SIAM J. NUMER. ANAL.
Vol. 38, No. 2, pp. 489–514

FORMULATIONS AND NUMERICAL METHODS OF THE BLACK OIL MODEL IN POROUS MEDIA*

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Abstract. The black oil model for describing the hydrocarbon equilibrium in porous media is considered in this paper. Various formulations of the governing equations that describe this model, including phase, weighted fluid, global, and pseudoglobal pressure-saturation formulations with the total velocity and flux, are first constructed. These formulations are more suitable for their mathematical and numerical analysis. Finite element approximate procedures are then analyzed. These procedures are based on the use of mixed finite element methods for the pressure equations and Galerkin finite element methods for the saturation equations. Error estimates are stated first for the case where capillary diffusion coefficients are assumed to be uniformly positive. Then an error analysis is carried out in detail for a degenerate case where these coefficients can be zero.

Key words. mixed methods, finite elements, the black oil model, porous media, error estimate, mass transfer, degeneracy

AMS subject classifications. 65N30, 65N10, 76S05, 76T05

PII. S0036142999304263

1. Introduction.

There has been extensive literature on numerical methods for solving the equations that describe fluid flow in porous media (see, e.g., [6, 13, 30, 39] and the references therein). In conjunction with this literature, there has been intensive research into the analysis of these methods (see, e.g., [5, 22, 25, 26, 27, 28, 29, 30, 32, 33, 34, 40]). However, most of the models analyzed in these papers dealt with incompressible flow. A slightly compressible miscible displacement problem was treated in [22, 28, 34, 40], but the single phase only was handled, gravitational terms were omitted, and quadratic terms in velocity were ignored. While finite difference and finite element methods were considered for the black oil model in the past years (see, e.g., [8, 9, 46] and the references therein), no analysis was given. Only recently has an initial attempt been made to analyze a compressible air-water model in groundwater hydrology using finite element methods [17, 19], where two-phase fluid flow has been considered and the gravitational and quadratic terms in velocity included, but no mass transfer effects have been considered.

In this paper we analyze the black oil model often exploited for petroleum reservoir simulation. This model is a simplified compositional model for describing multiphase flow with mass interchange between phases in a porous medium. It consists of three phases (gas, oil, and water), can predict compressibility and mass transfer effects, and can be used to model a low-volatility oil system, consisting mainly of methane and heavy components, using data from a conventional differential vaporization test on reservoir oil samples (see, e.g., [7, 39]).

We first derive various formulations of the governing equations that describe the black oil model in porous media. A phase formulation, which involves a phase pressure, a total velocity (respectively, a total flux), and two saturations, can be easily

*Received by the editors April 21, 1999; accepted for publication (in revised form) March 14, 2000; published electronically July 19, 2000. This research is supported in part by National Science Foundation grants DMS-9626179, DMS-9972147, and INT-9901498, and by a gift grant from the Mobil Technology Company.

http://www.siam.org/journals/sinum/38-2/30426.html

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obtained by manipulating these governing equations under physically reasonable conditions. The drawback of this formulation is a strong coupling between the pressure and saturation equations. On the other hand, a global formulation, which involves a global pressure, a total velocity (respectively, a total flux), and two saturations, can be derived under a so-called total differential condition on the shape of three-phase relative permeability and capillary pressure functions. The advantage of this global formulation is that much less coupling occurs between the pressure and saturation equations as in the two-phase flow [3, 13, 17, 19, 21]. Thus, this global approach is more efficient than the phase approach from the mathematical and computational point of view. In the two-phase flow, the governing equations can be manipulated to have the global form under physically reasonable assumptions. The complexity of the three-phase relative permeability and capillary pressure curves complicates the derivation of the global form for the three-phase flow. In fact, the total differential condition is necessary and sufficient for the governing equations to be written in terms of a global pressure and two saturations. Due to this, other formulations such as weighted fluid (with saturations as weights) and pseudoglobal formulations are also developed. A comparison between all these formulations is described. We mention that the global formulation with the total flux for the black oil model has been considered in [13] and other formulations derived here seem new for this model. Also, the "volume discrepancy" approach has been utilized in numerical methods of this model [1, 46, 47]. In this approach, the volume balance equation for the saturations is satisfied approximately, while it is satisfied exactly in our approach. Furthermore, in their formulations the capillary pressures have been neglected, while they are included here.

We then develop and analyze finite element approximate procedures for numerically solving the pressure and saturation equations in the various formulations. It is known that the physical transport dominates the diffusive effects in incompressible flow. In the black oil model studied in this paper, the transport again dominates the entire process. Hence, it is important to obtain good approximate velocities. This motivates the use of mixed finite element methods for the pressure equations [26]. Also, due to their convection-dominated feature, more efficient approximate methods should be used to solve the saturation equations (see, e.g., the references in [29, 18, 19]). However, since the black oil model is analyzed for the first time using finite element methods, it is of some importance to establish the standard finite element analysis. We mention that the mixed finite element method based on the Brezzi–Douglas–Marini space of degree one [12] has been recently used for the numerical solution of this model [9]. In the analysis in this paper, all existing mixed finite element spaces will be considered.

Error estimates are stated first for the case where capillary diffusion coefficients are assumed to be uniformly positive. In this case, error estimates of optimal order in the L^2-norm and almost optimal order in the L^∞-norm are obtained. The derivation of these error estimates follows from those obtained in [19] for two-phase immiscible flow. Then an error analysis is carried out in detail for a degenerate case where the diffusion coefficients can be zero. The error analysis does not use any regularization of the saturation equations. It is based directly on the fully degenerate equations, it does not impose any restriction on the nature of degeneracy in diffusivity, and it respects the minimal regularity on the solution of the differential systems. This is in strong contrast with the analysis given in [35, 42, 43] for much simpler flow problems, where a regularization of the saturation equations was utilized, the nature of degeneracy was imposed, and strong regularity on the solution was assumed. Sharp error estimates in various norms are obtained here for the degenerate case.

The rest of the paper is organized as follows. In section 2, we derive the formulations of the governing equations that describe the black oil model. Then, in section 3 we develop the finite element approximate procedures in the uniformly positive case; both semidiscrete and fully discrete versions are considered. Finally, in section 4 the degenerate case is described.

We end this section with three remarks. First, the derivation and analysis of the various formulations of the black oil model in this paper provide a mathematical background for the numerical solution of fluid flows exploiting this model in porous media. Second, the error analysis shows that optimal estimates can be obtained for the finite element procedure proposed here for this model in the case where the capillary diffusion coefficients are uniformly positive and the solutions are sufficiently smooth. However, in real applications, these coefficients can be zero and the solutions typically lack in regularity. Hence, these error estimates become useless in the realistic case since the constants appearing in them depend on the coefficients and solution regularity. It is for this reason that a technique is developed here, which respects the degeneracy and minimal regularity. Also, it leads to error estimates useful in practical computations. Third, it would be interesting to compare all the formulations developed from the computational point of view. This would involve tremendous work and will be a future investigation.

2. Formulations. In this section we formulate the black oil model in such a way that main physical properties inherent in the governing equations and constraints are preserved, the nonlinearity and coupling among the equations are weakened, and efficient numerical methods for the solution of the resulting system can be devised. In this model it is assumed that no mass transfer occurs between the water phase and the other two phases (gas and oil). In the hydrocarbon (gas-oil) system, only two components are considered. The "oil" component (also called stock-tank oil) is the residual liquid at atmospheric pressure left after a differential vaporization, while the "gas" component is the remaining fluid in a porous medium $\Omega \subset \Re^d$, $d = 2$ or 3.

Let ϕ and k denote the porosity and absolute permeability of the porous system, s_α, μ_α, ρ_α, p_α, u_α, b_α, $k_{r\alpha}$, and q_α the α-phase saturation, viscosity, density, pressure, volumetric velocity, formation factor, relative permeability, and external source term, respectively, $\alpha = g, o, w$, r_{so} the gas solubility, $\tilde{g}$ the gravitational, downward-pointing, constant vector, and $J = (0, T]$ $(T > 0)$ the time interval of interest. Set $\Omega_T = \Omega \times J$. Then the black oil model is described by (see, e.g., [7, 39])

$$\begin{aligned}
&\phi\frac{\partial}{\partial t}\left(\frac{s_g}{b_g} + \frac{r_{so}s_o}{b_o}\right) + \nabla\cdot\left(\frac{1}{b_g}u_g + \frac{r_{so}}{b_o}u_o\right) = q_g, \quad && (x,t) \in \Omega_T,\\
&\phi\frac{\partial}{\partial t}\left(\frac{s_o}{b_o}\right) + \nabla\cdot\left(\frac{1}{b_o}u_o\right) = q_o, && (x,t) \in \Omega_T,\\
&\phi\frac{\partial}{\partial t}\left(\frac{s_w}{b_w}\right) + \nabla\cdot\left(\frac{1}{b_w}u_w\right) = q_w, && (x,t) \in \Omega_T,
\end{aligned} \tag{2.1}$$

where the volumetric velocity of the α-phase is given by

$$u_\alpha = -\frac{kk_{r\alpha}}{\mu_\alpha}(\nabla p_\alpha - \rho_\alpha \tilde{g}), \quad (x,t) \in \Omega_T,\ \alpha = g, o, w. \tag{2.2}$$

The equations in (2.1) do not represent mass balances but, rather, balances on "standard volumes" [39]. In addition to (2.1) and (2.2), we have also the customary property for the saturations,

$$\sum_{\beta} s_\beta = 1, \tag{2.3}$$

where $\sum_\beta = \sum_{\beta=g,o,w}$, and we define, for notational convenience, the capillary pressure functions,

$$p_{c\alpha o} = p_\alpha - p_o, \quad \alpha = g, o, w, \tag{2.4}$$

where $p_{coo} \equiv 0$, p_{cgo} represents the gas phase capillary pressure and p_{cwo} is the negative water phase capillary pressure.

2.1. Phase formulation.

2.1.1. Phase formulation with the total velocity. For expositional convenience, we introduce the phase mobility functions

$$\lambda_\alpha = k_{r\alpha}/\mu_\alpha, \quad \alpha = g, o, w,$$

and the total mobility

$$\lambda = \sum_\beta \lambda_\beta.$$

Also, we define the fractional flow functions

$$f_\alpha = \lambda_\alpha/\lambda, \quad \alpha = g, o, w,$$

so that $\sum_\beta f_\beta = 1$.

