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Chapter 7

Shock modelling in petroleum engineering

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Abstract

A discussion of the situations in which petroleum reservoir models generate shocks, together with a general formulation of the jump conditions to be satisfied by them, is presented. In addition, a brief review of the procedures available for treating them is made and the front tracking method is explained with some detail. Then, an Eulerian-Lagrangian approach to the modeling of shocks, that was introduced by the authors in a previous paper, for treating the advance of a gas front into a region of occupied by undersaturated oil, is explained.

1 Introduction

This chapter stems from a previous paper,[1] in which a method for treating shocks occurring in variable bubble point problems of petroleum engineering was proposed. The procedure offers some novelty, in that it is an Eulerian-Lagrangian method for tracking the discontinuous fronts and in addition, it uses finite difference approximations which are applicable to discontinuous functions. In the present chapter, a more extensive discussion of the situations in which petroleum reservoir models generate shocks, including methods which are available for treating them, is presented.

For this purpose, one must distinguish between 'miscible' and 'immiscible' displacement. By immiscible displacement, it is usually understood[2] one in which

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1 Introduction

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For this purpose, one must distinguish between 'miscible' and 'immiscible' displacement. By immiscible displacement, it is usually understood[2] one in which

the different phases involved do not mix at all and there is no mass exchange between them. This is the case, for example, when water is injected through some wells, in secondary recovery.

On the other hand, if complete mixing or 'miscibility' is attained, so that only one phase is formed, the term 'miscible' displacement is most frequently applied. This is the case, for example, when CO_2 is injected to form a single fluid phase with the resident hydrocarbon.

Another situation that can occur is 'partial mixing', in which two or more phases can exchange mass but in which there is no complete mixing, so that each one of the different phases keeps its own identity. This is the case, for example, in reservoirs containing liquid oil and soluble gas, when the bubble point varies.

In actual reservoirs, diffusive processes are always present and discontinuities are smoothed out, so that shocks cannot occur. However, if the advection terms are dominant, very steep fronts may develop and the modeling of such continuous although rather sharp fronts, has been and still is, a very challenging problem of computational mechanics.

Many methods have been presented in the literature for representing such fronts accurately. A class of such methods, which has been specially successful, is based on the method of characteristics.[37] However, the shortcomings that such methods had, were the lack of mass conservation property and that they did not treat the boundary conditions properly. A generalization of such methods that has been developed recently,[8–10] overcomes these problems and is being implemented further (see for example Refs 11-15). Such generalization was obtained combining the modified method of characteristics (an Eulerian-Lagrangian approach) with the author's localized adjoint method[16–19] and it is known as ELLAM.

If the diffusive processes can be neglected, then shocks may occur. In the case of miscible displacement, the diffusive processes are associated with dispersion and it seems that in most cases of miscible displacement of practical interest, dispersion can not be left aside.[20] On the other hand, in reservoir models with several phases which are immiscible or only partially miscible, shocks can occur when capillary pressure is neglected.

The starting point for the understanding of shocks in immiscible displacement, was the classical Buckley-Leverett theory,[21–23] which was further enlighten by the work of Cardwell & Sheldon,[24,25] who explained clearly the way in which shocks are generated in such processes. A very important step forward was made, when the Buckley-Leverett theory was set in the framework of the general theory of 'hyperbolic conservation laws' (see, for example Ref. 26).

One of the most successful methods that have been proposed for modeling shocks in miscible displacement, is 'front tracking'. This was introduced by Richtmyer,[27] and was developed extensively by Glimm, McBryan *et al.* (see, for example Ref. 28). Many descriptions of the method at different states of development have been published (see, for example Ref. 29) and a very recent one has been presented by Bratvedt *et al.*[30]

On the other hand, shocks which occur when the phases are treated as partially miscible, as is the case when a gas front advances into a region occupied by undersaturated liquid oil, have not received as much attention.

Since the purpose of this Chapter is to discuss shocks, attention is restricted to phases which are miscible or partially miscible, and capillary pressure is neglected in all cases. The physical basis of the fundamental equations which govern the flow and transport of fluids in a reservoir, are the *balance equations of Continuum Mechanics.* Thus, the technical discussions, in Section 2, start by presenting the 'general jump conditions' which must be fulfilled in order to satisfy the balance equations. In Section 3, the classical Buckley-Leverett theory is revised and shock formation is explained in Section 4. The general framework of 'hyperbolic conservation laws' is introduced in Section 5, where the front tracking method for immiscible displacement, is discussed. The study of shocks in partially miscible displacement is begun in Section 6, where the jump conditions are applied and the velocity of a discontinuous front is derived. The Eulerian-Lagrangian method for modeling shocks that was introduced in Ref. 1, is presented in Section 7 and the finite difference formulas, which are an essential ingredient of this method, are explained in Section 8. Section 9 is devoted to present a numerical application to a variable bubble point problem.

