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Unified formulation of enhanced oil-recovery methods

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Resumen

En la actualidad las técnicas de recuperación mejorada de petróleo (EOR, por sus siglas en inglés) son esenciales para mantener los suministros de petróleo del mundo. A su vez, los modelos matemáticos y computacionales de los métodos EOR son fundamentales para su aplicación y perfeccionamiento. Debido a la gran diversidad de procesos que ocurren en la EOR, es valioso contar con procedimientos generales unificados para la construcción de los mismos, que puedan aplicarse fácilmente independientemente de la complejidad del sistema considerado. El objetivo de este trabajo es presentar un modelo matemático unificado, que incluya ambos: el sistema gobernante de las ecuaciones en derivadas parciales y las condiciones de choque. Éste se basa en una formulación axiomática, pues las formulaciones axiomáticas son el medio más eficaz para lograr generalidad, sencillez y claridad. En el enfoque que se propone aquí, la construcción del modelo matemático es en gran medida automática, todo lo que se requiere a fin de definir las ecuaciones en derivadas parciales y las condiciones de choque que constituyen un modelo básico consiste en identificar las fases y las propiedades extensivas que participan en el sistema de la EOR. Este modelo básico proporciona una base muy firme para incorporar la fenomenología. El procedimiento se ilustra derivando los modelos matemáticos más utilizados en la tecnología EOR; en particular, se derivan los modelos de petróleo negro y los composicionales, tanto en su versión isotérmica como sus variantes térmicas, en las cuales es indispensable incluir el balance de energía. Para ilustrar la aplicación de la formulación axiomática a modelos con discontinuidades, se realiza también una descripción exhaustiva de los choques que pueden ocurrir en el Modelo de Petróleo Negro.

Palabras clave: EOR, recuperación mejorada, modelación matemática, modelo del petróleo negro, modelo composicional, procesos térmicos.

Abstract

At present enhanced oil recovery (EOR) techniques are essential for maintaining the oil supplies of the world. In turn, mathematical and computational models of the processes that occur in EOR are fundamental for the application and advancement of such methods. Due to the great diversity of processes occurring in EOR, it is valuable to possess unified general procedures for constructing them, which can be easily applied independently of the complexity of the system considered. The *leitmotiv* of this paper is to present a unified mathematical model, including both: the governing system of partial differential equations and shock conditions. It is based on an axiomatic formulation, since axiomatic formulations are the most effective means for achieving generality, simplicity and clarity. In the approach here proposed, the construction of the mathematical model is to a large extent automatic; all what is required in order to define the partial differential equations and the shock conditions that constitute such a basic model is to identify the phases and *extensive properties* that participate in the EOR system. Such a basic model supplies a very firm basis on which the phenomenology is incorporated. The procedure is illustrated by deriving the mathematical models of the most commonly occurring EOR models: black-oil, compositional and non-isothermal compositional. An exhaustive description of the shocks that may occur in black-oil models is also included.

Key words: enhanced oil recovery, mathematical models, black-oil model, compositional model, non-isothermal compositional model.

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Introduction

Generally, three stages of oil recovery are identified in the production life of a petroleum reservoir: *primary, secondary and tertiary recovery* (Lake, 1989). *Primary recovery* refers to the production that is obtained using the energy inherent in the reservoir due to gas under pressure or a natural water drive. At a very early stage the reservoir essentially contains a single fluid such as gas or oil (the presence of immobile water can be usually neglected) and often the pressure is so high that the oil or gas is produced without any pumping of the wells. *Primary recovery* ends when the oil field and the atmosphere reach pressure equilibrium. The total recovery obtained at this stage is usually around 12-15% of the hydrocarbons contained in the reservoir (OIIP: oil initially in place).

The technique of *waterflooding* used to be considered as an *enhanced oil recovery* method, but nowadays *secondary recovery* most frequently refers to waterflooding. In this approach, water is injected into some wells *(injection wells)* to maintain the field pressure and flow rates, while oil is produced through other wells *(production wells)*. In secondary recovery, if the oil phase is above the bubble point, the flow is *two-phase immiscible* with water in one phase and oil in the other one. In such a case, there is no mass exchange between the phases. When the pressure drops below the bubble point, due to oil production, the hydrocarbon component of the system separates into two phases: oil and gas. In this case the *black-oil* model applies; in such a model the oil and gas phases exchange mass while the water phase does not. *Secondary recovery* yields an additional 15-20% of the OIIP.

After secondary recovery has been completed, 50% or more of the hydrocarbons often remains in the reservoir. The more advanced techniques that have been developed for recovering such a valuable volume of hydrocarbons are known as *tertiary recovery techniques* or by the more generic term *enhanced oil recovery (EOR)*.

The terms *primary*, *secondary* and *tertiary* may be confusing. For example, water injection (a secondary recovery strategy) is often implemented from the start in the North Sea and cyclic steam injection is also often applied from the start in heavy oil reservoirs. Actually, *EOR* methods are employed both to obtain additional yields from a reservoir after secondary recovery procedures have been applied and also to treat non-conventional fields which, due to their difficult characteristics, require advanced methods from the start. In this respect, the term *EOR* (also called *improved oil recovery; IOR*) is more adequate. A suitable definition of EOR is: *"enhanced oil recovery processes are those methods that use external sources of materials and energy to recover oil from a reservoir that cannot be produced economically by conventional means".*

The most important EOR methods can be grouped as follows:

1. waterflooding (conventional, water-alternating-gas, or WAG, polymer flooding);

2. miscible gas injection: hydrocarbon gas, CO_2, nitrogen, flue gas;

3. chemical injection: polymer/surfactant, caustic and micellar/polymer flooding; and

4. thermal oil recovery: cyclic steam injection, steam-flooding, hot-water drive, in-situ combustion.

At present a large part of the oil reserves of the world are located in mature oil-fields whose production is declining and for which the only possibility for expanding their yield is by application of EOR techniques. Another large fraction of oil reserves are non-conventional oil-fields that are very difficult to exploit, either because of the characteristics of their hydrocarbons -such as very large viscosity- or because of the characteristics of the soils and rocks in which they are contained. In both cases, such reservoirs can only be exploited applying EOR methods. Therefore, today, EOR is an important strategy for sustaining the oil supply of the world (Lake, 1989; Chen *et al.,* 2006).

On the other hand, mathematical and computational modeling (MCM) of oil reservoirs is fundamental for the development and application of EOR techniques, because it permits predicting and understanding the behavior of a reservoir when it is subjected to the complicated and varied processes that occur in EOR techniques (Lake, 1989; Chen *et al.*, 2006). Among other important capabilities supplied by MCM, applying it, it is possible to evaluate the different production strategies and choose that which maximizes oil recovery; also, to correct deviations from the reservoir expected-behavior when they occur, as well as to estimate its production life and overall yield.

Processes to be modeled

In primary production, the processes to be modeled are the motion of one phase or of two phases at most (Chen *et al*., 2006), without mass exchange between the phases. In secondary production, generally the motion of a three-phase fluid system has to be modeled; the phases being water, oil and gas. Mass exchange between the oil and gas phases must be included. The standard computational model to mimic such a system is technically known as the *black-oil model*. In Enhanced Oil Recovery, the processes to be modeled are extremely varied; among them, multiphase-multispecies transport in two modalities, isothermal conditions and non-isothermal conditions, and many more. A process especially complex is in-situ combustion, which is further complicated by the fact that sharp fronts (shocks) may need to be included.

Generally, when constructing a simulator for the processes occurring in EOR the following models have to be developed successively: a mathematical model, a numerical model and a computational model (Lake, 1989; Chen *et al.*, 2007). The *mathematical models* of petroleum reservoirs consist of a system of partial differential equations, usually non-linear, whose numerical solution by computational means permits predicting the reservoir behavior. Due to the great diversity of processes occurring in EOR, it is valuable to possess a *unified mathematical model* that can be applied independently of the complexity of the system considered. The *leitmotiv* of this paper is to present such a unified model.

Furthermore, this unified model includes the systematic manner of treating shocks (i.e., discontinuous solutions). The petroleum engineering community has been aware of the occurrence of shocks in oil-reservoir models since Buckley-Leverett reported them (Buckley and Leverett, 1942). Double discontinuity shocks that occur in Black-Oil models were more recently reported and studied (Herrera, 1996; Herrera and Camacho, 1997). Furthermore, an exhaustive account of those that may occur in Black-Oil models was presented by I. Herrera et al. (1993). As it is well known, shocks are useful approximations to abrupt changes of the values of physical properties that may occur in the real systems. In EOR technology, they may valuable for example when modeling combustion fronts (Akkutlu and Yortsos, 2003).