Oil being a continuous phase implies that p_o is well behaved, so we use the oil phase pressure as the pressure variable in this subsection:

$$p = p_o. \tag{2.5}$$

We now define the total velocity:

$$u = \sum_\beta u_\beta. \tag{2.6}$$

Then, we use (2.5) and (2.6), carry out the differentiation indicated in (2.1), and apply (2.2)–(2.4) to obtain the differential equations with $(x,t) \in \Omega_T$:

$$\begin{aligned} u &= -k\lambda \left(\nabla p - G_\lambda + \sum_\beta f_\beta \nabla p_{c\beta o} \right), \\ \nabla \cdot u &= \sum_\beta b_\beta \left(q_\beta - \phi s_\beta \frac{\partial}{\partial t}\left(\frac{1}{b_\beta}\right) - u_\beta \cdot \nabla \left(\frac{1}{b_\beta}\right)\right) \\ &\quad - b_g \left(r_{so} q_o + \frac{\phi s_o}{b_o}\frac{\partial r_{so}}{\partial t} + \frac{1}{b_o} u_o \cdot \nabla r_{so} \right) \end{aligned} \tag{2.7}$$

and

$$\begin{aligned}\phi\frac{\partial s_\alpha}{\partial t} + \nabla\cdot u_\alpha &= b_\alpha\left(q_\alpha - \phi s_\alpha\frac{\partial}{\partial t}\left(\frac{1}{b_\alpha}\right) - u_\alpha\cdot\nabla\left(\frac{1}{b_\alpha}\right)\right),\\ u_\alpha &= f_\alpha u + kf_\alpha\sum_\beta \lambda_\beta\big(\nabla(p_{c\beta o} - p_{c\alpha o}) - (\rho_\beta - \rho_\alpha)\tilde{g}\big)\end{aligned} \tag{2.8}$$

for $\alpha = o, w$, where

$$G_\lambda = \tilde{g}\sum_\beta f_\beta\rho_\beta.$$

The equations in (2.7) and (2.8) are, respectively, the pressure and saturation equations.

2.1.2. Phase formulation with the total flux. In the right-hand sides of the second equation of (2.7) and the first equation of (2.8) appear the quadratic terms in the velocities. To get rid of these terms, we now introduce the total flux. Toward that end, set

$$\lambda_g = \frac{k_{rg}}{b_g\mu_g},\quad \lambda_o = \frac{1+r_{so}}{b_o\mu_o}k_{ro},\quad \lambda_w = \frac{k_{rw}}{b_w\mu_w},\quad \lambda = \sum_\beta \lambda_\beta$$

and

$$f_\alpha = \lambda_\alpha/\lambda,\quad \alpha = g, o, w.$$

The pressure variable is defined as in (2.5) and the total flux is now given by

$$u = \sum_\beta \frac{1}{b_\beta}u_\beta + \frac{r_{so}}{b_o}u_o. \tag{2.9}$$

Then with the same manipulation on (2.1) as above, we have the pressure and saturation equations with $(x,t)\in\Omega_T$:

$$\begin{aligned} u &= -k\lambda\left(\nabla p - G_\lambda + \sum_\beta f_\beta\nabla p_{c\beta o}\right),\\ \phi\frac{\partial}{\partial t}&\left(\sum_\beta\frac{s_\beta}{b_\beta} + \frac{s_o r_{so}}{b_o}\right) + \nabla\cdot u = \sum_\beta q_\beta,\end{aligned} \tag{2.10}$$

and

$$\phi\frac{\partial}{\partial t}\left(\frac{s_\alpha}{b_\alpha}\right) + \nabla\cdot\left(\frac{1}{b_\alpha}u_\alpha\right) = q_\alpha,\quad \alpha = o, w, \tag{2.11}$$

where

$$\begin{aligned} u_o &= \frac{b_o}{1+r_{so}}\left\{f_o u + kf_o\sum_\beta\lambda_\beta\big(\nabla p_{c\beta o} - (\rho_\beta - \rho_o)\tilde{g}\big)\right\},\\ u_w &= b_w\left\{f_w u + kf_w\sum_\beta\lambda_\beta\big(\nabla(p_{c\beta o} - p_{cwo}) - (\rho_\beta - \rho_w)\tilde{g}\big)\right\}.\end{aligned} \tag{2.12}$$

2.2. Weighted fluid formulation. We now define a smoother pressure than the phase pressure given in (2.5). Namely, we define the weighted fluid pressure

$$p = \sum_{\alpha} s_\alpha p_\alpha. \tag{2.13}$$

Note that even if some saturation is zero (i.e., some phase disappears), we still have a nonzero smooth variable p. By (2.3) and (2.4), the phase pressures are given by

$$p_\alpha = p + p_{c\alpha o} - \sum_{\beta} s_\beta p_{c\beta o}, \qquad \alpha = g,\, o,\, w.$$

As an example, we develop the weighted fluid formulation with the total flux only; the total velocity formulation is similarly obtained as in section 2.1.1. Then we define the phase and total mobilities, the fractional flow functions, and the total flux as in section 2.1.2. Now, apply (2.1) and (2.2) to see that

$$\begin{aligned} u &= -k\lambda \left(\nabla p - G_\lambda + \sum_{\beta} f_\beta \nabla p_{c\beta o} - \sum_{\beta} \nabla (s_\beta p_{c\beta o}) \right), \\ \phi \frac{\partial}{\partial t} &\left(\sum_{\beta} \frac{s_\beta}{b_\beta} + \frac{s_o r_{so}}{b_o} \right) + \nabla \cdot u = \sum_{\beta} q_\beta. \end{aligned} \tag{2.14}$$

The saturation equations and the relationships between the phase velocities and the total flux are the same as in (2.11) and (2.12).

2.3. Global formulation.

2.3.1. Global formulation with the total velocity. The phase and total mobilities and the fractional flow functions are defined in the same manner as in section 2.1.1. To introduce a global pressure, we assume that the fractional flow functions f_α depend solely on the saturations s_w and s_g (for pressure-dependent functions f_α, see the next subsection) and there exists a function $(s_w, s_g) \longmapsto p_c(s_w, s_g)$ such that

$$\nabla p_c = f_w \nabla p_{cwo} + f_g \nabla p_{cgo}. \tag{2.15}$$

This holds if and only if the following equations are satisfied:

$$\begin{aligned} \frac{\partial p_c}{\partial s_w} &= f_w \frac{\partial p_{cwo}}{\partial s_w} + f_g \frac{\partial p_{cgo}}{\partial s_w}, \\ \frac{\partial p_c}{\partial s_g} &= f_w \frac{\partial p_{cwo}}{\partial s_g} + f_g \frac{\partial p_{cgo}}{\partial s_g}. \end{aligned} \tag{2.16}$$

A necessary and sufficient condition for existence of a function p_c satisfying (2.16) is

$$\frac{\partial f_w}{\partial s_g}\frac{\partial p_{cwo}}{\partial s_w} + \frac{\partial f_g}{\partial s_g}\frac{\partial p_{cgo}}{\partial s_w} = \frac{\partial f_w}{\partial s_w}\frac{\partial p_{cwo}}{\partial s_g} + \frac{\partial f_g}{\partial s_w}\frac{\partial p_{cgo}}{\partial s_g}. \tag{2.17}$$

This condition is referred to as the total differential condition [13, 20]. When the condition (2.17) is satisfied, the function p_c is determined by

$$\begin{aligned} p_c(s_w, s_g) = &\int_1^{s_w} \left\{ f_w(\xi, 0) \frac{\partial p_{cwo}}{\partial s_w}(\xi, 0) + f_g(\xi, 0) \frac{\partial p_{cgo}}{\partial s_w}(\xi, 0) \right\} d\xi \\ &+ \int_0^{s_g} \left\{ f_w(s_w, \xi) \frac{\partial p_{cwo}}{\partial s_g}(s_w, \xi) + f_g(s_w, \xi) \frac{\partial p_{cgo}}{\partial s_g}(s_w, \xi) \right\} d\xi, \end{aligned} \tag{2.18}$$

where we assume that the above integrals are well-defined, which is always true in practical situations [13]. We now introduce the global pressure by

$$p = p_o + p_c, \tag{2.19}$$

and we introduce the total velocity as in (2.6). Now, use the condition (2.17), the definitions in (2.18) and (2.19), and the same calculations as in section 2.1.1 to obtain the pressure and saturation equations with $(x,t) \in \Omega_T$:

$$\begin{aligned} u &= -k\lambda(\nabla p - G_\lambda), \\ \nabla \cdot u &= \sum_\beta b_\beta \left(q_\beta - \phi s_\beta \frac{\partial}{\partial t}\left(\frac{1}{b_\beta}\right) - u_\beta \cdot \nabla \left(\frac{1}{b_\beta}\right)\right) \\ &\quad - b_g \left(r_{so} q_o + \frac{\phi s_o}{b_o}\frac{\partial r_{so}}{\partial t} + \frac{1}{b_o} u_o \cdot \nabla r_{so}\right) \end{aligned} \tag{2.20}$$

and

$$\begin{aligned} &\phi \frac{\partial s_\alpha}{\partial t} + \nabla \cdot u_\alpha = b_\alpha \left(q_\alpha - \phi s_\alpha \frac{\partial}{\partial t}\left(\frac{1}{b_\alpha}\right) - u_\alpha \cdot \nabla\left(\frac{1}{b_\alpha}\right)\right), \\ &u_\alpha = f_\alpha u + k\lambda_\alpha\big(\nabla(p_c - p_{c\alpha o}) - \delta_\alpha\big), \end{aligned} \tag{2.21}$$

for $\alpha = o, w$, where

$$\begin{aligned} \delta_\alpha =& \left(f_\beta(\rho_\beta - \rho_\alpha) + f_\gamma(\rho_\gamma - \rho_\alpha)\right)\tilde{g}, \\ & \qquad \alpha, \beta, \gamma = g, o, w, \ \alpha \neq \beta, \beta \neq \gamma, \gamma \neq \alpha. \end{aligned}$$

2.3.2. Global formulation with the total flux. As in the phase formulation, to get rid of the quadratic terms in the velocities in the second equation of (2.20) and the first equation of (2.21), we define the phase and total mobilities, the fractional flow functions, and the total flux as in section 2.1.2. In the present case we assume that the solubility factor r_{so}, the formation factors b_α, and the viscosity functions μ_α depend only on their respective phase pressure. This assumption is physically reasonable [2, 13]. Furthermore, to derive a global pressure p, we assume that these functions essentially depend on p. The second assumption ignores the error caused by calculating them for the α-phase at p instead of p_α. For details on this error, which introduces lower order terms in partial differential equations, the reader is referred to [17] for a similar treatment in the two-phase flow. With these, the fractional flow functions f_α depend only on the saturations s_w and s_g and a global pressure p.