2 Jump conditions

To give to our developments a firm physical and mathematical basis, we start by revising the balance equations of continuum mechanics. The synthesis of this theory that has been given in Refs 31 and 32, is very convenient for our purposes. In the case of multi-phase systems, each α phase moves with its own velocity $\mathbf{v}^\alpha$. Here, $\alpha = 1, ...N$, where N is the total number of components. In any phase there may be several components, but all components contained in the same phase move with the same velocity. The balance equations satisfied by any intensive property ψ^α associated with component α, are:

$$\psi_t^\alpha + \nabla \cdot (\psi^\alpha \mathbf{v}^\alpha) - \nabla \cdot \boldsymbol{\tau}^\alpha = g^\alpha \tag{1}$$

and

$$[\psi^\alpha(\mathbf{v}^\alpha - \mathbf{v}_\Sigma) - \boldsymbol{\tau}^\alpha] \cdot \mathbf{n} = g_\Sigma^\alpha \tag{2}$$

Here, the vector $\boldsymbol{\tau}^\alpha$ is the **flux** of ψ^α across surfaces in space, while the quantities g^α and g_Σ^α represent **external supply** of ψ^α (Refs 31 and 32), per unit volume and unit time, in the case of g^α , while g_Σ^α represents **external supply** of ψ^α through the discontinuity, per unit area and unit time. In addition, $\mathbf{v}_\Sigma$ stands for the velocity with which the discontinuity moves. In all the applications that follow, the intensive properties are densities (mass per unit of total volume) of each one of the components of the systems to be considered.

Equation (1) is the 'general differential balance law', to be satisfied at every point of the space occupied by the continuous system. Equation (2) is the 'general jump condition', to be satisfied on surfaces of discontinuity. With respect to this latter

equation, it is assumed that there is a surface of discontinuity Σ (generally, space-time), which moves with velocity $\mathbf{v}_\Sigma$ and in which the physical variables may have jump discontinuities. In addition, the square brackets are defined as the 'jumps' accross the surface of discontinuity Σ. More precisely, for any function $[f] = f_+ - f_-$, where f_+ and f_- represent the limits of f as Σ is approached from the positive and negative sides, respectively. In what follows, unless otherwise stated, the positive side of Σ is chosen arbitrarily and then the unit normal vector $\mathbf{n}$, is chosen pointing towards the positive side of Σ. Finally, it must be mentioned that in the form presented here, eqn (2) is slightly more general than that of Refs 31 and 32, because the possibility of non-vanishing external supply through the discontinuity, has been included.

To illustrate the use of eqns (1) and (2), let us apply them to a black oil model. The black oil (or beta) model that will be considered is based on the following hypotheses:

a. There are three phases: water, liquid oil and gas;

b. Water and oil are immiscible, while gas is soluble only in liquid oil; i.e. the water and gas phases consist of only one component, while the liquid oil is made of two components (dissolved gas and nonvolatile oil). This implies that the total number of components are four and that $\mathbf{v}^\alpha$, in eqn (2), is the same for the latter two components.

c. No physical diffusion is present. This includes both, molecular diffusion and that induced by the randomness of the porous medium (dispersion).

With the mass of each one of the components there is associated one intensive property, which represents the mass per unit of total volume of that component. Thus, one can write:

$$\psi^{\mathrm{w}} = \phi S_{\mathrm{w}} \rho_{\mathrm{w}}, \quad \bar{\psi}^{\mathrm{o}} = \phi S_{\mathrm{o}} \bar{\rho}_{\mathrm{o}}, \quad \bar{\psi}^{\mathrm{dg}} = \phi S_{\mathrm{o}} \bar{\rho}_{\mathrm{dg}}, \quad \psi^{\mathrm{g}} = \phi S_{\mathrm{g}} \rho_{\mathrm{g}} \tag{3}$$

for the intensive properties associated with water, nonvolatile oil, dissolved gas and gas in the gas phase, respectively. The notations: $\bar{\rho}_{\mathrm{o}}$ and $\bar{\rho}_{\mathrm{o}}$ are used for the effective densities of nonvolatile oil and dissolved gas, respectively. Also, the **flux** τcorresponding to each one of these intensive properties vanishes identically, since no physical diffusion is assumed. Applying eqn (1) to each one of these intensive properties, one gets:

$$(\phi S_{\mathrm{w}} \rho_{\mathrm{w}})_t + \nabla \cdot (\phi \rho_{\mathrm{w}} S_{\mathrm{w}} \mathbf{v}^{\mathrm{w}}) = 0 \tag{4}$$

$$(\phi S_{\mathrm{o}} \bar{\rho}_{\mathrm{o}})_t + \nabla \cdot (\phi \bar{\rho}_{\mathrm{o}} S_{\mathrm{o}} \mathbf{v}^{\mathrm{o}}) = 0 \tag{5}$$

$$(\phi S_{\mathrm{o}} \bar{\rho}_{\mathrm{dg}})_t + \nabla \cdot (\phi \bar{\rho}_{\mathrm{dg}} S_{\mathrm{o}} \mathbf{v}^{\mathrm{o}}) = g^{\mathrm{o}}_{\mathrm{Ig}} \tag{6}$$

$$(\phi S_{\mathrm{g}} \rho_{\mathrm{g}})_t + \nabla \cdot (\phi \rho_{\mathrm{g}} S_{\mathrm{g}} \mathbf{v}^{\mathrm{g}}) = g^{\mathrm{g}}_{\mathrm{Io}} \tag{7}$$