Extensive properties and balance equations

Axiomatic formulations are the most effective means for achieving generality, simplicity and clarity. In particular, in what follows the use of an axiomatic approach will permit us to construct the *unified general model* for the very varied processes that occur, or may occur in the future, in *Enhanced Oil Recovery*.

There are two approaches to the study of matter and its motion: the microscopic and the macroscopic approaches. The former studies molecules, atoms and elemental particles, while the latter studies and models large systems. Oil reservoirs constitute macroscopic physical-chemical systems. The theoretical foundations of macroscopic models lie on Continuous Mechanics. The axiomatic method of Continuous Mechanics was established in the second half of the XX Century by a group of scholars and researchers two of whose most conspicuous leaders were Noll (1974). Recently, Allen *et al.* (1988), summarized the results that are essential for the axiomatic formulation of the basic mathematical models. A revised and, in some respects, improved presentation of the subject, in which we base the developments of the present paper, is due to appear soon (Herrera and Pinder, to appear).

Firstly, an abstract framework that is essential in the axiomatic approach will be introduced. The main thrust of this paper lies on the applications; so, when explaining the axiomatic formulation that will be applied to EOR processes, the theoretical foundations are explained as briefly as possible; details are included just enough to make them understandable and without sacrificing clarity. We start with a definition: An *'extensive property'* is a body property such that, for every body $\mathcal{B}$ and every time t, can be expressed as a volume integral over the domain, $B\,(t)$(see Figure 1), of the physical space occupied by the body; that is,

$$E\,(\mathcal{B},t) \equiv \int_{B(t)} \psi(\underline{x},\,t)d\,\underline{x} \tag{2.1}$$

The integrand $\psi(\underline{x},\,t)$ which represents the extensive property per unit volume, is said to be the *intensive property* associated with the *extensive property* E. The main extensive properties considered in EOR models are the mass of different components, as well as the energy, contained in each phase of an EOR system.

A model of a macroscopic system is said to contain a shock when there is a surface, $\Sigma(t)$, across which at least one of the *intensive properties* of the model is discontinuous. In our notation, $\Sigma(t)$ will be the union of the surfaces across which the intensive properties are discontinuous. In particular, if the model does not contain a shock, $\Sigma(t)$ is void. The kind of discontinuities that may occur across $\Sigma(t)$ are *'jump discontinuities'*, exclusively. By definition, a *jump discontinuity* of a function is one in which the limits from each side of $\Sigma(t)$ exist, but they are different from each other. Furthermore, the surface $\Sigma(t)$ is oriented arbitrarily (i.e., a *positive* and a *negative* side are defined) and a unit normal vector, $\underline{n}$, pointing towards the *positive* side is taken on it. The *jump* on $\Sigma(t)$ of any function, $f(\underline{x})$, is defined to be

$$[\![f]\!] \equiv f_{+} - f_{-}\,. \tag{2.2}$$

Here, f_+ and f_- are the limits on the positive and negative sides, respectively.

A Basic Axiom is: *"An extensive property can change in time, exclusively, because it enters into the body. In turn, it can enter into the body through its boundary or directly in its interior."* The mathematical expression of this Axiom is:

$$\frac{dE}{dt}(t) = \int_{B(t)} g\left(\underline{x},t\right)d\underline{x} + \int_{\partial B(t)} \underline{\tau}\left(\underline{x},t\right)\cdot\underline{n}\left(\underline{x},t\right)d\underline{x} + \int_{\Sigma(t)} g_\Sigma\left(\underline{x},t\right)d\underline{x}\,. \qquad (2.3)$$

In these statements the amount that *'enters'* may be positive or negative. With regards to Eq. (2.3), in the nomenclature of the general formulation of Continuum Mechanics, Allen *et al.* (1988), $g\,(\underline{x},t)$ is called the *external (distributed) supply* of the *extensive property* and $\underline{\tau}\,(\underline{x},t)$ is the *flux of the extensive property*. As for $g_\Sigma\,(\underline{x},t)$, it is also an *external supply*, but this one is concentrated on the surface $\Sigma(t)$; see: (Herrera and Pinder, to appear). The function $g\,(\underline{x},t)$ is the amount of the *extensive property* per unit volume per unit time that enters the body at the point $\underline{x}$ of the physical space at time t, while the function $g_\Sigma\,(\underline{x},t)$ is the amount of the *extensive property* per unit area per unit time that enters the body at the point $\underline{x}$ of the surface $\Sigma(t)$, at time t. The inclusion of such concentrated sources is essential in order to be able to treat shocks with sufficient generality; in particular, this will permit us to present in Section 5 an exhaustive description of shocks that may occur in Black-Oil models, which was originally reported in (Herrera *et. al.*, 1993) and includes Buckley-Leverett's shocks (Buckley and Leverett, 1942) as well as those reported by Herrera and Camacho (1997) and Herrera *et al.* (1993). In particular, the double-discontinuity models of shocks occurring in *variable-bubble-point* systems is an example in which, for some of the extensive properties that constitute the model, $g_\Sigma\,(\underline{x},t) \neq 0$ (Buckley and Leverett, 1942; Herrera *et al*., 1993; Herrera, 1996; Herrera and Camacho, 1997).

Finally, in Eq. (2.3), the function $\underline{\tau}(\underline{x},t)\bullet\underline{n}$ at the point $\underline{x}$ of the body external-boundary, $\partial B(t)$, is the amount of *extensive property* that enters the body there at time t (Figure 1), per unit area per unit time. In EOR models, $\underline{\tau}\,(\underline{x},t)$ represents the flux due to diffusion (mainly, material dispersion-diffusion or thermal diffusion).

A purely mathematical result (i.e., a *mathematical theorem*; see, Allen *et al*.,1988 and Herrera and Pinder, to appear) shows that Eq. (2.3) is fulfilled by each body of a continuous system, if and only if, the following *'balance conditions'* are satisfied:

$$\frac{\partial\psi}{\partial t} + \nabla\cdot\left(\underline{v}\psi\right) = \nabla\cdot\underline{\tau} + g, \ \ at\ every\ \underline{x}\in B\left(t\right)-\Sigma\left(t\right) \qquad (2.4)$$

and

$$\left[\!\left[\psi\left(\underline{v}-\underline{v}_\Sigma\right)\right]\!\right]\bullet\underline{n} = g_\Sigma,\ \ at\ every\ \underline{x}\in\Sigma\left(t\right) \qquad (2.5)$$

Eq. (2.4) will be referred to as the *"balance differential equation"*, while Eq. (2.5) is the *"jump condition"*. The systems of differential equations that constitute the mathematical models will be derived from Eq. (2.4), while the treatment of shocks will be based on Eq (2.5).

A unified model of EOR systems

Most EOR systems are multiphase systems, albeit there are a few that are one-phase systems. In any event, EOR systems are particular cases of the most general multiphase system treated in this Section. In the axiomatic approach that permits such a unified treatment any multiphase system is characterized by the following axioms:

1. A family of phases. Each phase of this family moves with its own velocity;

2. A family of extensive properties. Each extensive property of such a family is associated with one and only one phase; and

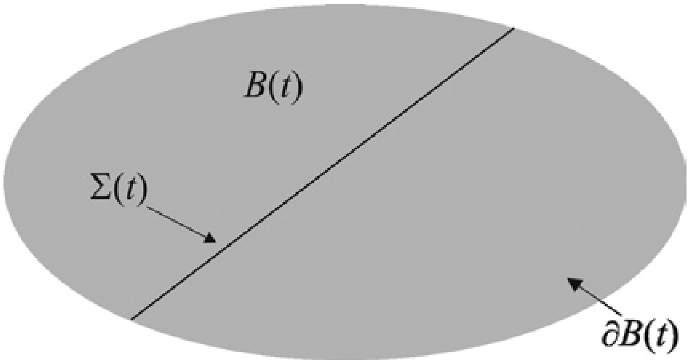

Figure 1. A fluid body and a shock in it.

3. The *basic mathematical model of the multiphase system* is constituted by the system of partial differential equations and jump conditions that is obtained when the *balance conditions* for each one of the extensive properties of the family is expressed in terms of the corresponding *intensive property*.

Once the axioms of multiphase systems have been described in this very brief manner, what remains is to state them with greater precision in mathematical terms, as we do next. In particular, with respect to Axiom 2, the manner in which *extensive properties* are associated with *phases* requires being described in greater detail.