We now assume that there exists a function $(s_w, s_g, p) \longmapsto p_c(s_w, s_g, p)$ satisfying

$$\nabla p_c = f_w \nabla p_{cwo} + f_g \nabla p_{cgo} + \frac{\partial p_c}{\partial p}\nabla p. \tag{2.22}$$

With the same argument as in section 2.3.1, a necessary and sufficient condition for existence of a function p_c satisfying (2.22) is (2.17), where p is treated as a parameter. Under this condition, the function p_c is described by

$$\begin{aligned} p_c(s_w, s_g, p) = & \int_1^{s_w} \left\{ f_w(\xi, 0, p)\frac{\partial p_{cwo}}{\partial s_w}(\xi, 0) + f_g(\xi, 0, p)\frac{\partial p_{cgo}}{\partial s_w}(\xi, 0)\right\} d\xi \\ & + \int_0^{s_g} \left\{ f_w(s_w, \xi, p)\frac{\partial p_{cwo}}{\partial s_g}(s_w, \xi) + f_g(s_w, \xi, p)\frac{\partial p_{cgo}}{\partial s_g}(s_w, \xi)\right\} d\xi. \end{aligned} \tag{2.23}$$

With the same global pressure as in (2.19), we can derive the pressure and saturation equations with $(x,t) \in \Omega_T$:

$$u = -k\lambda(\omega \nabla p - G_\lambda),$$

$$\phi \frac{\partial}{\partial t}\left(\sum_\beta \frac{s_\beta}{b_\beta} + \frac{s_o r_{so}}{b_o}\right) + \nabla \cdot u = \sum_\beta q_\beta \tag{2.24}$$

and

$$\phi \frac{\partial}{\partial t}\left(\frac{s_\alpha}{b_\alpha}\right) + \nabla \cdot \left(\frac{1}{b_\alpha} u_\alpha\right) = q_\alpha, \quad \alpha = o, w, \tag{2.25}$$

where

$$u_o = \frac{b_o}{1 + r_{so}}\left\{\omega^{-1} f_o u + k\lambda_o(\nabla p_c - \delta_o) - \omega^{-1}\frac{\partial p_c}{\partial p} G_\lambda\right\},$$
$$u_w = b_w\left\{\omega^{-1} f_w u + k\lambda_w(\nabla(p_c - p_{cwo}) - \delta_w) - \omega^{-1}\frac{\partial p_c}{\partial p} G_\lambda\right\}$$

and

$$\omega(s_w, s_g, p) = 1 - \frac{\partial p_c}{\partial p}.$$

2.4. Pseudoglobal pressure formulation. The global pressure formulation in the previous subsection requires the total differential condition (2.17) on the shape of three-phase relative permeability and capillary pressure functions. In this subsection, as introduced in [20] for immiscible problems, we finally consider a pseudoglobal pressure formulation, which does not require this condition. As an example, we consider this formulation with the total velocity. The formulation with the total flux can be obtained as in section 2.3.2.

Assume that the capillary pressures satisfy the usual condition

$$p_{cwo} = p_{cwo}(s_w), \quad p_{cgo} = p_{cgo}(s_g). \tag{2.26}$$

We then introduce the mean values

$$\widehat{f_w}(s_w) = \frac{1}{1 - s_w}\int_0^{1-s_w} f(s_w, \zeta) \mathrm{d}\zeta,$$
$$\widehat{f_g}(s_g) = \frac{1}{1 - s_g}\int_0^{1-s_g} f_g(\zeta, s_g) \mathrm{d}\zeta, \tag{2.27}$$

and the pseudoglobal pressure

$$p = p_o + \int_{s_{wc}}^{s_w} \widehat{f_w}(\zeta)\frac{dp_{cwo}(\zeta)}{ds_w}\mathrm{d}\zeta + \int_{s_{gc}}^{s_g} \widehat{f_g}(\zeta)\frac{dp_{cgo}(\zeta)}{ds_g}\mathrm{d}\zeta,$$

where s_{wc} and s_{gc} are such that $p_{cwo}(s_{wc}) = 0$ and $p_{cgo}(s_{gc}) = 0$. Now, apply these definitions to (2.7) to find that

$$u = -k\lambda\left\{\nabla p - G_\lambda + \sum_\alpha \left(f_\alpha - \widehat{f_\alpha}\right)\frac{dp_{c\alpha o}}{ds_\alpha}\nabla s_\alpha\right\},$$
$$\nabla \cdot u = \sum_\beta b_\beta\left(q_\beta - \phi s_\beta \frac{\partial}{\partial t}\left(\frac{1}{b_\beta}\right) - u_\beta \cdot \nabla\left(\frac{1}{b_\beta}\right)\right)$$
$$-b_g\left(r_{so} q_o + \frac{\phi s_o}{b_o}\frac{\partial r_{so}}{\partial t} + \frac{1}{b_o} u_o \cdot \nabla r_{so}\right).$$

Other equations are given as in (2.8).

2.5. Remarks on the formulations. The four pressure formulations developed above have similar structures as those developed in [20] for the flow of immiscible fluids, where a numerical comparison was given. A similar comparison for the black oil model under consideration is beyond the scope of this paper (an error analysis is emphasized instead). Here we just make a few remarks from the above derivations and observations made in [20].

The global formulation is far more efficient than the phase and pseudoglobal formulations from the computational point of view and also more suitable for mathematical analysis since the coupling between the pressure and saturation equations is much less. The weakness of the global formulation is the need of the satisfaction of the total differential condition (2.17) by the three-phase relative permeability and capillary pressure curves. In general, the phase (or the weighted fluid) formulation can be applied. However, if the fractional flow functions of the water and gas phases are close to their respective mean values as defined in (2.27), the pseudoglobal formulation is more useful. In the (unphysical) case where the capillary pressures p_{cgo} and p_{cwo} are zero, all the formulations are the same. Finally, we remark, as mentioned in the introduction, that the global formulation with the total flux for the black oil model has been considered in [13], and other formulations derived in this paper seem new for this model.

3. Finite elements in the positive case. In this and the next sections we develop finite element approximate procedures for numerically solving the partial differential equations developed in the previous section. As an example, we consider the global formulation with the total velocity, which is representative in that it involves the global concept so that the same analysis can be easily done for the global formulation with the total flux, and it contains the quadratic terms in velocity so that a similar analysis can be extended to other formulations. In this section we consider the case where capillary diffusion coefficients are assumed to be uniformly positive, and we indicate how to obtain error estimates from those in [17, 19].

3.1. The differential model. To adopt the numerical analysis used in the two-phase immiscible flow [17, 19], we now write the differential model in (2.20) and (2.21) in a slightly different form. For this, we introduce the following coefficients:

$$q(p) = \sum_\beta b_\beta q_\beta - b_g r_{so} q_o,$$

$$c(s_o, s_w, p) = \phi \left(\sum_\beta s_\beta b_\beta \frac{d}{dp}\left(\frac{1}{b_\beta}\right) + \frac{s_o b_g}{b_o}\frac{dr_{so}}{dp} \right),$$

$$d_0(s_o, s_w, p) = -\sum_\beta b_\beta \frac{d}{dp}\left(\frac{1}{b_\beta}\right) k\lambda_\beta \delta_\beta - \frac{b_g}{b_o}\frac{dr_{so}}{dp} k\lambda_o \delta_o,$$

$$d_1(s_o, s_w, p) = \sum_\beta b_\beta \frac{d}{dp}\left(\frac{1}{b_\beta}\right) f_\beta + \frac{b_g}{b_o}\frac{dr_{so}}{dp} f_o,$$

$$d_\alpha(s_o, s_w, p) = \sum_\beta b_\beta k\lambda_\beta \frac{d}{dp}\left(\frac{1}{b_\beta}\right) \frac{\partial(p_c - p_{c\beta o})}{\partial s_\alpha} + k\lambda_o \frac{b_g}{b_o}\frac{dr_{so}}{dp}\frac{\partial p_c}{\partial s_\alpha}, \quad \alpha = o, w,$$

$$\theta_\alpha(s_o, s_w, p) = b_\alpha \left(q_\alpha - \phi s_\alpha c^{-1} q(p) \frac{d}{dp}\left(\frac{1}{b_\alpha}\right) \right), \quad \alpha = o, w,$$

$$\eta_\alpha(s_o, s_w, p) = \phi s_\alpha b_\alpha c^{-1} \frac{d}{dp}\left(\frac{1}{b_\alpha}\right), \quad \alpha = o, w,$$

$$g_{\alpha 0}(s_o, s_w, p) = b_\alpha \left(\phi s_\alpha c^{-1} d_0 + k\lambda_\alpha \delta_\alpha\right) \frac{d}{dp}\left(\frac{1}{b_\alpha}\right), \quad \alpha = o, w,$$

$$g_{\alpha 1}(s_o, s_w, p) = b_\alpha \left(\phi s_\alpha c^{-1} d_1 - f_\alpha\right) \frac{d}{dp}\left(\frac{1}{b_\alpha}\right), \quad \alpha = o, w,$$

$$g_{\alpha\beta}(s_o, s_w, p) = b_\alpha \left(\phi s_\alpha c^{-1} d_\beta - k\lambda_\alpha \frac{\partial(p_c - p_{c\alpha o})}{\partial s_\beta}\right) \frac{d}{dp}\left(\frac{1}{b_\alpha}\right), \quad \alpha, \beta = o, w,$$

$$D_{\alpha\beta}(s_o, s_w) = -k\lambda_\alpha \frac{\partial(p_c - p_{c\alpha o})}{\partial s_\beta}, \quad \alpha, \beta = o, w.$$

Then (2.20) and (2.21) can be written as follows with $(x,t) \in \Omega_T$:

$$\begin{aligned} &u = -k\lambda(\nabla p - G_\lambda), \\ &c\frac{\partial p}{\partial t} + \nabla \cdot u = q(p) - \big(d_0 + d_1 u + d_o \nabla s_o + d_w \nabla s_w\big) \cdot \nabla p, \end{aligned} \tag{3.1}$$

and

$$\begin{aligned} \phi\frac{\partial s_\alpha}{\partial t} &- \nabla \cdot \big(D_{\alpha o}\nabla s_o + D_{\alpha w}\nabla s_w - f_\alpha u + k\lambda_\alpha \delta_\alpha\big) \\ &= \theta_\alpha + \eta_\alpha \nabla \cdot u + \big(g_{\alpha 0} + g_{\alpha 1} u + g_{\alpha o}\nabla s_o + g_{\alpha w}\nabla s_w\big) \cdot \nabla p, \quad \alpha = o, w. \end{aligned} \tag{3.2}$$

The model is completed by specifying the boundary and initial conditions. For simplicity we consider no flow boundary conditions

$$u_\alpha \cdot \nu = 0, \quad (x,t) \in \partial\Omega \times J, \quad \alpha = g, o, w, \tag{3.3}$$

where ν is the outer unit normal to $\partial\Omega$. Other types of boundary conditions can be handled similarly [17, 19, 21] (see how to handle the Dirichlet boundary condition in the next section, for example). From the definition of the total velocity (2.6), we have

$$u \cdot \nu = 0, \quad (x,t) \in \partial\Omega \times J, \tag{3.4}$$

and from the second equation of (2.21)

$$\begin{aligned} &\big(D_{\alpha o}\nabla s_o + D_{\alpha w}\nabla s_w - f_\alpha u + k\lambda_\alpha \delta_\alpha\big) \cdot \nu = 0, \\ &\qquad\qquad (x,t) \in \partial\Omega \times J, \quad \alpha = o, w. \end{aligned} \tag{3.5}$$

The initial conditions are given by

$$\begin{aligned} p(x,0) &= p^0(x), \qquad && x \in \Omega, \\ s_\alpha(x,0) &= s_\alpha^0(x), \qquad && x \in \Omega,\ \alpha = o, w. \end{aligned} \tag{3.6}$$

The unknowns are s_o, s_w, p, and u.