where g°_{Ig} is the mass of gas that is dissolved in the liquid oil per unit volume per unit time, while $g^{\mathrm{g}}_{\mathrm{Io}}$ is the mass of dissolved oil that goes into the gas phase, per unit volume per unit time, and the extraction terms have been set to zero. Clearly

$$g^{\circ}_{\mathrm{Ig}} + g^{g}_{\mathrm{Io}} = 0 \tag{8}$$

for mass conservation. Thus, adding up eqns (5) and (6), one gets

$$\{\phi(S_{\mathrm{o}}\bar{\rho}_{\mathrm{dg}} + S_{\mathrm{g}}\rho_{\mathrm{g}})\}_t + \nabla \cdot \{\phi(\bar{\rho}_{\mathrm{dg}}S_{\mathrm{o}}\mathbf{v}^{\mathrm{o}} + \rho_{\mathrm{g}}S_{\mathrm{g}}\mathbf{v}^{\mathrm{g}})\} = 0 \tag{9}$$

Introducing the formation volume factors, Darcy's Law, as well as the relation

$$\bar{\rho}_{\mathrm{dg}} = \frac{\rho_{\mathrm{gSTC}}}{\rho_{\mathrm{oSTC}}} R_{\mathrm{s}}\bar{\rho}_{\mathrm{o}} \tag{10}$$

the system of eqns (4), (5) and (9), becomes the familiar system of equations of black oil models:

$$\nabla \cdot [\lambda_{\mathrm{w}}(\nabla p_{\mathrm{w}} - \gamma_{\mathrm{w}}\nabla z)] = \frac{\partial}{\partial t}\left(\frac{\phi S_{\mathrm{w}}}{B_{\mathrm{w}}}\right) \tag{11}$$

$$\nabla \cdot [\lambda_{\mathrm{o}}(\nabla p_{\mathrm{o}} - \gamma_{\mathrm{o}}\nabla z)] = \frac{\partial}{\partial t}\left(\frac{\phi S_{\mathrm{o}}}{B_{\mathrm{o}}}\right) \tag{12}$$

$$\begin{aligned} \nabla \cdot & [R_{\mathrm{s}}\lambda_{\mathrm{o}}(\nabla p_{\mathrm{o}} - \gamma_{\mathrm{o}}\nabla z) + \lambda_{\mathrm{g}}(\nabla p_{\mathrm{g}} - \gamma_{\mathrm{g}}\nabla z)] \\ &= \frac{\partial}{\partial t}\left[\phi\left(R_{\mathrm{s}}\frac{S_{\mathrm{o}}}{B_{\mathrm{o}}} + \frac{S_{\mathrm{g}}}{B_{\mathrm{g}}}\right)\right] \end{aligned} \tag{13}$$

In a similar fashion applying eqn (2), to each one of the four components, the following are obtained:

$$[\phi\rho_{\mathrm{w}}S_{\mathrm{w}}(\mathbf{v}^{\mathrm{w}} - \mathbf{v}_{\Sigma})] \cdot \mathbf{n} = 0 \tag{14}$$

$$[\phi\bar{\rho}_{\mathrm{o}}S_{\mathrm{o}}(\mathbf{v}^{\mathrm{o}} - \mathbf{v}_{\Sigma})] \cdot \mathbf{n} = 0 \tag{15}$$

$$[\phi\bar{\rho}_{\mathrm{dg}}S_{\mathrm{o}}(\mathbf{v}^{\mathrm{o}} - \mathbf{v}_{\Sigma})] \cdot \mathbf{n} = g^{\circ}_{\Sigma_{\mathrm{g}}} \tag{16}$$

$$[\phi\rho_{\mathrm{g}}S_{\mathrm{g}}(\mathbf{v}^{\mathrm{g}} - \mathbf{v}_{\Sigma})] \cdot \mathbf{n} = g^{\mathrm{g}}_{\Sigma_{\mathrm{o}}} \tag{17}$$

In addition, Darcy's Law requires:

$$[p_l] = 0 \; ; \quad l = \mathrm{w},\ \mathrm{o},\ \mathrm{g} \tag{18}$$

Above, the quantities $g^{\circ}_{\Sigma_{\mathrm{g}}}$ and $g^{\mathrm{g}}_{\Sigma_{\mathrm{o}}}$ stand for the exchange of mass between the gaseous phase and the component of dissolved gas which is contained in the liquid oil phase. Mass conservation requires that:

$$g^{\circ}_{\Sigma_{\mathrm{g}}} + g^{\mathrm{g}}_{\Sigma_{\mathrm{o}}} = 0 \tag{19}$$

Thus, adding up eqns (16) and (17), it is obtained:

$$[\phi\bar{\rho}_{dg}S_o\mathbf{v}^o + \phi\rho_g S_g\mathbf{v}^g]\cdot\mathbf{n} - [\phi\bar{\rho}_{dg}S_o + \phi\rho_g S_g]\mathbf{v}_\Sigma\cdot\mathbf{n} = 0 \tag{20}$$