The number of phases and extensive properties of these families will be denoted by M and N, respectively. We observe that $N \geq M$, necessarily. It is assumed that at each time, at each point of the physical space, there are M particles; each one of them corresponds to one and only one phase. Furthermore, given any domain of the physical space, let $B_\xi(t)$ be the set of particles of phase ξ (ξ may be $1,\dots, M$) that are located at such a domain at time t. A family of M bodies $\{B_1(t),\dots,B_M(t)\}$, is defined in this manner.

Then, a precise statement of the association between *extensive properties* and *phases* referred to in Axiom 2 follows. Given any *extensive property* $E^\alpha \in \{E^1,\dots,E^N\}$, there is a unique ξ, to be denoted by $\xi(\alpha)$, such that it has the property

$$E^\alpha(t) = \int_{B_\xi(t)} \psi^\alpha(\underline{x},t)\,dx . \tag{3.1}$$

Clearly, here the range of α is $\{1,\dots,N\}$, while that of ξ is $\{1,\dots,M\}$. In Eq. (3.1), ψ^α is the unique *intensive property* associated with E^α. Thereby, we observe that corresponding to the family $\{E^1,\dots, E^N\}$ of *extensive properties*, we have a unique family $\{\psi^1(\underline{x},t),\dots,\psi^N(\underline{x},t)\}$ of *intensive properties*, since the correspondence $E^\alpha \leftrightarrow \psi^\alpha$, $\alpha = 1,\dots, N$ is one-to-one. Therefore, every *intensive property* is also associated with one and only one phase.

The *global balance conditions* for each extensive property $E^\alpha \in \{E^1,\dots, E^N\}$ can now be expressed, as follows (see Figure 2):

$$\frac{dE^\alpha}{dt} = \int_{B_\xi(t)} g^\alpha(\underline{x},t)\,d\underline{x} + \int_{\partial B_\xi(t)} \underline{\tau}^\alpha(\underline{x},t) \bullet \underline{n}\,d\underline{x} + \int_{\Sigma(t)} g_\Sigma^\alpha(\underline{x},t)\,d\underline{x}, \quad \alpha = 1,\dots,N . \tag{3.2}$$

Here, it is understood that $\xi = \xi(\alpha)$, where $\xi(\alpha)$ corresponds to the unique phase associated with extensive property E^α. Furthermore, g^α and g^α_Σ, are the *'supplies'* of the extensive property α, the first one distributed in $B_\xi(t)$ and the second one concentrated on $\Sigma(t)$, while $\underline{\tau}^\alpha$ is the *'flux'* field of the same extensive property. The *supply terms*, g^α and g^α_Σ, will also be referred to as the *source terms*. As was mentioned before, $\Sigma(t)$ is the surface where discontinuities of any of the *intensive properties* of the model may occur; we observe that this definition is independent of the *extensive property* considered. However, for many extensive properties to be considered we will have $g^\alpha_\Sigma = 0$, on $\Sigma(t)$.

As it was seen in Section 2, the balance equation of any *extensive property* can also be expressed in terms of its corresponding *intensive property* by means of Eqs. (2.4) and (2.5). So, instead of the system of Eqs. (3.2), in what follows we use

$$\left.\begin{aligned} &\frac{\partial \psi^\alpha}{\partial t} + \nabla \bullet \left(\underline{v}^{\xi(\alpha)} \psi^\alpha\right) = \nabla \bullet \tau^\alpha + g^\alpha \\ &\left[\!\left[\psi^\alpha \left(\underline{v}^{\xi(\alpha)} - \underline{v}_\Sigma\right) - \underline{\tau}^\alpha \right]\!\right] \bullet \underline{n} = g^\alpha_\Sigma \end{aligned}\right\}, \alpha = 1,\dots,N . \tag{3.3}$$

We recall that the *jump conditions* are fulfilled on $\Sigma(t)$, while the differential equations everywhere, except at $\Sigma(t)$ and the outer boundary of the continuous system.

This system of *partial differential equations and jump conditions* constitutes a unified mathematical model of EOR systems, which is the *leitmotiv* of the present article mentioned before;

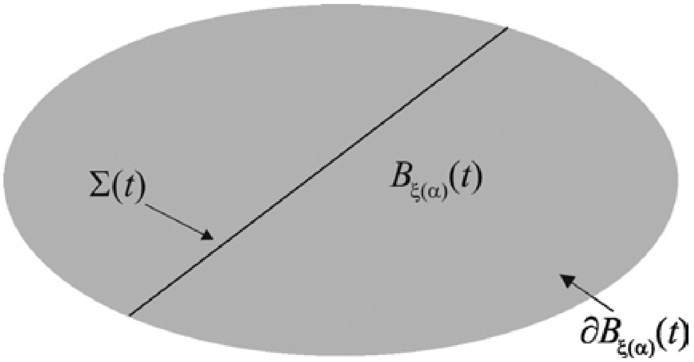

Figure 2. A body in a multiphase system.

it includes exhaustively the mathematical models of EOR systems. In the remaining of this article, this general model is specialized to obtain the most commonly used models of EOR technology. In particular, we will obtain the models discussed in the very comprehensive and complete treaty of EOR models, authored by Chen *et al*. (2006).

For models of *EOR* systems, it is useful to decompose the *source terms* g^α $(\alpha = 1,\ldots,N)$ into two parts whose origins can be traced back to the system *exterior* (g^α_e) and the system *interior* (g^α_I), respectively. Thus, we write

$$g^\alpha = g^\alpha_e + g^\alpha_I \tag{3.4}$$

The black-oil model

The basic mathematical model of a Black-Oil system corresponds to the case when in the *unified EOR model* of Section 3, the following conditions are satisfied; the family of phases is constituted by:

1. A water-phase,

2. An oil-phase (liquid), and

3. A gas-phase.

In Black-Oil and isothermal Compositional Models the phase constituted by the solid matrix of the oil reservoir is usually ignored because it does not move and it does not exchange mass with the fluid phases.

There are three different substances (or components): water, nonvolatile oil (usually called 'oil') and volatile oil (usually called 'gas'), and only the volatile-oil may be in more than one phase; namely, the oil and gas phases. The family of extensive properties has four members:

1. The *mass of water in the water-phase*,

2. The *mass of nonvolatile oil in the oil-phase*,

3. The *mass of volatile-oil contained in the oil-phase* ('dissolved gas'), and

4. The *mass of volatile-oil contained in the gas-phase*.

Let ψ^i $(i = 1,2,3,4)$ the *intensive properties* associated with each one of them. In this case the function $\xi(\alpha)$ is: $\xi(1)=1$, $\xi(2)=2$, $\xi(3)=2$ and $\xi(4)=3$. Then, the most basic mathematical model of Black-oil systems is given by Eq.(3.3); that is:

$$\begin{aligned}
&\frac{\partial \psi^1}{\partial t} + \nabla\bullet\left(\underline{v}^1\psi^1\right) = \nabla\bullet\underline{\tau}^1 + g^1\\
&\frac{\partial \psi^2}{\partial t} + \nabla\bullet\left(\underline{v}^2\psi^2\right) = \nabla\bullet\underline{\tau}^2 + g^2\\
&\frac{\partial \psi^3}{\partial t} + \nabla\bullet\left(\underline{v}^2\psi^3\right) = \nabla\bullet\underline{\tau}^3 + g^3\\
&\frac{\partial \psi^4}{\partial t} + \nabla\bullet\left(\underline{v}^3\psi^4\right) = \nabla\bullet\underline{\tau}^4 + g^4
\end{aligned} \tag{4.1}$$

The *jump conditions* are:

$$\left[\!\left[\psi^\alpha\left(\underline{v}^{\xi(\alpha)} - \underline{v}_\Sigma\right) - \underline{\tau}^\alpha\right]\!\right]\bullet n = g^\alpha_\Sigma, \alpha = 1,2,3,4 \ . \tag{4.2}$$

However, the jump conditions will not be discussed in this Section; instead, in the next one they will be used for making an exhaustive analysis of shocks that may occur in Black-Oil models.

Explicit expressions, as integrals, of these extensive properties are:

$$\begin{aligned}
E^1(t) &= \int_{B_1(t)} \phi S_w \rho_w dx\\
E^2(t) &= \int_{B_2(t)} \phi S_o \rho_{Oo} dx\\
E^3(t) &= \int_{B_2(t)} \phi S_o \rho_{Go} dx\\
E^4(t) &= \int_{B_3(t)} \phi S_g \rho_g dx
\end{aligned} \ . \tag{4.3}$$

So, the corresponding *intensive properties* are

$$\begin{aligned}
\psi^1(\underline{x},t) &= \phi S_w \rho_w\\
\psi^2(\underline{x},t) &= \phi S_o \rho_{Oo}\\
\psi^3(\underline{x},t) &= \phi S_o \rho_{Go}\\
\psi^4(\underline{x},t) &= \phi S_g \rho_g
\end{aligned} \ . \tag{4.4}$$

Furthermore, in what follows, we shall replace the superscripts $1,2,3,4,$ above, by w, Oo, Go and g, respectively.