The analysis for the nondegenerate case in this section is given under a number of assumptions. First, the solution is assumed smooth; i.e., the external source terms are smoothly distributed, the coefficients are smooth, the boundary and initial data satisfy the compatibility condition, and the domain has at least the regularity required for a standard elliptic problem to have $H^2(\Omega)$-regularity and more if error estimates of an order bigger than one are required. Second, the coefficients $a(s_o, s_w) = k\lambda$, ϕ, and $c(s_o, s_w, p)$ are assumed to be bounded positively below:

$$
\begin{aligned}
&0 < a_* \le a(s_o, s_w) \le a^* < \infty, \\
&0 < \phi_* \le \phi(x) \le \phi^* < \infty, \\
&0 < c_* \le c(s_o, s_w, p) \le c^* < \infty.
\end{aligned}
\tag{3.7}
$$

While the phase mobilities can be zero, the total mobility is always positive [39, 44]. The assumptions in (3.7) are physically reasonable. In the case of k being a tensor, we assume that $a(s_o, s_w)$ is uniformly positive definite. Also, the present analysis obviously applies to the incompressible case where $c(s_o, s_w, p) = 0$ (c is the total compressibility). In this case, the analysis is simpler since we have an elliptic pressure equation instead of the parabolic equation (3.2). Thus we assume that the condition in the third equation of (3.7) holds for the compressible case under consideration. Next, with the definition

$$
D(s_o, s_w) = \begin{pmatrix} D_{oo} & D_{ow} \\ D_{wo} & D_{ww} \end{pmatrix},
$$

we assume its uniform boundedness and positive definiteness,

$$
D_* \zeta^t \zeta \le \zeta^t D \zeta \le D^* \zeta^t \zeta, \qquad \zeta \in \Re^2,
\tag{3.8}
$$

with fixed constants D_*, $D^* > 0$, where ζ^t denotes the transpose of the column vector ζ. As a final remark, we mention that for the case where point sources and sinks occur in a porous medium, an argument was given in [33] for the incompressible miscible displacement problem and can be extended to the present case.

3.2. Semidiscrete version. Let

$$
\begin{aligned}
&H(\mathrm{div}, \Omega) = \{v \in (L^2(\Omega))^d : \nabla \cdot v \in L^2(\Omega),\ d = 2 \text{ or } 3\}, \\
&V = \{v \in H(\mathrm{div}, \Omega) : v \cdot \nu = 0 \text{ on } \partial\Omega\}.
\end{aligned}
$$

Below $\mathcal{C}$ denotes a generic positive constant. For $0 < h_p < 1$ and $0 < h < 1$, let T_{h_p} and T_h be quasi-uniform partitions into elements, say, simplexes, rectangular parallelepipeds, and/or prisms. In both partitions, we also need that adjacent elements completely share their common edge or face and that the boundary edge of a boundary element can be curved. Let $M_h \subset W^{1,\infty}(\Omega)$ be a standard C^0-finite element space associated with T_h such that

$$
\inf_{\psi \in M_h} \|v - \psi\|_{W^{1,\pi}(\Omega)} \le \mathcal{C} \left(\sum_K h_K^{2k} \|v\|^2_{W^{k+1,\pi}(K)} \right)^{1/2}, \qquad k \ge 1,\ 1 \le \pi \le \infty,
$$

where h_K =diam(K), $K \in T_h$, and $\|v\|_{W^{k,\pi}(K)}$ is the norm in the Sobolev space $W^{k,\pi}(K)$ (we have $H^k(K) = W^{k,2}(K)$ when $\pi = 2$). Also, let $V_h \times W_h = V_{h_p} \times W_{h_p} \subset V \times L^2(\Omega)$ be the Raviart–Thomas–Nédélec [41, 37], the Brezzi–Douglas–Fortin–Marini [11], the Brezzi–Douglas–Marini [12] (if $d = 2$), the Brezzi–Douglas–Durán–Fortin [10] (if $d = 3$), or the Chen–Douglas [16] mixed finite element space associated with the partition T_{h_p} of an index such that the approximation properties below are satisfied:

$$\inf_{\psi \in V_h} \|v-\psi\|_{L^2(\Omega)} \le C\left(\sum_K h_{p,K}^{2r}\|v\|_{H^r(K)}^2\right)^{1/2}, \qquad 0 \le r \le k^*+1,$$

$$\inf_{\psi \in V_h} \|\nabla\cdot(v-\psi)\|_{L^2(\Omega)} \le C\left(\sum_K h_{p,K}^{2r}\|\nabla\cdot v\|_{H^r(K)}^2\right)^{1/2}, \qquad 0 \le r \le k^{**},$$

$$\inf_{\psi \in W_h} \|w-\psi\|_{L^2(\Omega)} \le C\left(\sum_K h_{p,K}^{2r}\|w\|_{H^r(K)}^2\right)^{1/2}, \qquad 0 \le r \le k^{**},$$

where $h_{p,K}$ =diam(K), $K \in T_{h_p}$, $k^{**}=k^*+1$ for the first two spaces, $k^{**}=k^*$ for the second two spaces, and both cases are included in the last space.

The semidiscrete finite element approximate procedure is defined as follows. The approximation procedure for the pressure is defined by the mixed method for a pair of maps $\{u_h, p_h\} : J \to V_h \times W_h$ such that

$$\begin{aligned}
&(a_h^{-1}u_h, v) - (\nabla\cdot v, p_h) = (G_\lambda(s_{o,h}, s_{w,h}, p_h), v) && \forall v \in V_h,\\
&\left(c_h\frac{\partial p_h}{\partial t}, \psi\right) + (\nabla\cdot u_h, \psi) = (q(p_h), \psi)\\
&\quad -\big((d_{0,h}+d_{1,h}u_h+d_{o,h}\nabla s_{o,h}+d_{w,h}\nabla s_{w,h})\cdot\nabla p_h, \psi\big) && \forall \psi \in W_h,
\end{aligned} \tag{3.9}$$

where the discrete coefficients a_h^{-1}, etc. are calculated at $s_{o,h}$, $s_{w,h}$, and p_h,

$$\nabla p_h = -a^{-1}(s_{o,h}, s_{w,h})u_h + G_\lambda(s_{o,h}, s_{w,h}, p_h), \tag{3.10}$$

and $s_{o,h}$ and $s_{w,h} : J \to M_h$ are given by

$$\begin{aligned}
&\left(\phi\frac{\partial s_{\alpha,h}}{\partial t}, v\right) + (D_{\alpha o,h}\nabla s_{o,h} + D_{\alpha w,h}\nabla s_{w,h} - f_{\alpha,h}u_h + k\lambda_{\alpha,h}\delta_{\alpha,h}, \nabla v)\\
&\quad = (\theta_{\alpha,h} + \eta_{\alpha,h}\nabla\cdot u_h + (g_{\alpha 0,h} + g_{\alpha 1,h}u_h + g_{\alpha o,h}\nabla s_{o,h}\\
&\qquad + g_{\alpha w,h}\nabla s_{w,h})\cdot\nabla p_h, v) \qquad \forall v \in M_h,
\end{aligned} \tag{3.11}$$

for $\alpha = o$, w, where the discrete coefficients are again calculated at $s_{o,h}$, $s_{w,h}$, and p_h. The initial data $p_h(\cdot,0) = p_h^0$ and $s_{\alpha,h}(\cdot,0) = s_{\alpha,h}^0$ can be taken as their respective projections or interpolants of p^0 and s_α^0 in W_h and M_h, for example.

3.3. Error estimates. To see that the error analysis for the two-phase immiscible flow problem in [17] can be exploited for (3.9)–(3.11), we introduce the following vectors and matrix:

$$d_{ow} = \begin{pmatrix} d_o \\ d_w \end{pmatrix}, \quad s = \begin{pmatrix} s_o \\ s_w \end{pmatrix}, \quad f = \begin{pmatrix} f_o \\ f_w \end{pmatrix}, \quad \delta = \begin{pmatrix} \lambda_o\delta_o \\ \lambda_w\delta_w \end{pmatrix},$$

$$\theta = \begin{pmatrix} \theta_o \\ \theta_w \end{pmatrix}, \quad \eta = \begin{pmatrix} \eta_o \\ \eta_w \end{pmatrix}, \quad g_i = \begin{pmatrix} g_{oi} \\ g_{wi} \end{pmatrix}, \quad g = \begin{pmatrix} g_{oo} & g_{ow} \\ g_{wo} & g_{ww} \end{pmatrix}$$

for $i = 0, 1$. Then (3.1) and (3.2) can be written as a nonlinear system for p and s:

$$\begin{aligned}
&u = -k\lambda(\nabla p - G_\lambda),\\
&c\frac{\partial p}{\partial t} + \nabla\cdot u = q(p) - \big(d_0 + d_1 u + d_{ow}^t\nabla s\big)\cdot\nabla p,
\end{aligned} \tag{3.12}$$

and

$$\phi\frac{\partial s}{\partial t} - \nabla\cdot\big(D\nabla s - fu + k\delta\big) \\ = \theta + \eta\nabla\cdot u + (\nabla p\ I)\big(g_0 + g_1 u + g\nabla s\big), \tag{3.13}$$

where I is the two-by-two identity matrix. Now, we see that (3.12) and (3.13) in form resemble those in (2.9)–(2.11) in [17] with minor changes in lower order terms. Therefore, by the assumptions (3.7) and (3.8) and using the analysis in [17] for the semidiscrete version, we have the next convergence results in Theorems 3.1 and 3.2 below. Define

$$\begin{aligned}\mathcal{E} = &\sum_{K\in T_{h_p}} h_{p,K}^{k^{**}}\left(\|p\|_{L^\infty(J;H^{k^{**}}(K))} + \left\|\frac{\partial p}{\partial t}\right\|_{L^\infty(J;H^{k^{**}}(K))} + \left\|\frac{\partial^2 p}{\partial t^2}\right\|_{L^2(J;H^{k^{**}}(K))}\right)\\ &+ \sum_{K\in T_{h_p}} h_{p,K}^{k^*+1}\left(\|u\|_{L^\infty(J;H^{k^*+1}(K))} + \left\|\frac{\partial u}{\partial t}\right\|_{L^2(J;H^{k^*+1}(K))}\right)\\ &+ \sum_{K\in T_h} h_K^{k+1}\left(\|s\|_{L^\infty(J;H^{k+1}(K))} + \left\|\frac{\partial s}{\partial t}\right\|_{L^2(J;H^{k+1}(K))}\right).\end{aligned}$$

THEOREM 3.1. *Let* (u,p,s) *and* (u_h,p_h,s_h) *solve* (3.1), (3.2), *and* (3.9)–(3.11), *respectively, where* $s_h = (s_{o,h}, s_{w,h})^t$. *Then, under the assumptions* (3.7) *and* (3.8), *if the parameters* h_p *and* h *satisfy*

$$\big(h^{-d/2} + h_p^{-d/2}\big)\big(h_p^{k^*+1} + h_p^{k^{**}} + h^{k+1}\big) \to 0 \text{ as } h\to 0,\ d = 2 \text{ or } 3, \tag{3.14}$$

we have

$$\begin{aligned}&\|u-u_h\|_{L^\infty(J;L^2(\Omega))} + \|p-p_h\|_{L^\infty(J;L^2(\Omega))}\\ &+ \left\|\frac{\partial p}{\partial t} - \frac{\partial p_h}{\partial t}\right\|_{L^\infty(J;L^2(\Omega))} + \|s-s_h\|_{L^\infty(J;L^2(\Omega))}\\ &+ h\|s-s_h\|_{L^\infty(J;H^1(\Omega))} + \left\|\frac{\partial s}{\partial t} - \frac{\partial s_h}{\partial t}\right\|_{L^2(J;L^2(\Omega))} \le \mathcal{C}\mathcal{E},\end{aligned}$$

where $\mathcal{C}$ *depends upon the following quantities:*

$$\begin{aligned}\mathcal{C} = \mathcal{C}\Bigg(&\left\|\frac{\partial s}{\partial t}\right\|_{L^\infty(\Omega_T)}, \left\|\nabla\frac{\partial s}{\partial t}\right\|_{L^\infty(\Omega_T)}, \|\nabla s\|_{L^\infty(\Omega_T)},\\ &\left\|\frac{\partial p}{\partial t}\right\|_{L^\infty(\Omega_T)}, \left\|\frac{\partial^2 p}{\partial t^2}\right\|_{L^\infty(\Omega_T)}, \|u\|_{L^\infty(\Omega_T)}, \left\|\frac{\partial u}{\partial t}\right\|_{L^\infty(\Omega_T)}\Bigg).\end{aligned}$$

In the two-dimensional case, we also have the L^∞-estimates for the errors $s - s_h$ and $p - p_h$.