Since the pressures of the different phases are continuous, so is the porosity ϕ and ρ_w. This allows cancelling these factors in eqns (14), (15) and (20). Then, they can be written as:

$$[S_w]\mathbf{v}_\Sigma\cdot\mathbf{n} \;-\; [S_w\mathbf{v}^w]\cdot\mathbf{n} = 0 \tag{21}$$

$$[S_o/B_o]\mathbf{v}_\Sigma\cdot\mathbf{n} \;-\; [(S_o/B_o)\mathbf{v}^o]\cdot\mathbf{n} = 0 \tag{22}$$

$$[R_sS_o/B_o + S_g/B_g]\mathbf{v}_\Sigma\cdot\mathbf{n} - [(R_sS_o/B_o]\mathbf{v}^o + (S_g/B_g)\mathbf{v}^g]\cdot\mathbf{n} = 0 \tag{23}$$

where the formation volume factors have been introduced. Equations (21),(22) and (23), together with (18), constitute the desired system of jump conditions for the threephase (four component) oil reservoir. They relate the jumps of the physical variables with the velocity $\mathbf{v}_\Sigma$ of the advancing front. Observe that, in general, the jumps of the volume factor B_o and of R_s may be non-zero since they are functions of the bubble point, in addition to pressure.

3 Immiscible displacement: Buckley-Leverett theory

In this Section our discussion will be restricted to the case when only two phases are present and each one of them is made of one component: nonvolatile oil and the displacing fluid. No mass exchange between these phases is assumed and capillary pressure is neglected.

The Darcy velocities are defined by:

$$\mathbf{u}_\alpha = \phi S_\alpha\mathbf{v}^\alpha\,; \quad \alpha = o \text{ and } D \text{ (displacing fluid)} \tag{24}$$

Using them, eqns (4) and (5) can be written as:

$$(\phi S_D\rho_D)_t \;+\; \nabla\cdot(\rho_D\mathbf{u}_D) = 0 \tag{25}$$

$$(\phi S_o\rho_o)_t \;+\; \nabla\cdot(\rho_o\mathbf{u}_o) = 0 \tag{26}$$

The 'total Darcy velocity' is defined by

$$\mathbf{u}_T = \mathbf{u}_D + \mathbf{u}_o = \phi\{S_D\mathbf{v}^D + S_o\mathbf{v}^o\} \tag{27}$$

When capillary pressure and gravity forces are neglected, Darcy velocities are given by

$$\mathbf{u}_l = -\frac{\mathbf{k}k_{rl}}{\mu_l}\nabla p, \quad l = \mathrm{o},\mathrm{D} \tag{28}$$

and the total Darcy velocity, as well as the velocity of the displacing fluid, are colinear. Thus,

$$\mathbf{u}_D = f_D\mathbf{u}_T \tag{29}$$

where f_D is a proportionality factor. In view of this equation, one can replace $\mathbf{u}_D$ by $f_D\mathbf{u}_T$, in eqn (25), to obtain

$$(\phi S_D \rho_D)_t + \nabla \cdot (\rho_D f_D \mathbf{u}_T) = 0 \tag{30}$$

When the fluids are incompressible, the density of the displacing fluid can be cancelled out, in this equation. If in addition, the solid matrix is also incompressible, such equation reduces to

$$(S_D)_t + \phi^{-1} \nabla \cdot (f_D \mathbf{u}_T) = 0 \tag{31}$$

Equations (18) to (20), together imply

$$f_D(S_D) = \frac{1}{1 + \frac{k_{ro}\mu_D}{k_{rD}\mu_o}} \tag{32}$$

When the liquid phases and the solid matrix are incompressible, eqns (17) and (18) together imply that $\nabla \cdot \mathbf{u}_T = 0$. Hence, eqn (31), can be written as

$$(S_D)_t + \phi^{-1} f'_D \mathbf{u}_T \cdot \nabla S_D = 0 \tag{33}$$

because f_D is function of S_D, only. Here, f'_D stands for the derivative of f_D with respect to S_D. This equation is a first order differential equation for S_D and when complemented with suitable boundary conditions, it can be solved uniquely for S_D. Such equation states that the rate of advance of a point that has a certain fixed saturation, equals the total Darcy velocity $\mathbf{u}_T$, multiplied by the factor $\phi^{-1} f'_D$. Here, no gravity segregation has been taken into account, but it is not difficult to incorporate it (see, for example Ref 29).

Buckley & Leverett,[21,22] were the first to derive the one-dimensional version of eqn (33). For such a case, one has

$$(S_D)_t + \phi^{-1} f'_D \mathbf{u}_T \partial S_D / \partial x = 0 \tag{34}$$

Writing q_T for the total rate of flow through a section, the total Darcy velocity can be expressed as $\mathbf{u}_T = q_T/A$, where A is the cross-sectional area, and eqn (34) becomes:

$$(S_D)_t + (q_T/A\phi) f'_D \partial S_D / \partial x = 0 \tag{35}$$

This is the classical Buckley-Leverett equation. If f'_D is nonconstant, the space-time curves in which S_D remains constant will intersect, in general, leading to multi-valued solutions which are nonphysical. The problem is similar to that occurring in the study of compressible fluids, either supersonic flow or the piston problem, and is solved introducing discontinuous solutions or shocks. The same is done in multidimensional problems.

