assume (A2)–(A3) (Coats, 1999).

If capillary pressure effects are not ignored, then one needs to make explicit the terms $\partial P_m / \partial P$. These depend on the choice of P in Υ . As shown below, in general, (2) follows from (A1) to (A4).

3.2. TOTAL COMPRESSIBILITY IN UNSATURATED CASE

Let $N_G \geq 0$ be given with $R_o \leq R_s$, so that $S_g = 0$. The appropriate definition of \bar{c}_t follows from (20) where we select Υ and compute $\partial P_m / \partial P$. For instance, if $\Upsilon = (P_w, N_o, N_g)$, that is, $P = P_w$ then we calculate $\partial P_o / \partial P_w = 1 + P_{ow}^c \partial S_w / \partial P_w$ from (7) and obtain $\partial S_w / \partial P_w$ by implicit differentiation from $S_w = 1 - N_o B_o (P_w + P_{ow}^c(S_w))$ which follows from the definition of N_o and from (4). After some manipulations we get an expression for $\bar{c}_t = S_w c_w + N_o (-B'_o) 1 / (1 + N_o B'_o P_{ow}^c)$. In consequence, for $\bar{c}_t \geq 0$ (or for (2)) it is sufficient to have (10) and in view of (A1) to require also that $B'_o \leq 0$; the latter is consistent with requirement that the unsaturated oleic phase behaves “like a liquid” (see Remark 1). The expression for $\bar{\lambda}_t$ and analysis of when $\bar{\lambda}_t > 0$ follow from similar calculations and will be omitted.

For other choices of primary unknowns, calculations and conditions that guarantee $\bar{c}_t \geq 0, \bar{\lambda}_t > 0$ are similar. Some such calculations for all pos-

Table II. Definitions of $\bar{c}_t, \bar{\lambda}_t$ for various choices of Υ

Υ	$\frac{\partial S_w}{\partial P}$	$\frac{\partial P_{m'}}{\partial P}$	\bar{c}_t	$\bar{\lambda}_t$
(P_o, N_o)	+	≥ 1	$S_w c_w (1 - c_o S_o P_{ow}^c) + S_o c_o$	$\lambda_w (1 - c_o S_o P_{ow}^c) + \lambda_o$
(P_w, N_o)	+	$(0, 1]$	$S_w c_w + S_o c_o \frac{1}{(1 - c_o S_o P_{ow}^c)}$	$\lambda_w + \lambda_o \frac{1}{(1 - c_o S_o P_{ow}^c)}$
(P_w, N_w)	-	≥ 1	$S_w c_w + S_o c_o (1 - c_w S_w P_{ow}^c)$	$\lambda_w + \lambda_o (1 - c_w S_w P_{ow}^c)$
(P_o, N_w)	-	$(0, 1]$	$S_w c_w \frac{1}{(1 - c_w S_w P_{ow}^c)} + S_o c_o$	$\lambda_w \frac{1}{(1 - c_w S_w P_{ow}^c)} + \lambda_o$

Phase m' is the phase “other” than phase m for which P_m is included in Υ .

sible choices of Υ when $N_G = 0$ (dead-oil case) are given in Table II. We see that (A1) and (A2) are necessary and sufficient to ensure (2) that is, that the pressure equation is parabolic–elliptic. We note in passing that the same results can be obtained when P is a global or pseudo-pressure (not shown here). Finally, while we have demonstrated that the sign of $\bar{c}_t \bar{\lambda}_t^{-1}$ as well as the qualitative character of (17) are independent of the choice of P in Υ , we remark that the *magnitude* of $\bar{c}_t \bar{\lambda}_t^{-1}$ is strongly dependent on the selection of Υ ; the latter fact is significant for efficiency of associated iterative solvers but will not be pursued further.

3.3. TOTAL COMPRESSIBILITY IN SATURATED CASE

Let \bar{c}_t be defined as in (23) and $\Upsilon = (P, N_O, N_G)$ with P equal to P_o or P_w . By implicit differentiation applied to

$$S_g = [N_G - N_O R_s(P_o)] B_g(P_o + P_{go}^c(1 - S_g)) \tag{24}$$

we get

$$\frac{\partial S_g}{\partial P} = T \frac{\partial P_o}{\partial P}, \tag{25}$$

where $T := (a - N_O B_g R'_s) / (1 + a P_{go}^c)$ with $a := [N_G - N_O R_s] B'_g$. By (8) and (25)

$$\frac{\partial P_g}{\partial P} = \frac{\partial P_o}{\partial P} - P_{go}^c \frac{\partial S_g}{\partial P} = \frac{\partial P_o}{\partial P} [1 - P_{go}^c T]. \tag{26}$$

Since $S_o = N_O B_{so}(P_o)$ from Table I, we have $\partial S_o / \partial P = N_O B'_{so} \partial P_o / \partial P$. Substitute these in (4) differentiated with respect to P_w to get

$$0 = \frac{\partial S_w}{\partial P} + \frac{\partial S_o}{\partial P} + \frac{\partial S_g}{\partial P} = \frac{\partial S_w}{\partial P} + \frac{\partial P_o}{\partial P} T_1, \tag{27}$$

where $T_1 := N_O B'_{so} + T$. It follows that

$$\frac{\partial S_w}{\partial P} = -T_1 \frac{\partial P_o}{\partial P}. \tag{28}$$

It is immediate that (14), (13), (A1) imply $a \leq 0$ and $T \leq 0$.