Therefore, the *basic system of differential equations* of the Black-Oil model is constituted by the following system of equations

$$\begin{array}{l}
\dfrac{\partial \phi S_w \rho_w}{\partial t} + \nabla \bullet \left(\phi S_w \rho_w \underline{v}^w \right) = \nabla \bullet \underline{\tau}^w + g_e^w + g_I^w \\
\dfrac{\partial \phi S_o \rho_{Oo}}{\partial t} + \nabla \bullet \left(\phi S_o \rho_{Oo} \underline{v}^o \right) = \nabla \bullet \underline{\tau}^{Oo} + g_e^{Oo} + g_I^{Oo} \\
\dfrac{\partial \phi S_o \rho_{Go}}{\partial t} + \nabla \bullet \left(\phi S_o \rho_{Go} \underline{v}^o \right) = \nabla \bullet \underline{\tau}^{Go} + g_e^{Go} + g_I^{Go} \\
\dfrac{\partial \phi S_g \rho_g}{\partial t} + \nabla \bullet \left(\phi S_g \rho_g \underline{v}^g \right) = \nabla \bullet \underline{\tau}^g + g_e^g + g_I^g
\end{array} . \tag{4.5}$$

In the Black-Oil model *dispersion-diffusion processes* are neglected, so that $\underline{\tau}^\alpha = 0$ $(= w, Oo, Go, g)$. As for the *internal sources,* g^α_I, all them are zero except when $\alpha = Go, g$. In the absence of chemical reactions, as it is assumed in the Black-Oil Model, the mass of volatile oil is conserved and then:

$$g_I^{Go} + g_I^g = 0 \,. \tag{4.6}$$

Hence, Eq. (4.5) reduces to:

$$\begin{array}{l}
\dfrac{\partial \phi S_w \rho_w}{\partial t} + \nabla \bullet \left(\phi S_w \rho_w \underline{v}^w \right) = g_e^w \\
\dfrac{\partial \phi S_o \rho_{Oo}}{\partial t} + \nabla \bullet \left(\phi S_o \rho_{Oo} \underline{v}^o \right) = g_e^{Oo} \\
\dfrac{\partial \phi S_o \rho_{Go}}{\partial t} + \nabla \bullet \left(\phi S_o \rho_{Go} \underline{v}^o \right) = g_e^{Go} + g_I^{Go} \\
\dfrac{\partial \phi S_g \rho_g}{\partial t} + \nabla \bullet \left(\phi S_g \rho_g \underline{v}^g \right) = g_e^g + g_I^g
\end{array} . \tag{4.7}$$

Generally, the external sources g^α_e are due to wells; they are negative if extraction occurs and positive if injection takes place. In particular, the terms $-g^w_e$ and $-g^{Oo}_e$ represent the mass of water and non-volatile oil extracted from the water and oil phases, respectively, while $-g^{Go}_e$ and $-g^g_e$ represent the mass of nonvolatile-oil extracted from the oil and gas phases, respectively.

Starting with Eq. (4.7) it is easy to derive the standard forms of the mathematical model of Black-Oil reservoirs; in particular, for comparison we will use that presented in Chen *et al.* (2006). To this end we introduce the Darcy velocity, for each phase, which is defined by

$$\underline{u}_\xi = \phi S_\xi \underline{v}^\xi, \xi = w, o, g \tag{4.8}$$

Then, adding up the last two equalities of Eq. (4.7), we get

$$\begin{array}{l}
\dfrac{\partial \phi S_w \rho_w}{\partial t} + \nabla \bullet \left(\rho_w \underline{u}^w \right) = g_e^w \\
\dfrac{\partial \phi S_o \rho_{Oo}}{\partial t} + \nabla \bullet \left(\rho_{Oo} \underline{u}^o \right) = g_e^{Oo} \\
\dfrac{\partial \phi \left(S_o \rho_{Go} + S_g \rho_g \right)}{\partial t} + \nabla \bullet \left(\rho_{Go} \underline{u}^o + \rho_g \underline{u}^g \right) = g_e^{Go} + g_I^{Go}
\end{array} ; \tag{4.9}$$

together with

$$g_I^g = \frac{\partial \phi S_o \rho_{Go}}{\partial t} + \nabla \bullet \left(\rho_{Go} \underline{u}^o \right) - g_e^{Go} ; \tag{4.10}$$

or

$$g_I^{Go} = \frac{\partial \phi S_g \rho_g}{\partial t} + \nabla \bullet \left(\rho_g \underline{u}^g \right) - g_e^g \tag{4.11}$$

Eqs. (4.10) and (4.11) are not usually mentioned in the literature, since they are a sub-product of the methodology here applied for deriving the basic differential equations. However, they may be useful in some instances since either one of them can be applied for evaluating the *nonvolatile-oil* exchanged by the oil and gas phases.

The rest of the derivation is standard. Eqs. (4.9) can be transformed into (see Chen *et al*., 2006):

$$\begin{array}{l}
\dfrac{\partial}{\partial t}\left(\dfrac{\phi S_w \rho_{ws}}{B_w} \right) + \nabla \bullet \left(\dfrac{\rho_{ws} \underline{u}_w}{B_w} \right) = g_e^w \\
\dfrac{\partial}{\partial t}\left(\dfrac{\phi S_o \rho_{Os}}{B_0} \right) + \nabla \bullet \left(\dfrac{\rho_{Os} \underline{u}_o}{B_o} \right) = g_e^{Oo} \\
\dfrac{\partial \phi \left(\dfrac{S_g \rho_{Gs}}{B_g} + \dfrac{\rho_{Gs} S_o R_{so}}{B_o} \right)}{\partial t} + \\
\nabla \bullet \left\{ \left(\dfrac{\rho_{Gs}}{B_g} \underline{u}_g + \dfrac{\rho_{Gs} R_{so}}{B_o} \underline{u}_o \right) \right\} = g_e^{Go} + g_e^g
\end{array} . \tag{4.12}$$

This is achieved introducing the following notation (further details of the symbols used here are given at the end of this Section):

$$R_{so} \equiv \frac{\rho_{Os}}{\rho_{Gs}} \frac{\rho_{Go}}{\rho_{Oo}} \,. \tag{4.13}$$

The *formation volume factors*, B_w, B_0 and B_g are defined by

$$B_w \equiv \frac{\rho_{Ws}}{\rho_w}, B_o \equiv \frac{\rho_{Os} + R_{so} \rho_{Gs}}{\rho_o} \; and \; B_w \equiv \frac{\rho_{Gs}}{\rho_g} \,. \tag{4.14}$$

Eqs. (4.12) have to be complemented by several *constitutive equations* relating the variables occurring in them. In particular, Darcy's law

$$\underline{u}_\xi = -\frac{\underline{\underline{k}}_\xi}{\mu_\xi}\left(\nabla p_\xi + \rho_\xi \gamma_\xi \nabla z\right), \xi = w,o,g \tag{4.15}$$

the saturations identity

$$S_w + S_o + S_g = 1 \tag{4.16}$$

The capillary pressure equations

$$p_o - p_w = p_{cow} \text{ and } p_g - p_o = p_{cgo} \ , \tag{4.17}$$

which relate the phase pressures. Both p_{cow} and p_{cgo} are functions of other parameters of the reservoir system, the saturations in particular, which must be determined in advance, experimentally or otherwise. The *gas-oil ratio* equation of state:

$$R_{so} = R_{so}\left(p_o, T\right) \tag{4.18}$$

which is satisfied when $S_g > 0$; i.e., when the reservoir is truly a three-phase system.