Using eqn (24) and the incompressibility of the liquid phases, the jump conditions (14) and (15), can be written as:

$$[\mathbf{u}_D] \;=\; \phi [S_D] \mathbf{v}_\Sigma \tag{36}$$

$$[\mathbf{u}_o] = \phi[S_o]\mathbf{v}_\Sigma \tag{37}$$

Adding up these two equations, it is seen that

$$[\mathbf{u}_T] = 0 \tag{38}$$

i.e. the total Darcy velocity $\mathbf{v}_T$, is continuous. Making use of this result and of eqns (29) and (27), it is seen that

$$[\mathbf{u}_D] = [f_D]\mathbf{u}_T = \phi[f_D]\{S_D\mathbf{v}^D + S_o\mathbf{v}^o\} \tag{39}$$

which when combined with (36), yields

$$\mathbf{v}_\Sigma = \frac{[f_D]}{[S_D]}\{S_D\mathbf{v}^D + S_o\mathbf{v}^o\} = \phi^{-1}\frac{[f_D]}{[S_D]}\mathbf{u}_T \tag{40}$$

This relation was first derived by Sheldon & Cardwell,[25] for one-dimensional problems. As has been presented here, it applies to problems in several dimensions, as well.

4 Shock formation in immiscible displacement

According to the discussion presented in Section 3, for immiscible displacement, in the absence of capillary forces, the points in which the saturations remain constant move with velocity $\phi^{-1}f'_D\mathbf{u}_T$. Let $x_c(S_D, t)$, be the position at time t, of a point at which the saturation is S_D . Then, such point satisfies the differential equation

$$\frac{\partial x_c}{\partial t}(S_D, t) = \phi^{-1}f'_D(S_D)\mathbf{u}_T \tag{41}$$

The solutions of eqn (41), define straight lines in the space-time plane, since the slope is constant in each one of them.

Assume, $x_I(S_D)$ is the initial position, at time equal to zero, of a point in which the saturation of the displacing fluid is S_D . Then:

$$x_c(S_D, t) = x_I(S_D) + t\phi^{-1}_{f'_D}(S_D)\mathbf{u}_T \tag{42}$$

and the solution of the partial differential equation (34), will be single valued, unless the equation

$$\frac{\partial x_c}{\partial x}(S_D, t) = x'_I(S_D) + t\phi^{-1}f''_D(S_D)\mathbf{u}_T = 0 \tag{43}$$

is satisfied for some S_D . Clearing for t, one gets:

$$t = -\frac{\phi x'_I(S_D)}{f''_D(S_D)\mathbf{u}_T} = -\frac{\phi}{S'_{DI}f''_D(S_D)\mathbf{u}_T} \tag{44}$$

where $S_{DI}(x)$ is the initial distribution of S_D and a prime is used to denote the derivative of such function. A shock has to be introduced at the minimal time (t_{sh}) which satisfies (44). Under the assumption that the velocity $\mathbf{u}_T$ is positive, a t satisfying

end (44) would be positive, only if $S'_{DI} f''_D(S_D) < 0$. If this latter condition is fulfilled, t_{sh} is obtained when $|S'_{DI} f''_D(S_D)|$ is maximum, in eqn (44).

On the other hand, let $x_\Sigma(t)$ be the position of the shock at time t. According to eqn (40), one has

$$\frac{dx_\Sigma}{dt} = \phi^{-1} \frac{[f_D]}{[S_D]} \mathbf{u}_T \tag{45}$$

In general, the saturation S_D at the shock varies with time. A necessary condition for remaining constant, is that the shock moves with the velocity of a point which keeps fixed the value of S_D ; i.e.

$$\mathbf{v}_\Sigma = \frac{\partial x_c}{\partial t}(S_D, t) = \phi^{-1} f'_D(S_D) \mathbf{u}_T \tag{46}$$

In view of eqn (40), this condition is

$$f'_D(S_D) = \frac{[f_D]}{[S_D]} \tag{47}$$

Equation (47) can be fulfilled during a finite period of time, only if the shock advances into a region of constant S_D . A special case of this situation is when $S_D \equiv 0$ ahead of the shock ($S_{D+} = 0$). For this case:

$$f'_D(S_D) = \frac{f_D}{S_D} \tag{48}$$

since $f_D(0) = 0$. A point satisfying eqn (48), can be obtained drawing a tangent to the curve $f_D(S_D)$ from the origin. This is the graphical construction first suggested by Buckley & Leverett.[22] Such construction is the basis of the simplified method for computing oil recovery, due to Welge.[23]

In the more general situation in which S is a constant different from zero, ahead of the shock ($S_{D+} \neq 0$), the relation (47) in its more general form, must be fulfilled. It can be written more explicitly, as:

$$f'_D(S_D) = \frac{f_D(S_{D+}) - f_D(S_{D-})}{S_{D+} - S_{D-}} \tag{49}$$

A point S_{D+} satisfying such condition can be obtained drawing a tangent to the curve $f_D(S_D)$ from the point (S_{D-}, $f_D(S_{D-})$).