The remaining terms in \bar{c}_t by (25) can be written as

$$\begin{aligned} & -N_O [B'_{so} - B_g R'_s] \frac{\partial P_o}{\partial P} - [N_G - N_O R_s] B'_g \frac{\partial P_g}{\partial P} \\ & = \frac{\partial P_o}{\partial P} \left[-N_O [B'_{so} - B_g R'_s] - a [1 - P_{go}^c T] \right] = -\frac{\partial P_o}{\partial P} T_1. \end{aligned}$$

This can be seen, after we manipulate terms, as

$$\begin{aligned} & -N_O [B'_{so} - B_g R'_s] - a \left[1 - P_{go}^c T \right] \\ & = \frac{-N_O [B'_{so} - B_g R'_s] - a \left[1 + N_O P_{go}^c B'_{so} \right]}{1 + P_{go}^c a} = -T_1. \end{aligned}$$

It is clear then that in order for $\bar{c}_t \geq 0$ for any combination of phase saturations, we must have $-\partial P_o / \partial P T_1 \geq 0$. Hence, in addition to (A3) some growth condition on P_{go}^c which yields $T_1 \leq 0$ must be imposed. One can show that $T_1 \leq 0$ provided (A3), (A4) and (A1), (A2) hold.

In order to resolve the remaining relationships in \bar{c}_t we make a choice of P as either $P = P_o$ or $P = P_w$. In both cases (A1)–(A4) imply (2).

Case $\Upsilon = (P_o, N_O, N_G)$. Here we first calculate $\partial P_m / \partial P_o$ for $m = w, g$. Obviously $\partial P_o / \partial P_o = 1$. From (7) and (28) we find that $\partial P_w / \partial P_o = 1 + P_{ow}^c T_1$ and from (25) we have $\partial P_g / \partial P_o = 1 - P_{go}^c T$... Manipulating terms we get $\bar{c}_t = -N_w B'_w [1 + P_{ow}^c T_1] + T_1$ that is, $\bar{c}_t \geq 0$ provided (A3), (A4) hold. We also have

$$\bar{\lambda}_t := \lambda_w \frac{\partial P_w}{\partial P_o} + \lambda_o + \lambda_g \frac{\partial P_g}{\partial P_o} = \lambda_w \left[1 - P_{ow}^c \frac{\partial S_w}{\partial P_o} \right] + \lambda_o + \lambda_g \left[1 - P_{go}^c \frac{\partial S_g}{\partial P_o} \right].$$

and see $\bar{\lambda}_t > 0$ from (25) provided (A1)–(A4) hold.

Case $\Upsilon = (P_w, N_O, N_G)$. Here by (7) we have $\partial P_o / \partial P_w = 1 + P_{ow}^c \partial S_w / \partial P_w$ and resolving (28) we get $\partial S_w / \partial P_w = -T_1 / (1 + P_{ow}^c T_1)$, and $\partial P_o / \partial P_w = 1 + P_{ow}^c \partial S_w / \partial P_w = 1 / (1 + P_{ow}^c T_1)$. Rewriting (23) and eliminating terms we get $\bar{c}_t = -N_w B'_w - T_1 (\partial P_o / \partial P_w) = -N_w B'_w - T_1 / (1 + P_{ow}^c T_1)$. By (A1) we see that $1 \geq \partial P_o / \partial P_w \geq 0$; hence, $\bar{c}_t \geq 0$.

We also obtain similarly as above

$$\bar{\lambda}_t := \lambda_w + \lambda_o \frac{\partial P_o}{\partial P_w} + \lambda_g \frac{\partial P_g}{\partial P_w} = \lambda_w + \lambda_o \frac{\partial P_o}{\partial P_w} + \lambda_g \left[\frac{\partial P_o}{\partial P_w} - P_{go}^c T \frac{\partial P_o}{\partial P_w} \right] > 0$$

These calculations end the proof of the following proposition:

PROPOSITION 1. *In both unsaturated and saturated conditions the assumptions (A1)–(A4) guarantee (2) regardless of the choice of Υ .*

4. Resolution of Local Non-linearities

Consider the Newton step (15) and evaluation of F^n, DF^n , given Υ^n . This requires that we find the water saturation values S_w^n ; it turns out that the values of unknowns other than those in $\{\Upsilon, S_w\}$ and, hence, of F, DF , can then be computed explicitly. However, $\Upsilon^n \mapsto S_w^n$ is itself in general not