The following list of symbols complements the notation already explained in the text of this Section:

$$\left.\begin{array}{l}
\gamma \equiv \text{gravity acceleration} \\
\underline{\underline{k}}k_{r\xi} = \underline{\underline{k}}_\xi \equiv \text{effective permeability of phase } \xi \\
\underline{\underline{k}} \equiv \text{absolute permeability} \\
k_{r\xi} \equiv \text{relative permeability} \\
p_\xi \equiv \text{pressure of phase } \xi \\
\rho_\xi \equiv \text{density of phase } \xi \\
\rho_{Go} \equiv \text{mass of dissolved gas/volume of oil - phase} \\
\rho_{Gs} \equiv \text{gas - density at standard conditions} \\
\rho_{Oo} \equiv \text{mass of nonvolatile - oil/volume of oil - phase} \\
\rho_{Os} \equiv \text{oil - density at standard conditions} \\
\rho_{Ws} \equiv \text{water - density at standard conditions} \\
T \equiv \text{temperature}
\end{array}\right\} \xi = w,o,g$$

From the mere fact that the system consists of three phases and one of them contains two components, while each one of the other two contains only one, without any additional knowledge, we have derived the system of equations given by Eqs. (4.1) and (4.2). Such equations give a very firm basis for incorporating all the scientific and technological knowledge available about the system, as we have done, to obtain as final product the mathematical model of Black-Oil systems.

Analysis of shocks that may occur in black-oil models

To start with, we observe that Darcy's Law implies that the pressure is continuous and, if the solid-matrix does not have abrupt changes in properties, as in the contact between two geological formations of different origin, the porosity is also continuous. Then, the shock conditions of Eq. (4.2) when the external source terms vanish can be written as:

$$\begin{array}{ll}
[\![S_w\left(\underline{v}^w - \underline{v}_\Sigma\right)]\!]\bullet\underline{n} = 0 & \\
[\![S_o\rho_{Oo}\left(\underline{v}^o - \underline{v}_\Sigma\right)]\!]\bullet n = 0 & \\
\phi[\![R_s S_o\rho_{Oo}\left(\underline{v}^o - \underline{v}_\Sigma\right)]\!]\bullet\underline{n} = g^{Go}_{\Sigma g} & \text{with } g^{Go}_{\Sigma g} + g^{g}_{\Sigma Go} = 0 \\
\phi[\![S_g\rho_g\left(\underline{v}^g - \underline{v}_\Sigma\right)]\!]\bullet\underline{n} = g^{g}_{\Sigma Go} &
\end{array} \tag{5.1}$$

where $R_s(p, T)$is the *gas-oil ratio* defined by $\rho_{Go} = R_s\rho_{Oo}$.

A. In a region where the gas-phase is absent

The density ρ_{Oo} is continuous across the shock Σ because so is the pressure p_o. When the gas-phase is not present $S_g = 0$, so that Eq. (5.1) implies $g^{Go}_{\Sigma g} = g^{g}_{\Sigma Go} = 0$, and implies

$$[\![R_s]\!]\dot{\widehat{S_o\left(\underline{v}^o - \underline{v}_\Sigma\right)}}\cdot n = 0 \ , \tag{5.2}$$

where the notation is such that for any function f, $\dot{f} = \frac{f_+ + f_-}{2}$ is the the *average* of the function f across Σ.

From the first equality in Eq. (5.1) it follows that when $[\![S_w]\!] = -[\![S_o]\!] \neq 0$, the shock velocity is given by

$$\underline{v}_\Sigma\bullet\underline{n} = \frac{[\![S_w\underline{v}^w]\!]\bullet\underline{n}}{[\![S_w]\!]} \ . \tag{5.3}$$

On the other hand, from Eq. (5.2) it follows that when $[\![R_s]\!] \neq 0$, the shock velocity is given by

$$\underline{v}_\Sigma\bullet\underline{n} = \frac{\dot{\widehat{S_o\underline{v}_o}}\bullet\underline{n}}{\dot{\widehat{S_o}}} \tag{5.4}$$

Generally,

$$\frac{\dot{\widehat{S_o \underline{v}_o \bullet \underline{n}}}}{\dot{\widehat{S}}_o} \neq \frac{\llbracket S_w \underline{v}^w \rrbracket \bullet \underline{n}}{\llbracket S_w \rrbracket} . \tag{5.5}$$

Therefore, if these two kinds of shocks coincide at any time they will separate, since their velocities are different. Thus, at a shock either $\llbracket R_s \rrbracket = 0$, in which case $\llbracket S_w \rrbracket = -\llbracket S_o \rrbracket \neq 0$ and the velocity of the shock is given by Eq. (5.3), or $\llbracket S_w \rrbracket = -\llbracket S_o \rrbracket = 0$, in which case $\llbracket R_s \rrbracket \neq 0$ and the velocity of the shock is given by

$$\underline{v}_\Sigma = \underline{v}^o \tag{5.6}$$

B. At a gas front

For simplicity in what follows we only consider the case when the water phase is not present. At a front that advances into a region of under saturated oil, we take the unit normal vector pointing towards the under saturated region (Figure 3). Adding up the last two equalities in Eq. (5.1), one gets:

$$\llbracket R_s S_o \rho_{Oo} \left(\underline{v}^o - \underline{v}_\Sigma \right) \rrbracket \bullet \underline{n} + \llbracket S_g \rho_g \left(\underline{v}^g - \underline{v}_\Sigma \right) \rrbracket \bullet \underline{n} = 0 , \tag{5.7}$$

In the under-saturated oil region $Sg = 0$; i.e. $(S_g)_+ = 0$, on Σ.

According to the second equality in Eq. (5.1), $S_o(\underline{v}^o - \underline{v}_\Sigma)$ is continuous across the shock and therefore, from Eq. (5.7), it follows that

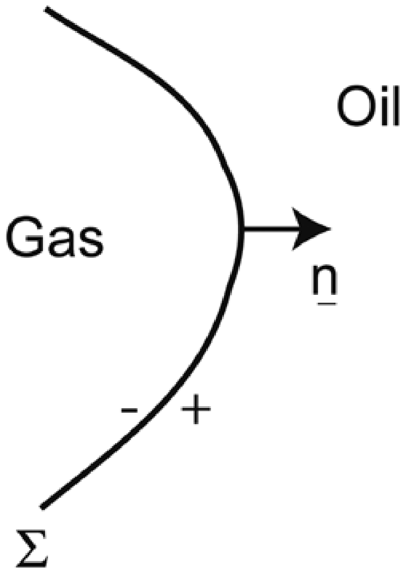

Figure 3. A gas-front that advances into a region of under saturated oil.

$$\llbracket R_s \rrbracket \frac{S_{o+} \rho_{Oo+}}{S_{g-} \rho_{g-}} \left(\underline{v}^o_+ - \underline{v}_\Sigma \right) \bullet \underline{n} = \left(\underline{v}^g_- - \underline{v}_\Sigma \right)_- \bullet \underline{n} . \tag{5.8}$$

Using the identity $\underline{v}^g_- - \underline{v}_\Sigma = \underline{v}^g_- - \underline{v}^o_+ + \underline{v}^o_+ - \underline{v}_\Sigma$, it can be seen that

$$\left(\underline{v}_\Sigma - \underline{v}^o_+ \right) \bullet \underline{n} = \varepsilon \left(\underline{v}^g_- - \underline{v}^o_+ \right) \bullet \underline{n} , \tag{5.9}$$

With

$$\varepsilon \equiv \frac{1}{1 + \llbracket R_s \rrbracket \dfrac{S_{o+} \rho_{Oo+}}{S_{g-} \rho_{g-}}} \leq 1 . \tag{5.10}$$

The physical interpretation of this result is that when a gas front advances into a region of under-saturated oil, it is retarded in its motion by the *'retardation factor'* ε (see Herrera, 1996, and Herrera and Camacho, 1997).

C. In a saturated oil-region (Buckley-Leverett theory)

This is the case of a biphasic system in which the gas-phase and the liquid oil-phase coexist, which was treated by Buckley-Leverett in their classical theory (Buckley and Leverett,1942). In this case $\llbracket R_S \rrbracket = 0$, because the oil is saturated and the pressure is continuous, Eq (5.1). reduce to

$$\begin{aligned} \llbracket S_o \left(\underline{v}^o - \underline{v}_\Sigma \right) \rrbracket \bullet \underline{n} = 0 \\ \llbracket S_g \left(\underline{v}^g - \underline{v}_\Sigma \right) \rrbracket \bullet \underline{n} = 0 \end{aligned} . \tag{5.11}$$

This is analogous to Eq. (5.2). Corresponding to Eq. (5.3), we now derive the equation:

$$\underline{v}_\Sigma \bullet \underline{n} = \frac{\llbracket S_g \underline{v}^g \rrbracket \bullet \underline{n}}{\llbracket S_g \rrbracket} , \tag{5.12}$$

or,

$$\underline{v}_\Sigma \bullet \underline{n} = \frac{\llbracket \underline{u}_g \rrbracket \bullet \underline{n}}{\phi \llbracket S_g \rrbracket} . \tag{5.13}$$

A special case of this equation is the immiscible and incompressible case considered by the classical Buckley-Theory, for which Eq. (5.13) becomes the well-known relation (see, for example, Herrera and Camacho, 1997):

$$\underline{v}_\Sigma \bullet \underline{n} = \phi^{-1} \frac{\llbracket f_g \rrbracket}{\llbracket S_g \rrbracket} \underline{u}_T \bullet \underline{n} . \tag{5.14}$$

Here,

$$\underline{u}_T \equiv \underline{u}_o + \underline{u}_g \text{ and } \underline{u}_g = f_g \underline{u}_T \quad . \tag{5.15}$$

The compositional model

In this Section we apply the general scheme of Section 3 to obtain the *basic mathematical model* of compositional oil reservoirs. The derivation need not be as formal as in Section 4, since the general protocol has already been illustrated there.