5 The Front Tracking Method

This Section is devoted to present the Front Tracking Method, which is well suited for treating shocks in immiscible displacement (see, for example Ref. 30). In general, such procedure is applicable to problems for which the basic equations can be written as a hyperbolic conservation law or a system of such laws. In several dimensions, a single conservation law is:

$$u_t + \nabla \cdot \mathbf{f}(u) = 0 \tag{50}$$

Comparing eqns (50) and (1), it is seen that a hyperbolic conservation law, can be interpreted as a balance equation for the 'intensive property u', defined in a macroscopic system in which the 'particles' move with velocity

$$\mathbf{v}(\mathbf{x},t) = \frac{\mathbf{f}(u)}{u} \tag{51}$$

Observe that the source terms (g), as well as the fluxes through the boundaries (τ), vanish. The corresponding jump conditions (eqn (2)) across a surface of discontinuity are:

$$[\mathbf{f}(u) - u\mathbf{v}_\Sigma] \cdot \mathbf{n} = 0 \tag{52}$$

This latter equation yields

$$\mathbf{v}_\Sigma \cdot \mathbf{n} = \frac{[\mathbf{f}(u)]}{[u]} \cdot \mathbf{n} = \frac{\mathbf{f}_+(u) - \mathbf{f}_-(u)}{u_+ - u_-} \tag{53}$$

This relation is usually referred to, as the Rankine-Hugoniot condition.

Equation (50) can be expanded to obtain

$$u_t + \mathbf{f}'(u) \cdot \nabla u = 0 \tag{54}$$

which states that any given value $\bar{u}$ of u, remains constant on a straight (characteristic) line, on which the position vector $\mathbf{x}(\bar{u},t)$ satisfies the condition

$$\frac{\partial \mathbf{x}}{\partial t}(\bar{u},t) = \mathbf{f}'(\bar{u}) \tag{55}$$

As in Section 4, when there is crossing of characteristics, a multi-valued solution will be obtained, which is non-physical and shocks, fulfilling the Rankine-Hugoniot condition (53), have to be introduced.

In one dimension, a single nonlinear conservation law reduces to

$$u_t + \frac{\partial}{\partial x} f(u(x,t)) = 0 \tag{56}$$

where f is a continuous and piecewise smooth, scalar function. A fundamental ingredient of the front tracking method, is the solution of the Riemann problem with initial data:

$$u(x,0) = \begin{cases} u_\mathrm{l}, & \text{for } x < 0 \\ u_\mathrm{r}, & \text{for } x > 0 \end{cases} \tag{57}$$

where it will be assumed that $u_\mathrm{l} < u_\mathrm{r}$. In general, the solution of this problem may be quite complex, but the complexity of the solution is determined by the number of inflection points that the graph of the function $f(u)$ has. Thus, it is easier to understand the general situation, analyzing first a case when $f(u)$ has only one inflection point, as in Fig. 1. In this case

$$f(u) = (u-1)^3 + 1 \tag{58}$$

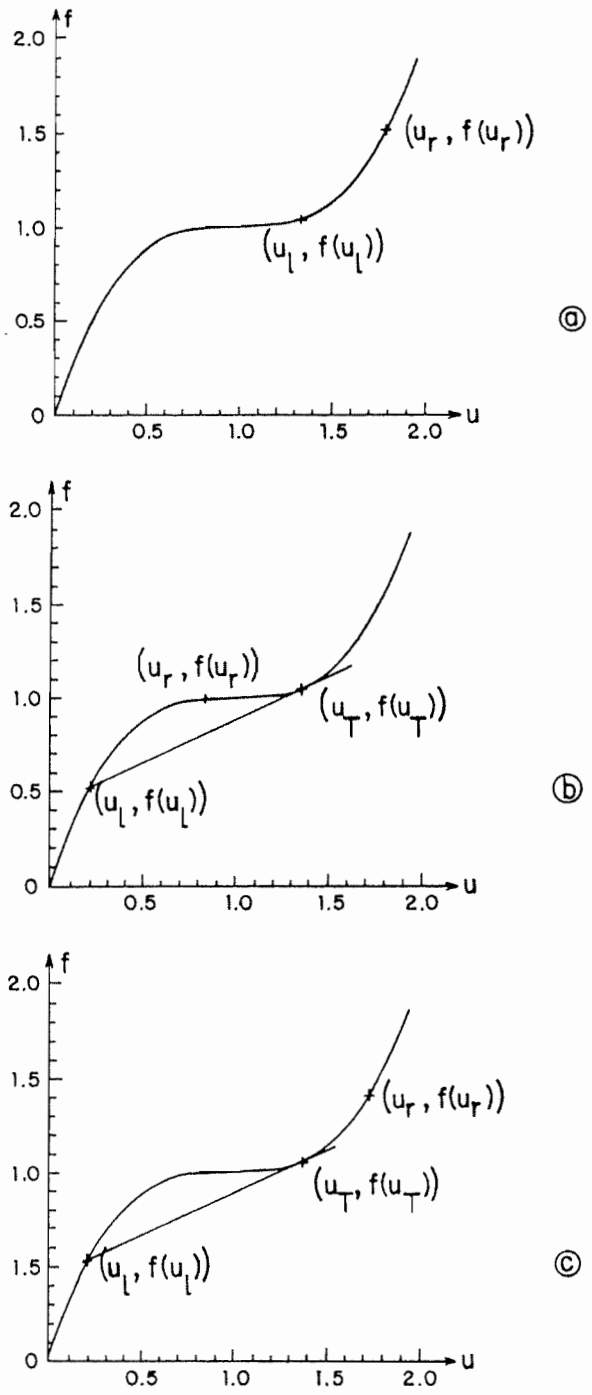


Figure 1: The Riemann problem. a) $u_l \geq 1$; b) $u_r \leq u_T$; c) $u_r > u_T$.