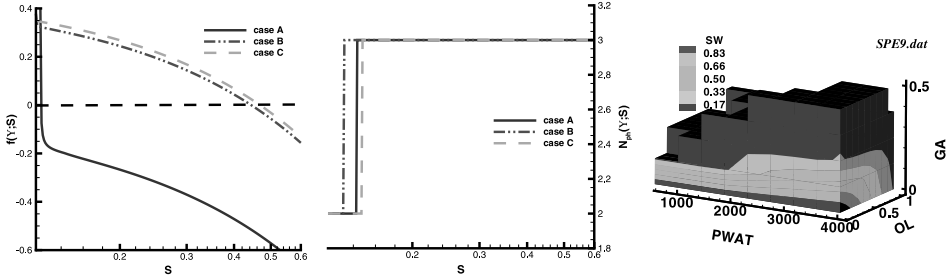


Figure 1. Left: behavior of $f(\mathbf{Y}; S)$ from case studies: (A) (Killough, 1995), (B) PVT data as in case (A) and capillary pressures as in Coats *et al.* (1995), and (C) PVT data typical for Prudhoe Bay (Minkoff *et al.*, 2003) and very small capillary pressures. In each case \mathbf{Y} is selected so that $S^*(\mathbf{Y}) \in \mathcal{A}_S$ exists, see plot of $N_{ph}(\mathbf{Y}; S)$ in the middle. Notice that the root S of $f(\mathbf{Y}; S)=0$ in case (A) is the root of $f_2(S)=0$ and in cases (B), (C) is the root of $f_3(S)=0$. Right: solution $S_w : f(\mathbf{Y}; S_w)=0$ found for various physical values of $\mathbf{Y}=(P_w, N_O, N_G) \in \mathcal{A}_Y$ (Case A).

explicit. It is given via the *local problem*

$$f(\mathbf{Y}; S_w) = 0 \quad S_w \in \mathcal{A}_S. \tag{29}$$

which must be solved numerically. Note that (29) must be solved for each spatial discretization point, at each time step, and for each Newtonian iteration n . This looks like a formidable additional computational burden.

Recall that a similar need to resolve local non-linearities associated with phase behavior and local equilibria exists in full EOS formulations for a compositional model, or, more generally, in chemical reaction modules. In that context the solvers for local implicit problems such as (29) are called *flash solvers*; these are typically multidimensional non-differentiable optimization algorithms and because of their complexity, capillary pressures are not taken into account. It is not practical to use flash solvers for (29) (see Lu *et al.*, 2001).

Next, consider alternatives to solving (29). These include time-lagging or iteration-lagging of S_w , that is, using some \tilde{S}_w from a previous time step or iteration. Another possibility is to use some explicit approximation \hat{S}_w^n to S_w^n , for example, by ignoring the capillary pressure. Such alternatives allow to bypass a potentially computationally expensive step of solving (29) numerically. Unfortunately, from our experience, it appears that they may lead to either a subsequent failure of Newtonian iteration, or to an excessive number of Newton steps required to solve (1), and as a result may cause costly iteration failures and time-step cutting. Such step or iteration failures are hard to deal with in coupled models.

The construction of a solver for (29) is complicated due to the singular character of $f(\mathbf{Y}; \cdot)$; the latter is likely the very cause of the failure of

lagging. The plots of $f(\Upsilon; \cdot)$ in Figure 1 illustrate the difficulties. These are overcome through a careful analysis which guides the construction of a robust and fast solver for (29). Additionally, this analysis provides insight into which values of Υ can be accepted as physically meaningful guesses which we associate with the requirement that the phase saturations computed from Υ satisfy (5). All physical guesses Υ are denoted as members of a set \mathcal{A}_Υ .

Finding \mathcal{A}_Υ is equivalent to deriving realistic bounds on the amount of components which can *fit within the available pore space*. Naively, since the phase compressibilities are positive, one should be able to fit any amount of fluids within a given volume, if only the pressure is high enough. However, infinite pressures are hardly the reality of reservoir exploration; realistically $P_{m,\min} \leq P_m \leq P_{m,\max}$. Also, (7) and (8) must hold.

Precise characterization of when $\Upsilon \in \mathcal{A}_\Upsilon$ is implicit; in what follows we find some useful *explicit* approximations $\mathcal{A}_\Upsilon^{\text{suff}} \subseteq \mathcal{A}_\Upsilon \subseteq \mathcal{A}_\Upsilon^{\text{nec}}$ which are easy to compute; these are extremely useful to determine whether the current Newton guess in (15), or an initial or boundary condition applied to (1), should be rejected or accepted.

4.1. CONSTRUCTION OF $f(\Upsilon; \cdot)$. PHYSICAL VALUES OF Υ

We consider $\Upsilon = (P_w, N_O, N_G)$ and $\Upsilon = (P_o, N_O, N_G)$ and discuss the map $f(\Upsilon, S_w)$ as well as conditions verifying whether Υ is physical, that is, whether $\Upsilon \in \mathcal{A}_\Upsilon$.