THEOREM 3.2. *Under the assumptions of Theorem* 3.1 *with* $d = 2$, *we have*

$$\begin{aligned}&\|p-p_h\|_{L^\infty(\Omega_T)} \le \mathcal{C}\log h_p^{-1}\big(\mathcal{E} + h_p^{k^{**}}\|p\|_{L^\infty(J;H^{k^{**}+1}(\Omega))}\big),\\ &\|s-s_h\|_{L^\infty(\Omega_T)} \le \mathcal{C}\big(\log h^{-1}\big)^\gamma\big(\mathcal{E} + h^{k+1}\|s\|_{L^\infty(J;W^{k+1,\infty}(\Omega))}\big),\end{aligned}$$

where $\gamma = 1$ *for* $k = 1$, $\gamma = 1/2$ *for* $k > 1$, *and* $\mathcal{C}$ *has the same dependence as in Theorem* 3.1.

As remarked in [21], the assumption (3.14) can be easily satisfied by the definition of k^*, k^{**}, and k. As a final remark, let us mention the existence and uniqueness of the approximate solution to the nonlinear system in (3.9)–(3.11). Introducing bases in V_h, W_h, and M_h, (3.9) and (3.10) can be written in matrix form as follows:

$$\begin{aligned} A(S)U - BP &= G_\lambda(S,P), \\ C(S,P)\frac{dP}{dt} + B^tU &= F(S,P), \end{aligned} \tag{3.15}$$

with $P(0)$ given, where $A(S)$ and $C(S,P)$ are positive definite by the first and third equations of (3.7); S, U, and P are the respective degrees of freedom of s_h, u_h, and p_h; and $F(S,P)$ denotes the right-hand side of the second equation of (3.9). Substituting the relation

$$U = A(S)^{-1}BP + A(S)^{-1}G_\lambda(S,P) \tag{3.16}$$

into the second equation of (3.15), we see that

$$C(S,P)\frac{dP}{dt} + B^tA(S)^{-1}BP + B^tA(S)^{-1}G_\lambda(S,P) = F(S,P),$$

which, in turn, produces the system

$$\frac{dP}{dt} = F_1(P,S). \tag{3.17}$$

Also, using the discrete counterpart of (3.13) and the same argument, it follows from (3.11) that

$$\frac{dS}{dt} = F_2(P,S), \tag{3.18}$$

with $S(0)$ given. Now, (3.17) and (3.18) can be regarded as a nonlinear system of ordinary differential equations for (P,S), which has a unique solution, at least locally and for h small enough. In fact, since we assumed that the coefficients in (3.1) and (3.2) are smooth, the vector valued function (F_1,F_2) is globally Lipschitz continuous, and the solution $(P(t),S(t))$ exists for all positive time t.

3.4. Fully discrete version. In this subsection we consider a fully discrete version of the finite element approximate procedure in (3.9)–(3.11). For this, let $\{t^n\}_{n=0}^{n_T}$ be a quasi-uniform partition of J, with $t^0=0$ and $t^{n_T}=T$, and set $\Delta t^n = t^n - t^{n-1}$, $\Delta t = \max\{\Delta t^n, 1\le n\le n_T\}$, and

$$\psi^n = \psi(t^n), \quad \partial\psi^n = (\psi^n - \psi^{n-1})/\Delta t^n.$$

The approximation procedure for the pressure is again defined by the mixed method for a pair of maps $\{u_h^n, p_h^n\}\in V_h\times W_h$, $n=1,2,\dots,n_T$, such that

$$\begin{aligned} &(a_h^{-1,n-1}u_h^n, v) - (\nabla\cdot v, p_h^n) = (G_\lambda(s_{o,h}^{n-1}, s_{w,h}^{n-1}, p_h^{n-1}), v) \qquad \forall v\in V_h, \\ &(c_h^{n-1}\partial p_h^n,\psi) + (\nabla\cdot u_h^n,\psi) = (q(p_h^{n-1}),\psi) - \big((d_{0,h}^{n-1} + d_{1,h}^{n-1}u_h^{n-1} \\ &\qquad + d_{o,h}^{n-1}\nabla s_{o,h}^{n-1} + d_{w,h}^{n-1}\nabla s_{w,h}^{n-1})\cdot\nabla p_h^{n-1},\psi\big) \quad \forall\psi\in W_h, \end{aligned} \tag{3.19}$$

where the discrete coefficients c_h^{n-1}, etc. are calculated at the previous time level $s_{o,h}^{n-1}$, $s_{w,h}^{n-1}$, and p_h^{n-1},

$$\nabla p_h^{n-1} = -a^{-1}(s_{o,h}^{n-1}, s_{w,h}^{n-1})u_h^{n-1} + G_\lambda(s_{o,h}^{n-1}, s_{w,h}^{n-1}, p_h^{n-1}), \tag{3.20}$$

and $s_{o,h}^n$ and $s_{w,h}^n : J \to M_h$ $(n = 1, 2, \dots, n_T)$ satisfy

$$\begin{aligned} &(\phi\partial s_{\alpha,h}^n, v) + (D_{\alpha o,h}^{n-1}\nabla s_{o,h}^n + D_{\alpha w,h}^{n-1}\nabla s_{w,h}^n - f_{\alpha,h}^{n-1}u_h^n + k\lambda_{\alpha,h}^{n-1}\delta_{\alpha,h}^{n-1}, \nabla v) \\ &\quad = (\theta_{\alpha,h}^{n-1} + \eta_{\alpha,h}^{n-1}\nabla\cdot u_h^n + (g_{\alpha 0,h}^{n-1} + g_{\alpha 1,h}^{n-1}u_h^n + g_{\alpha o,h}^{n-1}\nabla s_{o,h}^{n-1} \\ &\qquad\qquad + g_{\alpha w,h}^{n-1}\nabla s_{w,h}^{n-1})\cdot\nabla p_h^{n-1}, v) \quad \forall v \in M_h, \end{aligned} \tag{3.21}$$

where the coefficients are calculated at $s_{o,h}^{n-1}$, $s_{w,h}^{n-1}$, and p^n (i.e., the previous saturations and current pressure, e.g., $\delta_{\alpha,h}^{n-1} = \delta_\alpha(s_{o,h}^{n-1}, s_{w,h}^{n-1}, p^n)$) and the initial data p_h^0 and $s_{\alpha,h}^0$ can again be their respective projections or interpolants of p^0 and s_α^0 in W_h and M_h. Moreover, u_h^0, which is needed in (3.19) and (3.21), can be initially computed via the first equation of (3.1), for example.

After startup, for $n = 1, 2, \dots, n_T$, (3.19)–(3.21) are computed as follows. First, using $s_{\alpha,h}^{n-1}$, p_h^{n-1}, u_h^{n-1}, (3.19), and (3.20), evaluate $\{u_h^n, p_h^n\}$. Since it is linear, they have a unique solution for each n [15, 36]. Next, using $s_{\alpha,h}^{n-1}$, $\{u_h^n, p_h^n\}$, and (3.21), calculate s_h^n. Again, it has a unique solution for Δt^n sufficiently small for each n [45].

While the backward Euler scheme is used for the time discretization terms in (3.19) and (3.21), the Crank–Nicolson scheme and more accurate time stepping procedures (see, e.g., [31]) can be used and the present analysis applies to these schemes. Also, the nonlinearities in the pressure and saturation equations are handled by lagging in time. Consequently, a linear system of algebraic equations is solved at each time step instead of a nonlinear system. In this case a condition on the time step is needed; see (3.22) below. However, it turns out that this condition is not very restrictive. We point out that the analysis below extends to the nonlinear version where we calculate the coefficients fully at the current time level instead of the previous level (see the scheme in the next section). In the latter case the time step Δt in the condition (3.22) below would disappear. The drawback of this fully implicit scheme is that we have to solve a nonlinear system at each time step.

Again, using the version given in (3.12) and (3.13) and applying the analysis in [19], we have the next error estimates for the fully discrete scheme in Theorems 3.3 and 3.4 below. Set

$$\begin{aligned} \mathcal{E}_1 = &\Delta t \sum_{i=1}^{2} \left(\left\| \frac{\partial^i p}{\partial t^i} \right\|_{L^2(\Omega_T)} + \left\| \frac{\partial^i s}{\partial t^i} \right\|_{L^2(\Omega_T)} + \left\| \frac{\partial^i u}{\partial t^i} \right\|_{L^2(\Omega_T)} \right) \\ &+ \Delta t \left\| \frac{\partial^3 p}{\partial t^3} \right\|_{L^2(\Omega_T)} + \mathcal{E}. \end{aligned}$$

THEOREM 3.3. *Let (u, p, s) and (u_h, p_h, s_h) solve (3.1), (3.2), and (3.19)–(3.21), respectively. Then, if the parameters Δt, h_p, and h satisfy*

$$(h^{-d/2} + h_p^{-d/2})(\Delta t + h_p^{k^*+1} + h_p^{k^{**}} + h^{k+1}) \to 0 \text{ as } \Delta t,\ h \to 0,\ d = 2 \text{ or } 3, \tag{3.22}$$

we have

$$\max_{0\le n\le n_T}\Bigg\{\|u^n-u_h^n\|_{L^2(\Omega)}+\|p^n-p_h^n\|_{L^2(\Omega)}+\|s^n-s_h^n\|_{L^2(\Omega)}$$
$$+h\|\nabla(s^n-s_h^n)\|_{L^2(\Omega)}+\left\|\frac{\partial p^n}{\partial t}-\partial p_h^n\right\|_{L^2(\Omega)}\Bigg\}$$
$$+\left\{\sum_{n=1}^{n_T}\left\|\frac{\partial s^n}{\partial t}-\partial s_h^n\right\|^2_{L^2(\Omega)}\Delta t^n\right\}^{1/2}\le \mathcal{C}\mathcal{E}_1,$$

where $\mathcal{C}$ *has the same dependence as in Theorem* 3.1.