The characteristic features of *compositional models* are:

1. The *family of phases* is the same as before: the water-phase, the oil-phase and the gas-phase. The notation used for the velocities of such phases is also the same:

i) $\underline{v}^w$ is the velocity of the water-phase;

ii) $\underline{v}^o$ is the velocity of the oil-phase; and

iii) $\underline{v}^g$ is the velocity of the gas-phase.

2. Besides the water, we distinguish Nc chemical substances; these substances do not change chemical composition through time. However, through time, each one of them is exchanged by the oil and gas phases. The *family of extensive properties* consists of $2Nc + 1$ members; namely,

i) The *mass of the water-phase,* denoted by M^w;

ii) The *mass of the i-th component in the oil-phase,* denoted by $M^{io}(t)$, $i = 1,\ldots,Nc$; and

iii) The *mass of the i-th component in the gas-phase,* denoted by M^{ig}, $i = 1,\ldots,Nc$.

The notations used for the corresponding *intensive properties*, *supplies* (i.e., mass-sources) and *flux-fields* are:

$$\left.\begin{array}{l} M^w \leftrightarrow \psi^w \to g^w = g_e^w + g_I^w, g_\Sigma^w \to \underline{\tau}^w \\ M^{io} \leftrightarrow \psi^{io} \to g^{io} = g_e^{io} + g_I^{io}, g_\Sigma^{io} \to \underline{\tau}^{io} \\ M^{ig} \leftrightarrow \psi^{ig} \to g^{ig} = g_e^{ig} + g_I^{ig}, g_\Sigma^{ig} \to \underline{\tau}^{ig} \end{array}\right\} i = 1,\ldots,N_c \tag{6.1}$$

3. The *basic mathematical model of the multiphase system* is constituted by the *system of partial differential equations* and *jump conditions* of Eqs. (3.3); i.e.,

$$\begin{array}{l} \dfrac{\partial \psi^w}{\partial t} + \nabla\bullet\left(\psi^w \underline{v}^w\right) = g_e^w + g_I^w \\ \dfrac{\partial \psi^{io}}{\partial t} + \nabla\bullet\left(\psi^{io} \underline{v}^{io}\right) = g_e^{io} + g_I^{io} \quad , i = 1,\ldots,N_C \quad , \\ \dfrac{\partial \psi^{ig}}{\partial t} + \nabla\bullet\left(\psi^{ig} \underline{v}^{ig}\right) = g_e^{ig} + g_I^{ig} \end{array} \tag{6.2}$$

and

$$\begin{array}{l} \left[\!\left[\psi^w\left(\underline{v}^w - \underline{v}_\Sigma\right) - \underline{\tau}^w\right]\!\right]\bullet\underline{n} = g_\Sigma^w \\ \left[\!\left[\psi^{io}\left(\underline{v}^o - \underline{v}_\Sigma\right) - \underline{\tau}^{io}\right]\!\right]\bullet\underline{n} = g_\Sigma^{io} \\ \left[\!\left[\psi^{ig}\left(\underline{v}^g - \underline{v}_\Sigma\right) - \underline{\tau}^{ig}\right]\!\right]\bullet\underline{n} = g_\Sigma^{ig} \end{array} \tag{6.3}$$

In Eq. (6.2), the *source-terms* have been expressed as in Eq. (3.4).

Eqs. (6.2) and (6.3) constitute the *basic mathematical model of 'compositional' EOR systems*. A model capable of predicting the system behavior, when it is subjected to suitable initial and boundary conditions, will be derived from it by incorporating sufficient scientific and technical information about the actual system following the protocol *leitmotiv* of this article.

The integral expressions for each one of the $2Nc + 1$ extensive properties are:

$$\left.\begin{array}{l} M^w(t) = \displaystyle\int_{B_w(t)} \phi S_w \rho_w \, dx \\ M^{io}(t) = \displaystyle\int_{B_o(t)} \phi S_o \rho_{io} \, dx \\ M^{ig}(t) = \displaystyle\int_{B_g(t)} \phi S_g \rho_{ig} \, dx \end{array}\right\}, i = 1,\ldots,N_c \quad . \tag{6.4}$$

Therefore,

$$\left.\begin{array}{l} \psi^w(t) = \phi S_w \rho_w \\ \psi^{io}(t) = \phi S_o \rho_{io} \\ \psi^{ig}(t) = \phi S_g \rho_{ig} \end{array}\right\}, i = 1,\ldots,N_c \tag{6.5}$$

Furthermore, in the *Compositional Model* diffusion-dispersion processes of the components are neglected; this implies that all the *flux-fields* are zero; i.e.,

$$\left.\begin{array}{l} \underline{\tau}^w = 0 \\ \underline{\tau}^{oi} = 0 \\ \underline{\tau}^{gi} = 0 \end{array}\right\}, i = 1,\ldots,N_C \quad . \tag{6.6}$$

According to our assumptions $g_I^w = 0$, since no matter is exchanged with the water-phase.

When all this is taken into account, the *basic mathematical model* for compositional systems, of Eqs. (6.2) and (6.3), becomes:

$$\frac{\partial \phi S_w \rho_w}{\partial t} + \nabla \bullet \left(\phi S_w \rho_w \underline{v}^w \right) = g_e^w$$

$$\frac{\partial \phi S_o \rho_{io}}{\partial t} + \nabla \bullet \left(\phi S_o \rho_{Oo} \underline{v}^o \right) = g_e^{io} + g_I^{io} \quad ,$$

$$\frac{\partial \phi S_g \rho_{ig}}{\partial t} + \nabla \bullet \left(\phi S_g \rho_{ig} \underline{v}^g \right) = g_e^{ig} + g_I^{ig} \qquad (6.7)$$

and

$$\left[\!\left[\phi S_w \rho_w \left(\underline{v}^w - \underline{v}_\Sigma \right) \right]\!\right] \bullet \underline{n} = g_\Sigma^w$$

$$\left[\!\left[\phi S_o \rho_{io} \left(\underline{v}^o - \underline{v}_\Sigma \right) \right]\!\right] \bullet \underline{n} = g_\Sigma^{io} \ .$$

$$\left[\!\left[\phi S_g \rho_{ig} \left(\underline{v}^g - \underline{v}_\Sigma \right) \right]\!\right] \bullet \underline{n} = g_\Sigma^{ig} \qquad (6.8)$$

The contributions to ${g^\alpha}_e$, $\alpha = w, io, ig$, generally, are due to extraction or injection through wells. We observe that the following conditions are fulfilled:

$$g_I^{io} + g_I^{ig} = 0, i = 1, \ldots, N_C \qquad (6.9)$$

since the mass of each component must be conserved.

Mass interchange between phases is determined by the mass distribution of each component in the oil and gas phases through the condition of *stable thermodynamic equilibrium* (Chen *et al*, 2006). This condition is expressed by means of the equation

$$f_{io}\left(p_o, x_{1o}, x_{2o}, \ldots, x_{N_C o} \right) =$$
$$f_{ig}\left(p_g, x_{1g}, x_{2g}, \ldots, x_{N_C g} \right), i = 1, \ldots, N_c \ . \qquad (6.10)$$

Here, f_{io} and f_{ig} are the *fugacity functions* of the component in the oil and gas phases, respectively.