EXAMPLE 1. Let $\Upsilon = (P_o, N_O, N_G)$ be given, with $N_G = 0$ (dead-oil case). From (4) explicitly $S_w = 1 - N_O B_{\text{do}}(P_o)$. To ensure that S_w and Υ are physical we check (5). For this we must have $N_O \geq 0$, $N_O B_{\text{do}}(P_o) < 1 - S_{w,r}$. A sufficient condition by (11) is $N_O < (1 - S_{w,r}) / (B_{\text{do}}(P_{o,\min})) \leq 1 - S_{w,r}$; a necessary one is $N_O < (1 - S_{w,r}) / B_{\text{do}}(P_{o,\max})$. These two conditions define $\mathcal{A}_\Upsilon^{\text{suff}}$, $\mathcal{A}_\Upsilon^{\text{nec}}$, respectively.

Now consider $\Upsilon = (P_w, N_O, N_G)$ with $N_G = 0$. The equation $1 - N_O B_{\text{do}}(P_w + P_{ow}^c(S_w)) - S_w = 0$ is implicit in S_w . For Υ to be physical it is sufficient that $N_O < (1 - S_{w,r}) / B_{\text{do}}(P_w + P_{ow}^c(1))$; it is necessary that $N_O < (1 - S_{w,r}) / B_{\text{do}}(\infty)$, as otherwise (5) does not hold.

EXAMPLE 2. Here let $\Upsilon = (P_o, N_O, N_G)$ and $N_G > 0$. To find saturations, we first compute the value of $\bar{R}_s(P_o)$ and compare it to the ratio N_G / N_O . Following Table I we find whether $S_g = 0$ (unsaturated case) or $S_g > 0$ (saturated case).

In the unsaturated case solution of (29) is explicit: we compute S_o , then S_w from (4) with $S_g = 0$. In the saturated case we first solve for S_g the implicit relationship (24). Once S_g is known, we compute S_w from (4).

Finding S_g numerically is just one step of implicit calculations necessary in Example 3; as such, it is discussed in Section 4.3.

To find $\mathcal{A}_{\Upsilon}^{\text{suff}}$ we proceed similarly as in Example 1 and get the sufficient condition $N_O < (1 - S_{w,r})/B_o(P_{o,\min})$. Similarly, we get the necessary condition $N_O < (1 - S_{w,r})/B_o(P_{o,\max})$.

In the saturated conditions we bound both N_O and N_G from (5) $N_O B_{s_o} + [N_G - N_O R_s] B_g < 1 - S_{w,r}$. Here B_{s_o} and R_s are explicitly computed from P_o but the remaining parts are not explicit because $B_g = B_g(S_g)$. However, we obtain explicit conditions for $\Upsilon \in \mathcal{A}_{\Upsilon}^{\text{suff}}$ from (12), (14) as $N_O < (1 - S_{w,r})/B_{s_o}(P_{o,\max})$ and with (A1) we impose $N_O R_s < N_G < N_O R_s + (1 - S_{w,r})/B_g(P_o)$. A pair of necessary conditions is as follows $N_O < 1 - S_{w,r}$, $N_O R_s < N_G < N_O R_s + (1 - S_{w,r})/B_g(P_{g,\max})$. or $N_O R_s < N_G = N_O R_s < (1 - S_{w,r})/B_g(\infty)$. Finally, a useful sufficient and necessary condition on N_O in saturated conditions is that $0 < N_O < (1 - S_{w,r})/B_{s_o}(P_o)$.

EXAMPLE 3. Assume $\Upsilon = (P_w, N_O, N_G)$ is known with $N_G > 0$. Here it is not possible to know if $S_g = 0$ explicitly. This difficulty is one of the reasons why $\Upsilon = (P_o, N_O, N_G)$ may be preferred over $\Upsilon = (P_w, N_O, N_G)$. We discuss this situation in Section 4.2; in Section 4.3 we show how these difficulties can be overcome by an efficient numerical solution of (29).

Assume that *somehow* we *do* know whether $S_g = 0$ or not. If $S_g = 0$, then we find S_w as a fixed point of $S_w = 1 - N_O B_o(P_w + P_{ow}^c(S_w))$ and value of S_o follows from (4) with $S_g = 0$. If $S_g > 0$, then from (4), (7), (8) we solve for S_w

$$S_w = 1 - N_O B_o(P_w + P_{ow}^c(S_w)) - [N_G - N_O R_s (P_w + P_{ow}^c(S_w))] \times B_g \left(P_o + P_{go}^c(S_w + N_O B_o(P_w + P_{ow}^c(S_w))) \right). \quad (30)$$

Then we get P_o, S_o, S_g by (7) and (4).

In the unsaturated case, we find that $\Upsilon \in \mathcal{A}_{\Upsilon}^{\text{suff}}$ if only $N_O < (1 - S_{w,r})/B_o(P_w + P_c(1))$. Also, we must have $N_O < (1 - S_{w,r})/B_o(\infty)$ for $\Upsilon \in \mathcal{A}_{\Upsilon}^{\text{nec}}$.

In the saturated case, we derive that $\Upsilon \in \mathcal{A}_{\Upsilon}^{\text{suff}}$ if $N_O < (1 - S_{w,r}/B_{s_o})(\infty)$, $N_G < N_O R_s(P_w + P_{ow}^c(1)) + (1 - S_{w,r})/B_g(P_w + P_{ow}^c(1))$; also that we must have $N_O < 1 - S_{w,r}$, $N_O R_s(P_w + P_{ow}^c(1)) < N_G$, for $\Upsilon \in \mathcal{A}_{\Upsilon}^{\text{nec}}$.