THEOREM 3.4. *Under the assumptions of Theorem* 3.3 *with* $d=2$, *we have*

$$\max_{0\le n\le n_T}\|p^n-p_h^n\|_{L^\infty(\Omega)}\le \mathcal{C}\log h_p^{-1}\big(\mathcal{E}_1+h_p^{k^{**}}\|p\|_{L^\infty(J;H^{k^{**}+1}(\Omega))}\big),$$
$$\max_{0\le n\le n_T}\|s^n-s_h^n\|_{L^\infty(\Omega)}\le \mathcal{C}\big(\log h^{-1}\big)^{\gamma}\big(\mathcal{E}_1+h^{k+1}\|s\|_{L^\infty(J;W^{k+1,\infty}(\Omega))}\big),$$

where $\gamma=1$ *for* $k=1$, $\gamma=1/2$ *for* $k>1$, *and* $\mathcal{C}$ *has the same dependence as in Theorem* 3.1.

4. Finite elements in a degenerate case. In the previous section we assumed the uniform positiveness of $D(s)$ in (3.8). In this section we analyze a realistic case where $D(s)$ can be zero. As mentioned in section 3.1, the pressure equation is not degenerate, so we only analyze the saturation equation (3.2) or equivalently (3.13). To fix the idea, we write the saturation equation in the general form

$$\phi\frac{\partial s}{\partial t}-\nabla\cdot\big(D(s)\nabla s-f(s)u+\delta(s,p)\big)=q_w(s,p),\qquad (x,t)\in\Omega_T, \tag{4.1a}$$

where (u,p) is determined by the pressure equation. Also, to avoid unnecessary complications we treat s as a scalar function. Then, to analyze (4.1a), we introduce the Kirchhoff transformation

$$\sigma=\int_0^s D(\xi)\mathrm{d}\xi,\qquad 0\le s\le 1, \tag{4.2}$$

and let $\mathcal{S}(\sigma)$ be the inverse of (4.2) for $0\le\sigma\le\sigma^*$ with

$$\sigma^*=\int_0^1 D(\xi)\mathrm{d}\xi.$$

It is assumed below that $\mathcal{S}$ is strictly monotone increasing in σ. Moreover, it satisfies that

$$\|\sigma_1-\sigma_2\|^2_{L^2(\Omega)}\le\beta^*(\sigma_1-\sigma_2,s_1-s_2),\ 0\le\sigma_1,\,\sigma_2\le\sigma^*,\ s_i=\mathcal{S}(\sigma_i),\ i=1,2. \tag{4.3}$$

A sufficient condition for (4.3) to hold is

$$0\le D(s)\le\beta^*<\infty,\qquad 0\le s\le 1.$$

This is physically reasonable. It also says that the saturation equation can be degenerate. In practice, all the functions of s are normally defined on $[0,1]$. In the numerical approximation here, the possibility that $s \notin [0,1]$ is allowed. All functions of s are extended constantly outside $[0,1]$ except $\mathcal{S}$, which is extended as follows:

$$s = \text{extended } \mathcal{S}(\sigma) = \begin{cases} \sigma & \text{for} \quad \sigma < 0, \\ \mathcal{S}(\sigma) & \text{for} \quad 0 \le \sigma \le \sigma^*, \\ \sigma + 1 - \sigma^* & \text{for} \quad \sigma^* < \sigma. \end{cases}$$

The reason behind this extension will become clear from the proof of Lemma 4.1 later. Also, this extension is a good choice in the theoretical analysis of simpler fluid flow problems [4, 14].

We conclude with the boundary and initial conditions

$$\begin{aligned} &\sigma = \sigma_D, && (x,t) \in \partial\Omega \times J, \\ &s(x,0) = s^0(x), && x \in \Omega. \end{aligned} \tag{4.1b}$$

As an example in this section, we indicate how to handle the Dirichlet boundary condition; an extension to other types of boundary conditions is possible.

4.1. Preliminaries. Again, let $M_h \subset H^1(\Omega)$ be a standard C^0-finite element space associated with T_h such that

$$\inf_{v_h \in M_h} \|v - v_h\|_{H^1(\Omega)} \le \mathcal{C}h\|v\|_{H^2(\Omega)}. \tag{4.4}$$

In this section we consider only lowest-order C^0-finite elements such that (4.4) is satisfied; due to lacking in regularity on the solution, no improvement in the asymptotic convergence rate results from taking higher order finite element spaces. Finally, set $M_h(0) = M_h \cap H_0^1(\Omega)$.

We define the Green operator $G : H^{-1}(\Omega) \to H_0^1(\Omega)$ by

$$(\nabla Gv, \nabla w) = (\phi v, w) \qquad \forall w \in H_0^1(\Omega),\ v \in H^{-1}(\Omega). \tag{4.5}$$

Assume that the regularity result holds

$$\|Gv\|_{H^2(\Omega)} \le \mathcal{C}\|v\|_{L^2(\Omega)} \quad \text{for any } v \in L^2(\Omega). \tag{4.6}$$

Also, we can define

$$\|v\|^2_{H^{-1}(\Omega)} \equiv (\phi v, Gv) = (\nabla Gv, \nabla Gv) \qquad \forall v \in H^{-1}(\Omega), \tag{4.7}$$

which is equivalent to the usual norm on $H^{-1}(\Omega)$.

The discrete Green operator $G_h : H^{-1}(\Omega) \to M_h(0)$ is given by

$$(\nabla G_h v, \nabla w) = (\phi v, w) \qquad \forall w \in M_h(0),\ v \in H^{-1}(\Omega). \tag{4.8}$$

By the regularity of T_h and G, we have the following approximation property [23]:

$$\|(G - G_h)v\|_{H^l(\Omega)} \le \mathcal{C}h^{2-(l+\pi)}\|v\|_{B^{-\pi}(\Omega)}, \qquad 0 \le l, \pi \le 1, \tag{4.9}$$

where $B^{-\pi}(\Omega) = [L^2(\Omega), H^{-1}(\Omega)]_\pi$ is the interpolation space. Moreover, it follows from (4.7) that

$$\|\nabla G_h v\|_{L^2(\Omega)} \le \mathcal{C}\|v\|_{H^{-1}(\Omega)} \qquad \forall v \in H^{-1}(\Omega). \tag{4.10}$$

To handle the Dirichlet boundary condition, we introduce the set

$$M(g) = \{v \in H^1(\Omega) : v = g \text{ on } \partial\Omega\}$$

for $g \in H^{1/2}(\partial\Omega)$. Also, for $g \in C^0(\bar{\Omega})$ define

$$M_h(g) = \{v \in M_h : v = I_h g \text{ on } \partial\Omega\},$$

where $I_h g$ indicates the interpolant of g in M_h. We now define the discrete operator $E_h : M(g) \to M_h(g)$ by

$$(\nabla[v - E_h v], \nabla w) = 0 \qquad \forall w \in M_h(0),\ v \in M(g). \tag{4.11}$$

By (4.9), we see that

$$\|v - E_h v\|_{H^l(\Omega)} \leq \mathcal{C} h^{2-(l+\pi)} \|v\|_{H^{2-\pi}(\Omega)}, \qquad 0 \leq l, \pi \leq 1, \tag{4.12}$$

for $v \in M(g)$, with $g \in C^{0,1}(\partial\Omega)$. Finally, we denote by P_h the L^2-projection into M_h, which satisfies that

$$\|v - P_h v\|_{H^{-1}(\Omega)} \leq \mathcal{C} h \|v\|_{L^2(\Omega)} \qquad \forall v \in L^2(\Omega). \tag{4.13}$$

4.2. Finite element method. As an example, we analyze only a fully discrete approximation for problem (4.1). The semidiscrete version can be defined as in section 3.2 and can be analyzed similarly.

We recall the notation in section 3.4; for each positive integer n_T, let $0 = t^0 < t^1 < \cdots < t^{n_T} = T$ be a partition of J into subintervals $J^n = (t^{n-1}, t^n]$ with length $\Delta t^n = t^n - t^{n-1}$, $1 \leq n \leq n_T$. Also, set $v^n = v(\cdot, t^n)$. Finally, we indicate the time difference operator by

$$\partial v^n = \frac{v^n - v^{n-1}}{\Delta t^n}, \quad 1 \leq n \leq n_T.$$

We extend σ_D to Ω as the solution of the problem: Find $\psi \in M(\sigma_D)$ such that

$$(\nabla\psi, \nabla v) = 0 \qquad \forall v \in M(0);$$

we still indicate this extension by σ_D. Also, we set $\sigma_{D,h} = E_h \sigma_D$, where E_h is defined in (4.11).

The fully discrete approximation is given as follows: For any $1 \leq n \leq n_T$, find $\sigma_h^n \in M_h(\sigma_{D,h}^n)$ such that

$$\begin{aligned} &(\phi s_h^n, v) + \sum_{j=1}^{n} (\nabla \sigma_h^j - f(s_h^j) u^j + \delta(s_h^j, p^j), \nabla v) \Delta t^j \\ &\quad = \sum_{j=1}^{n} (q_w(s_h^j, p^j), v) \Delta t^j + (\phi s_h^0, v) \qquad \forall v \in M_h(0), \end{aligned} \tag{4.14}$$

where $s_h = \mathcal{S}(\sigma_h)$. The numerical initial datum $s_h(\cdot, 0) = s_h^0$ is defined as the L^2-projection of s^0 in M_h:

$$s_h^0 = P_h s^0.$$

In practical computations, we can use an equivalent form of (4.14). Take the difference of the equations at time levels n and $n-1$ and divide by Δt^n to see that

$$\begin{aligned} &(\phi \partial s_h^n, v) + (\nabla \sigma_h^n - f(s_h^n) u^n + \delta(s_h^n, p^n), \nabla v) \\ &\quad = (q_w(s_h^n, p^n), v) \qquad \forall v \in M_h(0). \end{aligned} \tag{4.15}$$

4.3. A priori estimates. We establish a priori estimates for (4.14), which will be used in the error analysis. Below we implicitly assume that $u \in L^\infty(\Omega_T)$. Also, the functions of s, f, δ, and q_w are assumed to be bounded in the following norms:

$$|||f|||_{L^2(\Omega_T)}, \quad |||\delta|||_{L^2(\Omega_T)}, \quad |||q_w|||_{L^2(J;H^{-1}(\Omega))},$$

where the norm $|||\cdot|||$ is defined by $|||v||| = \left\| \sup_{s\in[0,1]} |v(x,s)| \right\|$ for $v = v(x,s)$ and any given norm $\|\cdot\|$. Finally, the data s^0 and σ_D are bounded in the norms:

$$\|s^0\|_{L^2(\Omega)}, \quad \|\sigma_D\|_{L^2(J;H^{1/2}(\partial\Omega))}.$$

Below ε is a positive constant, as small as we please. A similar stability and error analysis was given in [38] for free boundary problems.