For the application of the *stable thermodynamic equilibrium* condition, the following notation and nomenclature is relevant:

$$\left. \begin{array}{l} \xi_w = \rho_w / W_w \\ \xi_{io} = \rho_{io} / W_i \\ \xi_{ig} = \rho_{ig} / W_i \end{array} \right\}, \ i = 1, \ldots, N_C \quad .$$

$$\xi_\alpha = \sum_{i=1}^{N_C} \xi_{i\alpha} \ and \ \chi_{i\alpha} = \xi_{i\alpha} / \xi_\alpha \qquad (6.11)$$

Here, W_w and W_i are the *"molar masses"*. On the other hand ξ_w, ξ_{io}, and ξ_{ig} are the *"molar densities"* of the water, the $i-th$ component in the oil-phase and of the $i-th$ component in the gas-phase, respectively. Furthermore, ξ_α is the *"molar density of phase α"*. The *"mole fraction of component i in phase α"*, is $\chi_{i\alpha}$. Since the condition of *stable thermodynamic equilibrium* is expressed in terms of the *mole fraction of component i in phase α*, it is advantageous to express the basic equations of the *compositional model* in terms of such parameters. Then

$$\left. \begin{array}{l} \dfrac{\partial \phi \xi_w S_w}{\partial t} + \nabla \bullet \left(\xi_w \underline{u}^w \right) = g^w / W_w \equiv q_w \\ \dfrac{\partial \phi \chi_{io} \xi_o S_o}{\partial t} + \nabla \bullet \left(\chi_{io} \xi_o \underline{u}^o \right) = \left(g^{io} + g_{ig}^{io} \right) / W_i \\ \dfrac{\partial \phi \chi_{ig} \xi_g S_g}{\partial t} + \nabla \bullet \left(\chi_{ig} \xi_g \underline{u}^g \right) = \left(g^{ig} + g_{io}^{ig} \right) / W_i \end{array} \right\}, \ i = 1, \ldots, N_C \qquad (6.12)$$

Adding up the last two equalities appearing in Eq. (6.12) and using Eq. (6.9), we get

$$\left. \begin{array}{l} \dfrac{\partial \phi \xi_w S_w}{\partial t} + \nabla \bullet \left(\xi_w \underline{u}^w \right) = q_w \\ \dfrac{\partial \phi \left(\chi_{io} \xi_o S_o + \chi_{ig} \xi_g S_g \right)}{\partial t} + \\ \nabla \bullet \left(\chi_{io} \xi_o \underline{u}^o + \chi_{ig} \xi_g \underline{u}^g \right) = \chi_{io} q_o + \chi_{ig} q_g \end{array} \right\}, \ i = 1, \ldots, N_C \ . \qquad (6.13)$$

As in the case of the Black-Oil model, the last two equalities in Eq. (6.12), can be used to evaluate the supplies ${g^{io}}_{ig}$ and ${g^{ig}}_{io}$ due to exchange. We recall that for saturated flows, these equations are supplemented with the saturation identity:

$$S_w + S_o + S_g = 1 \ . \qquad (6.14)$$

Other equations that are applied in order to obtain a model capable of predicting the system behavior are:

Darcy's Law,

$$\underline{u}^\beta = -\frac{k_{r\beta}}{\mu_\beta} \underline{\underline{k}} \left(\nabla p_\beta - \rho_\beta \gamma \nabla z \right), \beta = w, o, g \ , \qquad (6.15)$$

where $k_{r\beta}$ and μ_β are the relative permeability and the dynamic viscosity of the β phase, and $\underline{\underline{k}}$ is the absolute permeability.

Mole fractions identities,

$$\sum_{i=1}^{N_c}\chi_{io} = 1 \; and \; \sum_{i=1}^{N_c}\chi_{ig} = 1 \tag{6.16}$$

Capillary relations,

$$p_{cow} = p_o - p_w \; and \; p_{cgo} = p_g - p_o \;, \tag{6.17}$$

here p_{cow} and p_{cgo} are the capillarity pressures of oil and water and gas and oil, respectively, and p_β is the pressure of the β phase. Equations (6.13)-(6.17), together with the *stable thermodynamic equilibrium* condition of Eq. (6.10) constitute a $2N_c + 9$ system of equations for the $2N_c + 9$ dependent variables χ_{io}, χ_{ig}, $\underline{u}_\alpha$, p_α and S_α, $\alpha = w, o, g, \; i = 1,...,N_c$, which when subjected to suitable boundary and initial conditions provide a model capable of predicting the behavior of the compositional system.

The non-isothermal models

As stated before, in Black-Oil and Isothermal Compositional Models the phase constituted by the solid matrix of the oil reservoir is usually ignored because it does not move and it does not exchange mass with the fluid phases. However, the solid matrix cannot be ignored when formulating non-isothermal models since then energy balances have to be included and the solid phase plays a significant role in them. In turn, this is due to the fact that rocks and other materials that form the solid matrices of oil reservoirs have large heat capacities, frequently larger than the fluid phases participating in the reservoir systems.

Thus, the basic mathematical model of the non-isothermal compositional systems here discussed, has the general features that follow. The family of phases has four members: the solid matrix, the water-phase, the oil-phase and the gas-phase. The velocity of the solid phase is zero, while the notation used for the velocities of the other phases is the same that has been used in previous Sections. The family of extensive properties has $2N_c + 5$ members. The first $2N_c + 1$ are the same as for the Compositional Model. So, we only discuss here the other four; they are:

i) The *total energy of the water-phase,* denoted by $E^w(t)$;

ii) The *total energy of the oil-phase,* denoted by, $E^o(t)$;

iii) The *total energy of the gas-phase,* denoted by, $E^g(t)$; and

iv) The *total energy of the solid-phase,* denoted by, $E^S(t)$

For simplicity jump conditions will not be discussed. The differential equations required to complete the *non-thermal compositional model* are obtained applying Eq. (3.3). The *total energy* of each one of the phases is given by

$$\begin{aligned}\mathrm{E}^\alpha(t) &= \int\limits_{B_w(t)} \phi\rho_\alpha S_\alpha\left(\frac{1}{2}\left|\underline{v}^\alpha\right|^2 + U_\alpha\right)dx, \alpha = w,o,g \\ \mathrm{E}^s(t) &= \int\limits_{B_g(t)} (1-\phi)\rho_s U_s \, dx\end{aligned} \tag{7.1}$$

Where U_α is the specific internal energy (per unit mass) of phase α. Due to the smallness of the velocities occurring in flow of fluids through porous media, inertial effects are neglected and the kinetic energy is taken to be identically zero. Therefore, we take

$$\mathrm{E}^\alpha(t) = \int\limits_{B_w(t)} \phi\rho_\alpha S_\alpha U_\alpha \, dx, \alpha = w,o,g \quad , \tag{7.2}$$

Using Eqs. (7.1) and (7.2) it is seen that the *intensive properties* that correspond to the total-energies of the different phases are

$$\left.\begin{aligned}\psi^\alpha(t) &= \phi\rho_\alpha S_\alpha U_\alpha \\ \psi^s(t) &= (1-\phi)\rho_s U_s\end{aligned}\right\}, \alpha = w,o,g \tag{7.3}$$

Since we are dealing with total energy, the energy sources should be decomposed into two parts: heat sources and mechanical-energy sources (Herrera and Pinder, to appear). A similar decomposition applies to the energy fluxes. This is better understood making the analysis in integral form. In such a form, the balance equations for the *extensive properties* associated with the different fluid phases ($\alpha = w,o,g$) are:

$$\begin{aligned}\frac{dE^\alpha}{dt}(t) = \int_{B_\alpha(t)} \left\{\rho_\alpha\left[\phi S_\alpha h_\alpha - \gamma\left(\underline{u}_\alpha\right)_z\right] - q_L^\alpha + g_I^{E\alpha}\right\} dx \; + \\ \int_{\partial B_\alpha(t)} \left(\phi S_\alpha \underline{\underline{\sigma}}^\alpha \underline{v}^\alpha + \underline{q}^\alpha\right) \bullet \underline{n} \, dx \;.\end{aligned} \tag{7.4}$$