Now we put together the above examples; we emphasize the ‘‘harder’’ case $\Upsilon = (P_w, N_O, N_G)$ from Example 3. We define f in (29) as

$$f(\Upsilon; S) := \begin{cases} f_2(\Upsilon; S), & N_{\text{ph}}(\Upsilon; S) = 2, \\ f_3(\Upsilon; S), & N_{\text{ph}}(\Upsilon; S) = 3, \end{cases} \quad (31)$$

$$f_2(\Upsilon; S) := 1 - S - N_O B_o(\tilde{P}_o(S)), \quad (32)$$

$$f_3(\Upsilon; S) := 1 - S - N_O B_{so}(\tilde{\mathcal{P}}_o(S)) \quad (33)$$

$$- \left[N_G - N_O R_s(\tilde{\mathcal{P}}_o(S)) \right] B_g(\tilde{\mathcal{P}}_g(S)), \quad (34)$$

where $\tilde{\mathcal{P}}_g(S) := \tilde{\mathcal{P}}_g(\Upsilon; S) = \tilde{\mathcal{P}}_o(S) + P_{go}^c(S + N_O B_{so}(\tilde{\mathcal{P}}_o(S)))$; $\tilde{\mathcal{P}}_o(S) := \tilde{\mathcal{P}}_o(\Upsilon; S) = P_w + P_{ow}^c(S)$, and

$$N_{ph}(\Upsilon; S) := \begin{cases} 2, & N_G \leq N_O R_s(\tilde{\mathcal{P}}_o(\Upsilon; S)), \\ 3, & N_G > N_O R_s(\tilde{\mathcal{P}}_o(\Upsilon; S)). \end{cases} \quad (35)$$

As is apparent from examples in Figure 1, the function $f(\Upsilon; S)$ is decreasing and equals $f_2(\Upsilon; S)$ close to $S_{w,r}$ where its derivative has a pole. These general properties of f are proven below; they help (i) to see that (29) has a unique solution as well as (ii) to find an appropriate numerical solver for (29) which can handle the special character of f .

4.2. ANALYSIS OF THE LOCAL MAP $\Upsilon \mapsto S_w$

Here we prove the properties of f defined by (31) and establish that the local problem (29) has a unique solution provided that Υ is physical and that the data satisfy (A1)–(A4); these are the same conditions as those which guarantee (2). The significance of these technical results is that the choice of $\Upsilon = (P_w, N_O, N_G)$ in the implicit black-oil model with internally consistent data is sound.

LEMMA 1. *Let (A1), (A2) hold. Then (i) $N_{ph}(\Upsilon; S)$ is nondecreasing in S . In addition, (ii) it satisfies $N_{ph}(\Upsilon; S_{w,r}^+) = 2$.*

Proof. We need only to consider N_{ph} across the “phase change” point $S^*(\Upsilon)$ defined by

$$S^*(\Upsilon): N_G = N_O R_s(\tilde{\mathcal{P}}_o(\Upsilon; S^*)), \quad S^* \in \mathcal{A}_S, \quad (36)$$

if it exists. Note that $S^*(\Upsilon)$ does not exist if $N_G < N_O R_s(P_w + P_{ow}^c(1))$ in which case the value of $P^*(N_G/N_O) - P_w$ is outside the range of P_{ow}^c . If S^* does not exist, then we have $N_{ph}(\Upsilon; S) = 2, \forall S \in \mathcal{A}_S$. However, if $S^*(\Upsilon)$ exists, then by (A1) $\tilde{\mathcal{P}}_o(\Upsilon; S)$ is nonincreasing as a function of S and, by (13), so is $R_s(\tilde{\mathcal{P}}_o(S))$. Fix $\Upsilon \in \mathcal{A}_\Upsilon$ and $S^* = S^*(\Upsilon)$. If $S < S^*$, then $R_s(\tilde{\mathcal{P}}_o(S)) \geq R_s(\tilde{\mathcal{P}}_o(S^*))$ hence $N_{ph}(S) = 2 = N_{ph}(S^*)$. On the other hand, if $S > S^*$, we have $R_s(\tilde{\mathcal{P}}_o(S)) \leq R_s(\tilde{\mathcal{P}}_o(S^*))$, hence $N_{ph}(S) = 3 > 2 = N_{ph}(S^*)$. This completes the proof of (i).

To show (ii), we see from (A1) and (13) that for a given N_G, N_O , we can always find a small enough $\tilde{S} > S_{w,r}$ and a large enough $\tilde{P}_o(\tilde{S}), R_s(\tilde{P}_o(\tilde{S}))$ so that $N_{ph}((P_w, N_O, N_G); \tilde{S}) = 2$. \square

LEMMA 2. Let (A1), (A2) hold. Then (i) $f: (\mathbb{R}_0^+)^3 \times \mathcal{A}_S \rightarrow \mathbb{R}$ is uniformly continuous. Also, (ii) f is differentiable except possibly at $S^*(\Upsilon)$ and (iii) if $\lim_{P \rightarrow \infty} B'_o(P) < 0$, then $f' := \partial f / \partial S$ is unbounded as $S \rightarrow S_{w,r}^+$.