LEMMA 4.1. *For the solution (s_h, σ_h) of (4.14), there is a constant $\mathcal{C}$ independent of h and Δt^n, $n = 1, \ldots, n_T$, such that*

$$\max_{1\le n\le n_T} \left\{ \|s_h^n\|^2_{L^2(\Omega)} + \|\sigma_h^n\|^2_{L^2(\Omega)} \right\} + \sum_{n=1}^{n_T} \|\nabla\sigma_h^n\|^2_{L^2(\Omega)} \Delta t^n \le \mathcal{C}.$$

Proof. Take $v = \sigma_h^n - \sigma_{D,h}^n \in M_h(0)$ in (4.15) to see that

$$\begin{aligned}(\phi\partial s_h^n, \sigma_h^n - \sigma_{D,h}^n) + (\nabla\sigma_h^n - f(s_h^n)u^n + \delta(s_h^n, p^n), \nabla[\sigma_h^n - \sigma_{D,h}^n])\\ = (q_w(s_h^n, p^n), \sigma_h^n - \sigma_{D,h}^n).\end{aligned}$$

Summing over n from 1 to n_T, this equation can be written as follows:

$$\begin{aligned}&\sum_{n=1}^{n_T} \left\{ \left(\phi(s_h^n - s_h^{n-1}), \sigma_h^n - \sigma_{D,h}^n\right) + \left(\nabla\sigma_h^n, \nabla[\sigma_h^n - \sigma_{D,h}^n]\right) \Delta t^n \right\}\\ &\quad = \sum_{n=1}^{n_T} \Big\{ (q_w(s_h^n, p^n), \sigma_h^n - \sigma_{D,h}^n)\\ &\qquad\qquad + (f(s_h^n)u^n - \delta(s_h^n, p^n), \nabla[\sigma_h^n - \sigma_{D,h}^n]) \Big\} \Delta t^n.\end{aligned} \tag{4.16}$$

Note that

$$\begin{aligned}&\left|(\nabla\sigma_h^n, \nabla\sigma_{D,h}^n)\right| \le \varepsilon\|\nabla\sigma_h^n\|^2_{L^2(\Omega)} + \mathcal{C}\|\nabla\sigma_{D,h}^n\|^2_{L^2(\Omega)},\\ &\left|(q_w(s_h^n, p^n), \sigma_h^n - \sigma_{D,h}^n)\right| \le \varepsilon\|\sigma_h^n\|^2_{H^1(\Omega)} + \mathcal{C}\left(|||q_w^n|||^2_{H^{-1}(\Omega)} + \|\sigma_{D,h}^n\|^2_{H^1(\Omega)} \right),\\ &\left|(f(s_h^n)u^n, \nabla[\sigma_h^n - \sigma_{D,h}^n])\right| \le \varepsilon\|\nabla\sigma_h^n\|^2_{L^2(\Omega)} + \mathcal{C}\left(|||f^n|||^2_{L^2(\Omega)} + \|\nabla\sigma_{D,h}^n\|^2_{L^2(\Omega)} \right),\\ &\left|(\delta(s_h^n, p^n), \nabla[\sigma_h^n - \sigma_{D,h}^n])\right| \le \varepsilon\|\nabla\sigma_h^n\|^2_{L^2(\Omega)} + \mathcal{C}\left(|||\delta^n|||^2_{L^2(\Omega)} + \|\nabla\sigma_{D,h}^n\|^2_{L^2(\Omega)} \right).\end{aligned}$$

Also, define

$$\Phi(\tau) = \int_0^\tau \sigma(\xi)\mathrm{d}\xi.$$

Then we see that

$$(s_h^n - s_h^{n-1})\sigma_h^n \ge \Phi(s_h^n) - \Phi(s_h^{n-1}),$$

so,

$$\sum_{n=1}^{n_T}(\phi[s_h^n - s_h^{n-1}], \sigma_h^n) \geq \sum_{n=1}^{n_T}\left(\phi[\Phi(s_h^n) - \Phi(s_h^{n-1})], 1\right) = \left(\phi[\Phi(s_h^{n_T}) - \Phi(s_h^0)], 1\right).$$

By (4.3), we have

$$\Phi(s_h^{n_T}) \geq \frac{1}{2\beta^*}(\sigma_h^{n_T})^2 \quad \text{and} \quad \Phi(s_h^0) \leq \frac{\beta^*}{2}(s_h^0)^2.$$

Thus, by (3.7), we obtain

$$\sum_{n=1}^{n_T}(\phi[u_h^n - u_h^{n-1}], \sigma_h^n) \geq \frac{\phi_*}{2\beta^*}\|\sigma_h^{n_T}\|^2_{L^2(\Omega)} - \frac{\phi^*\beta^*}{2}\|s_h^0\|^2_{L^2(\Omega)}.$$

Also, by the extension of $\mathcal{S}$, we have

$$\left|\left(\phi(s_h^n - s_h^{n-1}), \sigma_{D,h}^n\right)\right| \leq \varepsilon\left(\|\sigma_h^n\|^2_{L^2(\Omega)} + \|\sigma_h^{n-1}\|^2_{L^2(\Omega)}\right) + \mathcal{C}\left(1 + \|\sigma_{D,h}^n\|^2_{L^2(\Omega)}\right).$$

Finally, substitute these inequalities into (4.16) and use the Gronwall inequality, the extension of σ_D, the definition of $\sigma_{D,h}$, and the Poincare inequality to yield the desired result. □

Set

$$\Delta t = \max_{1\leq n\leq n_T} \Delta t^n.$$

LEMMA 4.2. *For the solution* (s_h, σ_h) *of* (4.14), *if* $h = O(\Delta t)$, *there is a constant* $\mathcal{C}$ *independent of* h *and* Δt^n, $n = 1, \dots, n_T$, *such that*

$$\sum_{n=1}^{n_T}\|\partial s_h^n\|^2_{H^{-1}(\Omega)}\Delta t^n \leq \mathcal{C}.$$

Proof. Choose $v = G_h(\partial s_h^n)$ in (4.15) to see that

$$\begin{aligned}(\phi\partial s_h^n, G_h(\partial s_h^n)) + (\nabla\sigma_h^n - f(s_h^n)u^n + \delta(s_h^n, p^n), \nabla G_h(\partial s_h^n)) \\ = (q_w(s_h^n, p^n), G_h(\partial s_h^n)).\end{aligned} \tag{4.17}$$

By (4.10), we see that

$$\begin{aligned}&|(\nabla\sigma_h^n - f(s_h^n)u^n + \delta(s_h^n, p^n), \nabla G_h(\partial s_h^n))| \\ &\quad\leq \varepsilon\|\partial s_h^n\|^2_{H^{-1}(\Omega)} + \mathcal{C}\left\{\|\nabla\sigma_h^n\|^2_{L^2(\Omega)} + |||f^n|||^2_{L^2(\Omega)} + |||\delta^n|||^2_{L^2(\Omega)}\right\},\end{aligned}$$

and

$$|(q_w(s_h^n, p^n), G_h(\partial s_h^n))| \leq \varepsilon\|\partial s_h^n\|^2_{H^{-1}(\Omega)} + \mathcal{C}|||q_w^n|||^2_{H^{-1}(\Omega)}.$$

Note that

$$(\phi\partial s_h^n, G_h(\partial s_h^n)) = (\phi\partial s_h^n, G(\partial s_h^n)) + (\phi\partial s_h^n, G_h(\partial s_h^n) - G(\partial s_h^n)),$$

so that, by (4.7) and (4.9),

$$|(\phi\partial s_h^n, G_h(\partial s_h^n))| \geq \mathcal{C}\left\{\|\partial s_h^n\|^2_{H^{-1}(\Omega)} - h^2\|\partial s_h^n\|^2_{L^2(\Omega)}\right\}.$$

Substitute these inequalities into (4.17) and use Lemma 4.1 to finish the proof. □

4.4. Error estimate I. For the result in this section we need the minimal regularity on the solution and on the boundary datum:

$$\begin{aligned} &s \in L^2(\Omega_T), \quad \frac{\partial s}{\partial t} \in L^2(J; H^{-1}(\Omega)), \\ &\sigma \in L^2(J; H^1(\Omega)), \quad \sigma_D \in H^1(J; H^{1/2}(\partial\Omega)). \end{aligned} \tag{4.18}$$

Also, we assume that the coefficients satisfy

$$\begin{aligned} &\|f(s_1) - f(s_2)\|^2_{L^2(\Omega)} + \|\delta(s_1, \cdot) - \delta(s_2, \cdot)\|^2_{L^2(\Omega)} \\ &+\|q_w(s_1, \cdot) - q_w(s_2, \cdot)\|^2_{H^{-1}(\Omega)} \leq \mathcal{C}(s_1 - s_2, \sigma_1 - \sigma_2), \\ &0 \leq \sigma_1, \, \sigma_2 \leq \sigma^*, \, s_i = \mathcal{S}(\sigma_i), \, i = 1, 2, \, t \in J. \end{aligned} \tag{4.19}$$

Note that if f satisfies that

(4.20)

$$|f(s_1) - f(s_2)|^2 \leq \mathcal{C}(s_1 - s_2)(\sigma_1 - \sigma_2), \quad 0 \leq \sigma_1, \, \sigma_2 \leq \sigma^*, \text{ almost everywhere (a.e.) on } \Omega_T,$$

assumption (4.19) is true for f. A necessary and sufficient condition for (4.20) to hold is that

$$|f_s|^2 \leq \mathcal{C}\mathcal{S}_s^{-1} \qquad \forall s \in [0, 1], \text{ a.e. on } \Omega_T. \tag{4.21}$$

The same remark can be made for other functions in (4.19). Essentially, (4.21) implies that f_s vanishes with $\mathcal{S}_s^{-1}$, which is physically reasonable.

Introduce the notation

$$\overline{v}^n = \frac{1}{\Delta t^n} \int_{J^n} v(\cdot, t) \mathrm{d}t, \qquad 1 \leq n \leq n_T.$$

Also, set

$$s_h(\cdot, t) = s_h^n(\cdot), \quad \sigma_h(\cdot, t) = \sigma_h^n(\cdot) \quad \text{ for } t \in J^n, \quad n = 1, \ldots, n_T.$$

Note that (4.1) can be written in the weak form: Find $\sigma \in H_0^1(\Omega) + \sigma_D$ such that

$$\left(\phi \frac{\partial s}{\partial t}, v\right) + (\nabla\sigma - f(s)u + \delta(s, p), \nabla v) = (q_w(s, p), v), \quad v \in H_0^1(\Omega).$$

Integrate this equation over J^n to see that

$$(\phi \partial s^n, v) + (\nabla\overline{\sigma}^n - \overline{fu}^n + \overline{\delta}^n, \nabla v) = (\overline{q}_w^n, v), \quad v \in H_0^1(\Omega), \tag{4.22}$$

for $n = 1, \ldots, n_T$, where $\overline{\delta}^n = \overline{\delta(s, p)}^n$, etc. To fix the ideas, the errors $\overline{u}^n - u^n$ and $\overline{p}^n - p^n$ are omitted below.