Here, the heat sources are: $\phi S_\alpha \rho_\alpha h_\alpha$ and $q^\alpha{}_L$. The former represents the rate per unit volume of the physical space at which internal energy is supplied to the α phase by sources distributed in the body-interior (due, for example, to exothermal chemical reactions), while $q^\alpha{}_L$ is the heat loss of the α phase to the overburden and underburden, also per unit volume of the physical space. The term $-\gamma\rho_\alpha(\underline{u}_\alpha)_z$ (γ is the gravity acceleration and $(\underline{u}_\alpha)_z$ is the component of $\underline{u}_\alpha$ in the z direction) represents the mechanical work done by the gravity force on phase α. Furthermore, we put together the exchange of energy between the phases in the term $g^{E\alpha}{}_{I}$, which represents the total energy that enters phase α from other phases. As for energy fluxes that enter the α phase through its boundary, they are given by q^{α} and $\phi S^{\alpha}\underline{\underline{\sigma}}^{\alpha}\underline{v}^{\alpha}$. The former is the heat flux, while the latter comes from mechanical work done on the boundary of α bodies. Finally, we observe that

$$\sum_{\alpha=w,o,g,s} g_{I}^{E\alpha} = 0 \tag{7.5}$$

For the *non-isothermal compositional model* to be developed, the mechanical work done by the gravity force will be neglected (i.e., $\gamma(\underline{u}_{\alpha})_{z}\, 0$). Also, the work done by viscous forces will be neglected and, so, the stress tensor acting on phase α will be $\underline{\underline{\sigma}}^{\alpha} = -p_{\alpha}\underline{\underline{I}}$. Therefore,

$$\int_{\partial B(t)} \left(\phi S_{\alpha} \underline{\underline{\sigma}}^{\alpha} \bullet \underline{v}^{\alpha} \right) \bullet \underline{n}\, dx = -\int_{\partial B(t)} p_{\alpha} \underline{u}_{\alpha} \bullet \underline{n}\, dx \, ; \tag{7.6}$$

and Eq. (7.4) becomes

$$\int_{\partial B(t)} \left(\phi S_{\alpha} \underline{\underline{\sigma}}^{\alpha} \bullet \underline{v}^{\alpha} \right) \bullet \underline{n}\, dx = -\int_{\partial B(t)} p_{\alpha} \underline{u}_{\alpha} \bullet \underline{n}\, dx \, ; \tag{7.7}$$

This balance equation, when expressed in terms of the *intensive property,* becomes

$$\frac{\partial \phi \rho_{\alpha} S_{\alpha} U_{\alpha}}{\partial t} + \nabla \bullet \left(\rho_{\alpha} U_{\alpha} \underline{u}_{\alpha} \right) = \nabla \bullet \left(\underline{q}^{\alpha} - p_{\alpha} \underline{u}_{\alpha} \right) + \rho_{\alpha} \phi S_{\alpha} h_{\alpha} - q_{L}^{\alpha} + g_{I}^{E\alpha} \tag{7.8}$$

It can also be written as

$$\frac{\partial \phi \rho_{\alpha} S_{\alpha} U_{\alpha}}{\partial t} + \nabla \bullet \left\{ \rho_{\alpha} \underline{u}_{\alpha} \left[U_{\alpha} + p_{\alpha} \left(\rho_{\alpha} \right)^{-1} \right] \right\} = \nabla \bullet \left(\underline{q}^{\alpha} \right) + \rho_{\alpha} \phi S_{\alpha} h_{\alpha} - q_{L}^{\alpha} + g_{I}^{E\alpha} \tag{7.9}$$

By definition, the *"enthalpy per unit mass"* of the fluid phase H_{α} $(\alpha = w, o, g)$, satisfies

$$H_{\alpha} \equiv U_{\alpha} + p_{\alpha} \left(\rho_{\alpha} \right)^{-1} \tag{7.10}$$

Therefore, for $\alpha = w, o, g$, Eq. (7.9) is

$$\frac{\partial \phi \rho_{\alpha} S_{\alpha} U_{\alpha}}{\partial t} + \nabla \bullet \left\{ \rho_{\alpha} \underline{u}_{\alpha} H_{\alpha} \right\} = \nabla \bullet \underline{q}^{\alpha} + \rho_{\alpha} \phi S_{\alpha} h_{\alpha} - q_{L}^{\alpha} + g_{I}^{E\alpha} \, . \tag{7.11}$$

The balance equation for the *extensive property* associated with the energy of the solid phase is:

$$\frac{dE^{s}}{dt}\left(t \right) = \int_{B(t)} \left(g_{I}^{Es} - q_{L}^{s} \right) dx + \int_{\partial B(t)} \underline{q}^{s} \bullet \underline{n}\, dx \, . \tag{7.12}$$

This balance equation, when expressed in terms of the *intensive property*, is:

$$\frac{\partial \left(1 - \phi \right) \rho_{s} U_{s}}{\partial t} = \nabla \bullet \left(\underline{q}^{s} \right) + g_{I}^{Es} - q_{L}^{s} \, . \tag{7.13}$$

Adding up Eq. (7.13) and the four equalities of Eq. (7.11), we get

$$\frac{\partial}{\partial t} \left(\phi \sum_{\alpha=w,o,g} \rho_{\alpha} S_{\alpha} U_{\alpha} + \left(1 - \phi \right) U_{s} \right) + \nabla \bullet \sum_{\alpha=w,o,g} \rho_{\alpha} \underline{u}_{\alpha} H_{\alpha} - \nabla \bullet \underline{q} = \sum_{\alpha=w,o,g} \rho_{\alpha} \phi S_{\alpha} h_{\alpha} - q_{L} \tag{7.14}$$

Here, we have applied Eq. (7.5) and written $\underline{q} \equiv \sum_{\alpha=w,o,g,s} \underline{q}^{\alpha}$ as well as $q_{L} \equiv \sum_{\alpha=w,o,g,s} q_{L}^{\alpha}$. They are referred to as *total heat flux* and *overall heat source term*, respectively.

A very important assumption that is made in the *non-isothermal compositional model* that we are presenting is that, at each point of the oil reservoir, the different phases reach thermal equilibrium instantly, which implies that all the phases have the same temperature, denoted by T, at each point. Then, the *total heat flux* is given by an overall Fourier Law:

$$\underline{q} = \underline{\underline{k}}_{T} \nabla T \, . \tag{7.15}$$

This leads to the following form, of Eq. (7.14):

$$\frac{\partial}{\partial t} \left(\phi \sum_{\alpha=w}^{g} \rho_{\alpha} S_{\alpha} U_{\alpha} + \left(1 - \phi \right) U_{s} \right) + \nabla \bullet \sum_{\alpha=w}^{g} \rho_{\alpha} \underline{u}_{\alpha} H_{\alpha} - \nabla \bullet \left(\underline{\underline{k}}_{T} \nabla T \right) = q_{c} - q_{L} \, . \tag{7.16}$$

Here, q_{c} is referred to as the overall *heat source term* and it is defined by

$$q_{c} \equiv \sum_{\alpha=w}^{g} \rho_{\alpha} \phi S_{\alpha} h_{\alpha} \, . \tag{7.17}$$

Conclusions

Mathematical and computational models of the processes that occur in enhanced oil recovery (EOR) technology are fundamental for the application and advancement of such methods. At least the following three stages can be distinguished in the development of EOR models: construction of a mathematical, a numerical and a computational model, respectively. In particular, the construction of the mathematical model is the starting point and base on which the remaining construction is built. Due to the great diversity of processes occurring in EOR, it is valuable to possess a general and systematic procedure for constructing their mathematical models, which can be used as a unified protocol when building the corresponding computational simulators. In this paper we have presented such a procedure, based on an axiomatic formulation of Continuous Mechanics (Allen *et al*., 1988), which is systematic, rigorous and easy to apply independently of the complexity of the system considered.

As it is here explained, mathematical models of EOR processes are constituted by a system of partial differential equations together with a system of conditions, the *jump conditions*, which model discontinuities must fulfill when and where they occur; albeit, in standard treatments the *jump conditions* are not usually discussed. When building the mathematical model of an EOR system, the following stages can be distinguished: firstly, a basic system of partial differential equations and *jump conditions* that only depend on the number of phases and components in each phase are established –given in Eq. (3.3)-; and secondly, the phenomenology is incorporated into it. In this paper, the system of partial differential equations and *jump conditions* derived in the first step is referred to as the '*basic mathematical model*'. This supplies a very sound and firm basis for a second step, which consists in incorporating other scientific and technological information that is required to complete the mathematical model; this latter purpose is achieved by means of certain number of *constitutive equations* such as Darcy's Law, chemical laws, results of field measurements and many more. Specific applications of the procedures here introduced have already been made in the development of EOR projects such as water-alternating-gas injection and air injection methods.

In standard approaches, the system of partial differential equations of the *basic mathematical model* is derived by means of balances that are carried out in cubes (or parallelepipeds) of the physical space, putting together the different phases of the system and the *jump conditions* are not usually discussed. In the protocol here proposed, on the other hand, such balances in cubes are not required since instead the starting point is the system of *partial differential equations* and *shock conditions* of Eq. (3.3). The procedure is systematic, rigorous and easy to apply independently of the complexity of the system considered. In Sections 4 to 6, we have shown that when this approach is used for constructing the basic mathematical models, such construction is to a large extent automatic; all what is required in order to define the partial differential equations and the jump conditions of the mathematical model is to identify the phases and species, as well the energy sources, that participate in the EOR system.

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