Proof. By Lemma 1 we rewrite $f(\Upsilon; S)$ as

$$f(\Upsilon; S) := \begin{cases} f_2(\Upsilon; S), & S^*(\Upsilon) \notin \mathcal{A}_S, \\ \begin{cases} f_2(\Upsilon; S), & S \leq S^*(\Upsilon) \\ f_3(\Upsilon; S), & S > S^*(\Upsilon) \end{cases}, & S^*(\Upsilon) \in \mathcal{A}_S, \end{cases}$$

To show continuity of f we see that if $S^*(\Upsilon)$ exists then $f_2(S^*) = f_3(S^*)$. To show uniform continuity we extend $f(\Upsilon; \cdot)$ from \mathcal{A}_S to $S_{w,r}$; by Lemma 1, we see $\lim_{S \rightarrow S_{w,r}} f(S) = \lim_{S \rightarrow S_{w,r}} f_2(\Upsilon; S) = 1 - S_{w,r} - N_O B_o(\infty)$ which is finite. That is, we have shown (i).

To show (ii), by (A1), (A2) we see that each of f_2, f_3 is differentiable. We compute

$$\frac{\partial f_2}{\partial S} = \frac{\partial}{\partial S} \left[1 - N_O \left[B_o(\tilde{\mathcal{P}}_o(S)) \right] - S \right] = -1 - N_O P_{ow}^c B'_o, \quad (37)$$

$$\frac{\partial f_3}{\partial S} = -1 - N_o \left[B'_{so} - B_g R'_{so} \right] P_{ow}^c - B'_g \left[N_G - N_O R_s \right] \frac{\partial \tilde{\mathcal{P}}_g}{\partial S}, \quad (38)$$

with $\partial \tilde{\mathcal{P}}_g / \partial S = P_{ow}^c [1 + P_{go}^c N_o B'_{so}] + P_{go}^c$. We see that in general $f'_2(S^*) \neq f'_3(S^*)$ hence f is not differentiable at S^* which completes (ii).

By Lemma 1 we see that close to $S_{w,r}$, $f = f_2$ and we have $\partial f_2 / \partial S = -1 - N_O B'_o P_{ow}^c(S) \rightarrow -\infty$, as $S \rightarrow S_{w,r}$ which shows (iii). \square

LEMMA 3. Let (A1), (A2) hold. Then $f(\Upsilon, \cdot)$ has different signs at two endpoints of \mathcal{A}_S , i.e. it is *bracketed* on \mathcal{A}_S . Specifically, (i) $f(\Upsilon; 1) \leq 0$ for any $\Upsilon \in (\mathbb{R}_0^+)^3$. In addition, for (ii) $f(\Upsilon; S_{w,r}^+) \geq 0$ to be satisfied, it is sufficient that $\Upsilon \in \mathcal{A}_\Upsilon^{\text{suff}}$. For (ii) it is also necessary, respectively, that $\Upsilon \in \mathcal{A}_\Upsilon^{\text{nec}}$. These sets are defined

$$\mathcal{A}_\Upsilon^{\text{suff}} := \mathbb{R}_0^+ \times \left\{ N_O : 0 \leq N_O < \frac{1 - S_{w,r}}{B_o(\tilde{\mathcal{P}}_o(1))} \right\} \times \mathbb{R}_0^+, \quad (39)$$

$$\mathcal{A}_\Upsilon^{\text{nec}} := \mathbb{R}_0^+ \times \left\{ N_O : 0 \leq N_O \leq \frac{1 - S_{w,r}}{B_o(\infty)} \right\} \times \mathbb{R}_0^+. \quad (40)$$

Proof. Part (i) is a consequence of $N_O \geq 0$ and $f(\Upsilon; 1) = -C$ with $C = N_O B_{so}(\tilde{\mathcal{P}}_o(1)) + [N_G - N_O R_s(\tilde{\mathcal{P}}_o(1))] B_g$, if $N_{\text{ph}}(\Upsilon; 1) = 3$, and $C = N_O B_o(\tilde{\mathcal{P}}_o(1))$, if $N_{\text{ph}}(\Upsilon; 1) = 2$. We note $f(\Upsilon; 1) = 0$ only if $N_O = N_G = 0$ and $S = 1$ is the only solution to (29).