THEOREM 4.3. *For the solution* (s_h, σ_h) *of* (4.14), *under assumptions* (4.3), (4.18), *and* (4.19), *we have*

$$\|s - s_h\|_{L^\infty(J; H^{-1}(\Omega))} + \|\sigma - \sigma_h\|_{L^2(\Omega_T)} \leq \mathcal{C}(h^{1/2} + \Delta t^{1/2}).$$

Proof. Set $e_s^n = \overline{s}^n - s_h^n$ and $e_\sigma^n = \overline{\sigma}^n - \sigma_h^n$ for any $1 \leq n \leq n_T$. Choose $v = \Delta t^n G_h e_s^n \in M_h(0)$ in (4.15) and $v = \Delta t^n G e_s^n \in H_0^1(\Omega)$ in (4.22), subtract the resulting two equations, apply the definition of G, G_h, σ_D, and $\sigma_{D,h}$, and sum over n from 1 to n_T to see that

$$
\begin{aligned}
&\sum_{n=1}^{n_T}(\phi\partial[s^n - s_h^n], Ge_s^n)\Delta t^n + \sum_{n=1}^{n_T}(\phi e_\sigma^n, e_s^n)\Delta t^n \\
&\quad = \sum_{n=1}^{n_T}\left\{(\overline{q}_w^n, Ge_s^n) - (q_w(s_h^n, p^n), G_h e_s^n)\right\}\Delta t^n \\
&\qquad + \sum_{n=1}^{n_T}\left\{(\overline{fu}^n, \nabla Ge_s^n) - (f(s_h^n)u^n, \nabla G_h e_s^n)\right\}\Delta t^n \\
&\qquad - \sum_{n=1}^{n_T}\left\{(\overline{\delta}^n, \nabla Ge_s^n) - (\delta(s_h^n, p^n), \nabla G_h e_s^n)\right\}\Delta t^n \\
&\qquad + \sum_{n=1}^{n_T}(\phi[\overline{\sigma}_D^n - \sigma_{D,h}^n], e_s^n)\Delta t^n - \sum_{n=1}^{n_T}(\phi\partial s_h^n, Ge_s^n - G_h e_s^n)\Delta t^n.
\end{aligned}
\tag{4.23}
$$

Each of the terms in this equation is estimated as follows.

First, note that

$$
\begin{aligned}
&\sum_{n=1}^{n_T}(\phi\partial[s^n - s_h^n], Ge_s^n)\Delta t^n \\
&= \sum_{n=1}^{n_T}(\phi\partial[\overline{s}^n - s_h^n], Ge_s^n)\Delta t^n + \sum_{n=1}^{n_T}(\phi\partial[s^n - \overline{s}^n], Ge_s^n)\Delta t^n \equiv I + II.
\end{aligned}
$$

By elementary calculations, (4.5), and (4.13), we see that

$$
\begin{aligned}
I &= \sum_{n=1}^{n_T} a(Ge_s^n - Ge_s^{n-1}, Ge_s^n) \\
&= \frac{1}{2}a(Ge_s^{n_T}, Ge_s^{n_T}) - \frac{1}{2}a(Ge_s^0, Ge_s^0) + \frac{1}{2}\sum_{n=1}^{n_T} a(G[e_s^n - e_s^{n-1}], G[e_s^n - e_s^{n-1}]) \\
&\geq \frac{1}{2}\|e_s^n\|_{H^{-1}(\Omega)}^2 + \frac{1}{2}\sum_{n=1}^{n_T}\|e_s^n - e_s^{n-1}\|_{H^{-1}(\Omega)}^2 - Ch^2.
\end{aligned}
$$

Also, apply summation by parts to have

$$
\begin{aligned}
II &= (\phi[s^{n_T} - \overline{s}^{n_T}], Ge_s^{n_T}) - \sum_{n=2}^{n_T}(\phi[s^{n-1} - \overline{s}^{n-1}], G[e_s^n - e_s^{n-1}]) \\
&= a(G[s^{n_T} - \overline{s}^{n_T}], Ge_s^{n_T}) - \sum_{n=2}^{n_T} a(G[s^{n-1} - \overline{s}^{n-1}], G[e_s^n - e_s^{n-1}]) \\
&\leq C\Delta t\sum_{n=1}^{n_T}\|\partial_t s\|_{L^2(J^n;H^{-1}(\Omega))}^2 + \varepsilon\left(\|e_s^{n_T}\|_{H^{-1}(\Omega)}^2 + \sum_{n=2}^{n_T}\|e_s^n - e_s^{n-1}\|_{H^{-1}(\Omega)}^2\right).
\end{aligned}
$$

Second, observe that

$$
\begin{aligned}
&\sum_{n=1}^{n_T}(\phi e_\sigma^n, e_s^n)\Delta t^n \\
&= \sum_{n=1}^{n_T}\int_{J^n}(\phi[s(t) - s_h^n], \sigma(t) - \sigma_h^n)\mathrm{d}t + \sum_{n=1}^{n_T}\int_{J^n}(\phi[\overline{s}^n - s(t)], \sigma(t) - \sigma_h^n)\mathrm{d}t \\
&\geq \sum_{n=1}^{n_T}\int_{J^n}(\phi[s(t) - s_h^n], \sigma(t) - \sigma_h^n)\mathrm{d}t - C\Delta t\|\partial_t s\|_{L^2(J;H^{-1}(\Omega))}\|\sigma - \sigma_h\|_{L^2(J;H^1(\Omega))}.
\end{aligned}
$$

Third, notice that

$$\begin{aligned}&\sum_{n=1}^{n_T}\left\{(\overline{q}_w^n, Ge_s^n) - (q_w(s_h^n,p^n), G_h e_s^n)\right\}\Delta t^n\\&=\sum_{n=1}^{n_T}\left\{(\overline{q}_w^n - q_w(s_h^n,p^n), G_h e_s^n) + (\overline{q}_w^n, Ge_s^n - G_h e_s^n)\right\}\Delta t^n = III + IV,\end{aligned}$$

where, by (4.10),

$$\begin{aligned}III=&\sum_{n=1}^{n_T}\int_{J^n}(q_w(s,p) - q_w(s_h^n,p^n), G_h e_s^n)\mathrm{d}t\\&\le \varepsilon\sum_{n=1}^{n_T}\int_{J^n}\|q_w(s,p) - q_w(s_h^n,p^n)\|^2_{H^{-1}(\Omega)} + C\sum_{n=1}^{n}\|e_s^n\|^2_{H^{-1}(\Omega)}\Delta t^n\end{aligned}$$

and, by (4.9),

$$|IV| \le Ch|||q_w|||_{L^2(J;H^{-1}(\Omega))}\|e_s\|_{L^2(\Omega_T)}.$$

Fourth, in a similar manner we have

$$\begin{aligned}&\sum_{n=1}^{n_T}\left\{(\overline{fu}^n, \nabla Ge_s^n) - (f(s_h^n)u^n, \nabla G_h e_s^n)\right\}\Delta t^n\\&=\sum_{n=1}^{n_T}\left\{(\overline{fu}^n - f(s_h^n)u^n, \nabla G_h e_s^n) + (\overline{fu}^n, \nabla[Ge_s^n - G_h e_s^n])\right\}\Delta t^n \equiv V + VI,\end{aligned}$$

where

$$|V| \le \varepsilon\sum_{n=1}^{n_T}\int_{J^n}\|f(s) - f(s_h^n)\|^2_{L^2(\Omega)}\mathrm{d}t + C\sum_{n=1}^{n_T}\|e_s^n\|^2_{H^{-1}(\Omega)}\Delta t^n$$

and

$$|VI| \le Ch|||f|||_{L^2(\Omega_T)}\|e_s\|_{L^2(\Omega_T)}.$$

Fifth, the same argument also gives

$$\begin{aligned}&\sum_{n=1}^{n_T}\left\{(\overline{\delta}^n, \nabla Ge_s^n) - (\delta(s_h^n,p^n), \nabla G_h e_s^n)\right\}\Delta t^n\\&=\sum_{n=1}^{n_T}\left\{(\overline{\delta}^n - \delta(s_h^n,p^n), \nabla G_h e_s^n) + (\overline{\delta}^n, \nabla[Ge_s^n - G_h e_s^n])\right\}\Delta t^n \equiv VII + VIII,\end{aligned}$$

where

$$|VII| \le \varepsilon\sum_{n=1}^{n_T}\int_{J^n}\|\delta(s,p) - \delta(s_h^n,p^n)\|^2_{L^2(\Omega)}\mathrm{d}t + C\sum_{n=1}^{n_T}\|e_s^n\|^2_{H^{-1}(\Omega)}\Delta t^n$$

and

$$|VIII| \le Ch|||\delta|||_{L^2(\Omega_T)}\|e_s\|_{L^2(\Omega_T)}.$$

Sixth, by the extension of σ_D and the definition of $\sigma_{D,h}$, we have

$$\begin{aligned}
&\sum_{n=1}^{n_T}(\phi[\overline{\sigma}_D^n - \sigma_{D,h}^n], e_s^n)\Delta t^n \\
&= \sum_{n=1}^{n_T}\left\{(\phi[\overline{\sigma}_D^n - \overline{\sigma}_{D,h}^n], e_s^n) + (\phi[\overline{\sigma}_{D,h}^n - \sigma_{D,h}^n], e_s^n)\right\}\Delta t^n \\
&\leq \mathcal{C}\left(\Delta t\|\partial_t\sigma_D\|_{L^2(J;H^{1/2}(\partial\Omega))}\|e_s\|_{L^2(J;H^{-1}(\Omega))} + h\|\sigma_D\|_{L^2(J;H^{1/2}(\partial\Omega))}\|e_s\|_{L^2(\Omega_T)}\right).
\end{aligned}$$

Seventh, by (4.9), we observe that

$$\sum_{n=1}^{n_T}(\phi\partial s_h^n, Ge_s^n - G_h e_s^n)\Delta t^n \leq \mathcal{C}h\sum_{n=1}^{n_T}\|\partial s_h^n\|_{H^{-1}(\Omega)}\|e_s^n\|_{L^2(\Omega)}\Delta t^n.$$

Finally, substitute all these inequalities into (4.23) and use Lemmas 4.1 and 4.2, assumptions (4.3), (4.18), and (4.19), and the Gronwall inequality to obtain the desired result. □

4.5. Error estimate II. In this subsection we consider an assumption different from (4.3):

$$\|s_1 - s_2\|_{L^2(\Omega)}^2 \leq \beta_*(\sigma_1 - \sigma_2, s_1 - s_2),\ 0 \leq \sigma_1,\ \sigma_2 \leq \sigma^*,\ s_i = \mathcal{S}(\sigma_i),\ i = 1, 2. \tag{4.24}$$

THEOREM 4.4. *For the solution (s_h, σ_h) of (4.14), if (4.18) and (4.24) are satisfied and if the functions f, δ, and q_w are Lipschitz continuous in s, then*

$$\|s - s_h\|_{L^\infty(J;H^{-1}(\Omega))} + \|s - s_h\|_{L^2(\Omega_T)} \leq \mathcal{C}(h + \Delta t^{1/2}).$$

This theorem can be proven analogously. We remark that (4.3) means that the diffusion coefficient in (4.1a) can be zero, while (4.24) says that the coefficient in the time differentiation term can be zero.

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