To show (ii) we see that as $S \rightarrow S_{w,r}^+$, $\tilde{\mathcal{P}}_o(S) \rightarrow \infty$, $B_o(\tilde{\mathcal{P}}_o(S)) \rightarrow B_o^{\text{min}}$ and $f(S_{w,r}^+) = f_2(S_{w,r}^+) = 1 - S_{w,r} - N_O B_o^{\text{min}}$. Thus, (ii) is equivalent to $N_O B_o^{\text{min}} < 1 - S_{w,r}$. To complete the proof, see the discussion in Examples 1–3. \square

LEMMA 4. *Let (A1), (A2) hold. Then (i) f_2 is strictly decreasing. In addition, let $S^*(\Upsilon)$ exist and let (A3) hold everywhere and (A4) hold for $S \geq S^*(\Upsilon)$. Then (ii) f_3 is strictly decreasing and, in consequence, f is strictly decreasing for all $S \in \mathcal{A}_S$.*

Proof. Part (i) follows directly from (A1), (A2) and Remark 1.

To show (ii), we investigate the terms in (38) to see that by (A1), (A3), the term $[B'_{so} - B_g R'_{so}] P'_{ow} \geq 0$, hence the second term in (38) is nonpositive. Next, we consider the term $\partial \tilde{\mathcal{P}}_g / \partial S$ in (38). We will have shown (ii) if we ensure that the first term in $\frac{\partial \tilde{\mathcal{P}}_g}{\partial S}$ is nonpositive; by $P'_{ow} \leq 0$, this follows if we bound $|P'_{go}(S)|$ for $S \in [S^* + N_O B_{so}(\tilde{\mathcal{P}}_o(S^*)), 1]$, which follows from (A4). Finally combining this with (14) we see $\partial f_3 / \partial S \leq -1 < 0$ which proves (ii). \square

Combining Lemmas 2–4 we get the following result, a direct application of the Intermediate Value Theorem and monotonicity of f . We remark that unique solvability of (29) follows from the same conditions as those which guarantee $\bar{c}_t \geq 0$.

PROPOSITION 2. *Let (A1)–(A4) be satisfied. If $\Upsilon \in \mathcal{A}_\Upsilon^{\text{suff}}$, then the solution to (29) exists and is unique. If, on the other hand, $\Upsilon \in \mathcal{A}_\Upsilon \setminus \mathcal{A}_\Upsilon^{\text{nec}}$, then the solution to (29) does not exist.*

It is worthwhile to note that if the solution to (29) is found in \mathcal{A}_S (that is, it is physical), then it can be shown that the other saturations S_o, S_g satisfy (5).

4.3. LOCAL NUMERICAL SOLVER

Now we show how to construct a robust and efficient solver for the local problem (29) based on the qualitative information about f found above. We also relate our practical numerical experience.

As a direct result of this section, one sees that there is no significant advantage to using $\Upsilon = (P_o, N_O, N_G)$ over $\Upsilon = (P_w, N_O, N_G)$ as primary unknowns. As an indirect result, our construction can serve as a template for similar situations where analysis of the problem reveals its natural physical structure in spite of that apparent complexity of an implicit equation such as (29) appears prohibitive.

Consider a numerical method for solving (29); this requires that we evaluate f and possibly also f' at the current guess S . The fastest root-solving methods based on Newton’s method converge (quadratically) if f' exists and is smooth and bounded away from 0. However, f' is unbounded close to $S_{w,r}$ and f is not defined outside \mathcal{A}_S . (f is also not differentiable at S^* but this plays a small role since f remains monotone). Hence, the applicable method(s) must keep the subsequent guesses bracketed in \mathcal{A}_S ;

in such algorithms derived from the *falsi* rule, the subsequent iterates are given by the Newton' step unless they fall out of the established bracket in which case the method takes a bisection-like step. The associated convergence order is superlinear (Press *et al.*, 1992).

4.3.1. *Initial Bracket*

First, consider $\mathcal{A}_S^\beta := [S_\beta, 1] \subset \mathcal{A}_S$ where $S_\beta := S_{w,r}(1 + \beta) < 1$, $\beta > 0$. Since f' is bounded on \mathcal{A}_S^β , one is tempted to solve, instead of (29), the problem $f(\Upsilon; S_w) = 0, S_w \in \mathcal{A}_S^\beta$. Its solution may however fail to exist, if β is too large. In our experience $\beta \approx 10^{-3}$ led to failure but $\beta \approx 10^{-6}$ proved to be successful.

4.3.2. *Stopping Criteria*

The iterations for (1) and (29) stop when, respectively, $\|F(\Upsilon^n)\|_F \leq \eta_F$, and $|f(\Upsilon^n; S_w^n)| \leq \xi$. with η_F and ξ predefined convergence tolerances for the global and local problem. In general, η_F represents a combination of both absolute and relative tolerances; it depends on how many significant digits in the mass balance need to be preserved which is expressed by a problem-independent tolerance η (Aziz and Settari, 1979); η_F can vary in time, and is problem dependent.

The value of ξ controls how exactly (29) is solved. A small ξ results in more accurate values of Jacobian DF and residual F , however, it may require many local iterations and may be unnecessary if η is large; a large ξ may cause lack of accuracy in evaluation of DF or F and consequently difficulties in subsequent global Newtonian iterations (1). Our experiments show that ξ should be two or three orders of magnitude smaller than η ; see also general discussion in Kelley (1995).

4.3.3. *Fixed-Point Improvement of Initial Bracket*

Now we discuss an enhancement of a numerical solver which is useful when $f \equiv f_2$. This can accelerate the numerical solution of (29).

First we determine explicitly if $f \equiv f_2$ on \mathcal{A}_S . Consider the following decomposition of $(\mathbb{R}_0^+)^3$ depending on the values of P_w and N_O as $(\mathbb{R}_0^+)^3 = \mathcal{A}^{\text{dead}} \cup \mathcal{A}^{\text{unsat}} \cup \mathcal{A}^{\text{sat}}$ where $\mathcal{A}^{\text{dead}} = (\mathbb{R}_0^+)^2 \times \{0\}$, $\mathcal{A}^{\text{unsat}} = (\mathbb{R}_0^+)^2 \times \{N_G \in \mathbb{R}_0^+ : 0 < N_G \leq N_O R_s(\tilde{P}_o(1))\}$, and where \mathcal{A}^{sat} is their complement. Note that $f(\Upsilon; S)|_{\mathcal{A}^{\text{dead}} \cup \mathcal{A}^{\text{unsat}}} = f_2(\Upsilon; S)$.

Next we find an improved initial guess for (29) away from the singularity at $S_{w,r}$. We define $\tilde{S}_w(\Upsilon; S) := S + f(\Upsilon; S)$. It is clear that S_w is a solution to (29) iff it is a fixed point of

$$\tilde{S}_w(\Upsilon; S_w) = S_w. \tag{41}$$

From the proof of Lemma 2 we see that as $S \rightarrow S_{w,r}^+$, $\tilde{P}_o(S) \rightarrow \infty$ and $\tilde{S}_w(S_{w,r}^+) = 1 - N_O B_o^{\min}$. Consider $\Upsilon \in \mathcal{A}^{\text{dead}}$, $S \in \mathcal{A}_S$. From $\partial \tilde{S}_w(S) / \partial S = \partial f(\Upsilon; S) / \partial S + 1 \leq 0$, we get $\tilde{S}_w(S_{w,r}^+) > \tilde{S}_w(S) \geq \tilde{S}_w(1)$. Therefore, a solution S_w must satisfy $\tilde{S}_w(S_{w,r}) > S_w = \tilde{S}_w(S_w) \geq \tilde{S}_w(1) = 1 - N_O B_{do}(\tilde{P}_o(1))$. This lower bound can be used to find the *left bracket* $S_{w,\min} = \max\{\tilde{S}_w(1), S_{w,r}\}$ for S_w which, if only $N_O < (1 - S_{w,r}) / B_{do}(\tilde{P}_o(1))$, is away from singularity. We can further iterate on this argument since now $S_{w,\min} \leq S_w$ therefore $S_w = \tilde{S}_w(S_w) \leq \tilde{S}_w(S_{w,\min})$ which allows us to find the *right bracket* $S_{w,\max} = \min\{\tilde{S}_w(S_{w,\min}), 1\}$ away from $S = 1$.

It is not difficult to see that the above procedure is similar to Picard's iteration $S^{k+1} = \tilde{S}_w(S^k)$, $k = 1, 2, \dots$ with the initial guess $S^0 = 1$. In general, its convergence is not guaranteed and thus it could not replace the solver. However, it can substantially reduce the size of the initial bracket when $\Upsilon \in \mathcal{A}_\Upsilon^{\text{dead}} \cup \mathcal{A}_\Upsilon^{\text{unsat}}$ and in some cases also when $\Upsilon \in \mathcal{A}_\Upsilon^{\text{sat}}$. Our computational experiments showed that the bracketing procedure can reduce the number of iterations of the local solver to just a few (two or three) depending on the case.

4.3.4. Summary: Comparison of $\Upsilon = (P_o, N_O, N_G)$ and $\Upsilon = (P_w, N_O, N_G)$

As reported in Examples 2 and 3, the apparent difficulty associated with choosing P_w in Υ is that it leads to a local nonlinear problem which can be computationally expensive. On the other hand, if P_o is included in Υ , then an implicit relationship arises only in three-phase conditions. In other words, in the map $\Upsilon \mapsto S_w$, $\Upsilon \in \mathcal{A}_\Upsilon^{\text{dead}} \cup \mathcal{A}_\Upsilon^{\text{unsat}}$ is explicit when P_o is used but is implicit when P_w is used.

It is natural therefore to compare the efficiency of the local solver of (29) to the cost of its explicit evaluation when $\Upsilon \in \mathcal{A}_\Upsilon^{\text{dead}} \cup \mathcal{A}_\Upsilon^{\text{unsat}}$. Thanks to the fixed-point bracketing method which works well if $\Upsilon \in \mathcal{A}_\Upsilon^{\text{dead}} \cup \mathcal{A}_\Upsilon^{\text{unsat}}$, (29) can be solved in just a few iterations. Since the explicit calculation can be considered as an equivalent of one iteration, no significant disadvantage in using $\Upsilon = (P_w, N_O, N_G)$ over $\Upsilon = (P_o, N_O, N_G)$ exists, at least, as concerns the resolution of the local map (29). More comprehensive comparison is outside our scope.

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