so that

$$f'(u) = 3(u-1)^2 \text{ and } f''(u) = 6(u-1) \tag{59}$$

and the only inflection point occurs at $u = 1$. If $u_l \geq 1$ (Fig. 1a), then the graph of $f(u)$ between u_l and u_r is convex and the solution of the Riemann problem is made of two space-time regions in which u is constant, connected by a rarefraction wave without a shock. Assuming $u_l < 1$, define u_T as the value u at the point of contact of a tangent drawn from $(u_l, f(u_l))$ to the graph of $f(u)$, as illustrated in Fig. 1b. Then, one of the following possibilities takes place:

A. $u_r \leq u_T$ In this case, the two space-time regions in which u is constant, are joined by a straight shock, whose constant speed of propagation is determined by the Rankine-Hugoniot condition.

B. $u_r > u_T$ In this case, the space-time region in which $u \equiv u_l$, is limited by a shock whose speed of propagation, as given by the Rankine-Hugoniot condition, is $f'(u_T)$. Between this shock and the space-time region in which $u \equiv u_r$, there is a rarefaction wave which joins smoothly with this latter region.

The more general situation in which there may be an arbitrary number of inflection points between u_l and u_r , is a combination of the case described above and can be treated in a very systematic manner introducing the concept of **lower convex envelop**,[30] to be denoted by f_c . This is defined with respect to the interval $[u_l, u_r]$, in which a partition: $u_l = u_0 < u_1 < ... < u_N = u_r$, is introduced, with the property that either $f_c(u) = f(u)$ or $f_c(u) < f(u)$ holds, in each one of the subintervals. If $f_c(u) = f(u)$, the solution is a rarefraction wave, and the solution satisfies $u(x,t) = (f_c)^{-1}(\xi)$ there, where $\xi = x/t$. On the other hand, at a subinterval at which $f_c(u) < f(u)$ there is a shock, whose speed is $\{f_c(u_{i+1}) - f_c(u_i)\}/(u_{i+1} - u_i)$, by virtue of the Rankine-Hugoniot relation. The value of the solution is u_i and u_{i+1}, at the left and right of the shock, respectively.

The actual implementation of the above solution may be difficult and simplifications have been introduced to improve its efficiency.[33,34] Thus, the original function f may be approximated by piecewise linear functions and its convex envelop is also piecewise linear. Furthermore, the rarefraction waves are also replaced by shocks moving with the speeds predicted by the Rankine-Hugoniot condition. In this manner, the Riemann problem solution consists of constant states exclusively, separated by shocks.

To apply the method to problems occurring in practice, the solution $u(x, t_n)$, at time t_n , is represented by piecewise constant functions on a grid whose spacing satisfies a Courant- Friedrichs-Lewy condition. This avoids interactions between the solutions of the collection of Riemann problems generated in this manner and allows the construction of the overall solution as a superposition of them. The front tracking method is not limited to one-dimensional problems, although its extension to several dimensions is not straight forward. The general two-dimensional Riemann problem solution is quite complicated and apparently the most successful approach has been operator splitting.[29,30]

6 The shock velocity in partially miscible displacement

In this Section, a front of gas advancing into a non-saturated liquid oil, is considered. In the developments, a formula for the 'jump of a product' that has been used in previous work by the author,[16–19] will be applied. It is:

$$[rs] = \dot{r}[s] + \dot{s}[r] \tag{60}$$

where the dot stands for the 'average' across the surface of discontinuity. More precisely, for any function 'r', one has

$$\dot{r} = (r_+ + r_-)/2 \tag{61}$$

To treat the case of a front of gas advancing into a non-saturated liquid oil, the unit normal $\mathbf{n}$ to the gas front Σ, will be taken with its sense opposite to $\mathbf{v}^g$(i.e. $\mathbf{v}^g \cdot \mathbf{n} \leq 0$), so that the positive side of Σ is that in which the advancing gas is located. For simplicity, the residual saturation of the gas will be neglected, so that $S_{g-} = 0$ and the only properties of the gas phase which are relevant, are those defined on the positive side of Σ. Due to this fact, it is convenient to drop the 'plus' sign as a subindex, when it refers to a property of the gas phase. Thus, for example, we write B_g instead of B_{g+}. Using this convention, we define the parameters η, ζ and ω, by means of the relations:

$$\mathbf{v}_\Sigma \cdot \mathbf{n} = \eta \mathbf{v}^g \cdot \mathbf{n} \quad \mathbf{v}^o \cdot \mathbf{n} = \zeta \mathbf{v}^g \cdot \mathbf{n} \tag{62}$$

and

$$\omega = \frac{S_o B_g}{B_o S_g} \tag{63}$$

Then, eqs (21) and (23), can be written as:

$$[\omega(\zeta - \eta)] = 0 \tag{64}$$

$$[R_s \omega(\zeta - \eta)] + 1 - \eta = 0 \tag{65}$$

Using formula (60), eqn (64) can be transformed into:

$$\dot{\zeta}[\omega] + \dot{\omega}[\zeta] = \eta[\omega] \tag{66}$$

from which it follows that

$$\dot{\zeta} = \eta - \dot{\omega}\frac{[\zeta]}{[\omega]} \tag{67}$$

On the other hand, eqn (64), when use is made of the identity (60) and after simplifying by means of eqn (64), can be written as:

$$[R_s]\dot{\overline{\omega(\zeta - \eta)}} + 1 - \eta = 0 \tag{68}$$

Here, as in what follows, use is made of a bar to indicate that the average refers to the whole expression covered by it. From (68), it follows that

$$[R_s](\dot{\overline{\omega\zeta}} - \dot{\omega}\eta)] + 1 - \eta = 0 \tag{69}$$

which can be further simplified by means of an algebraic identity closely related with (60); this is: $\dot{\overline{\omega\zeta}} = [\omega][\zeta]/4 + \dot{\omega}\dot{\zeta}$. Applying this identity and combining the resulting equation with eqn (67), one gets:

$$\eta = 1 - [R_s]\frac{[\zeta]}{[\omega]}\omega_+\omega_- \tag{70}$$

Equations (62), (67) and (70), determine the velocity of the advancing front, but as they stand, they look criptic. However, they become more transparent when they are written in terms of a 'retardation factor ε', which exhibits how the relative velocities (with respect to the velocity of the oil) of the advancing front Σ and of the gas, are related. Thus, define the 'retardation factor ε' by means of the equation:

$$(\mathbf{v}_\Sigma - \mathbf{v}^o{}_+) \cdot \mathbf{n} = \varepsilon(\mathbf{v}^g - \mathbf{v}^o{}_+) \cdot \mathbf{n} \tag{71}$$

Using eqn (62), it can be seen that

$$\varepsilon = \frac{\eta - \zeta_+}{1 - \zeta_+} \tag{72}$$

When the auxiliary relations:

$$\eta - \zeta_+ = \frac{[\zeta]}{[\omega]}\omega_-; \quad 1 - \zeta_+ = \{1 + [R_s]\omega_+\}\frac{[\zeta]}{[\omega]}\omega_- \tag{73}$$

which are implied by eqns (67) and (70), after some algebraic manipulations, are used in eqn (72), the expression:

$$\varepsilon = \frac{1}{1 + [R_s]\omega_+} = \frac{1}{1 + [R_s]\frac{B_g S_{o+}}{S_g B_{o+}}} \tag{74}$$

for the retardation factor 'ε', is obtained. Equation (74), together with (71) yields the velocity of the advancing gas front. Observe that $R_{s+} \geq R_{s-}$, so that $0 < \varepsilon \leq 1$.

7 Eulerian-Lagrangian modeling of shocks

Equations (71) and (74) are informative and permit acquiring insight into the manner in which the advance of the gas front takes place. However, for numerical applications it was better to start from eqns (21)-(23) and transform them in the manner explained in Ref. 1.

For simplicity, in what follows only two phases will be considered: oil and gas. In addition, only a 1-D formulation will be presented, so that gravity effects will be left

out and as in Section 6, it will be assumed that the gas moves towards the left (i.e. $v_\Sigma < 0$). In this case the jump conditions can be transformed into (see Ref. 1, for details):

$$\dot{\lambda}_o \mathcal{S} + \left[\frac{\phi S_o}{B_o}\right] v_\Sigma + [\lambda_o]\,\mathcal{M} = 0 \tag{75}$$

$$(2\dot{\overline{R_s\lambda_o}} + \lambda_{g+})\mathcal{S} + 2\left[\phi\left(R_s\frac{S_o}{B_o} + \frac{S_g}{B_g}\right)\right] v_\Sigma + 2(\lambda_{g+} + [R_s\lambda_o])\mathcal{M} = 0 \tag{76}$$

Here the notations

$$\mathcal{S} = \left[\frac{\partial p_o}{\partial x}\right]; \quad \mathcal{M} = \dot{\overline{\frac{\partial p_o}{\partial x}}} \tag{77}$$

are understood and capilary pressure has been neglected. In Ref. 1, for the numerical treatment, eqns (75) and (76) were used as a system of equations for the unknowns $\mathcal{S}$, v_Σ and $\mathcal{M}$, all of them defined on the space-time surface of discontinuity $\Sigma(t)$. However, this system is not determined since it is 2 by 3. The additional equation that was needed, was obtained weighting the differential equations (12) and (13) in a suitable manner, as it is explained next.

The one-dimensional versions of eqns (12) and (13), are:

$$\frac{\partial}{\partial x}\left(\lambda_o\frac{\partial p_o}{\partial x}\right) - \frac{\partial}{\partial t}\left(\frac{\phi S_o}{B_o}\right) = 0 \tag{78}$$

$$\frac{\partial}{\partial x}\left(R_s\lambda_o\frac{\partial p_o}{\partial x} + \lambda_g\frac{\partial p_g}{\partial x}\right) - \frac{\partial}{\partial t}\left\{\phi\left(R_s\frac{S_o}{B_o} + \frac{S_g}{B_g}\right)\right\} = 0 \tag{79}$$

In this Section these equations will be weighted using convenient space-time weights, deriving in this manner equations suitable for discretization. The weights that will be chosen lead to what is essentially, a cells method.

It will be assumed that $Cu = -V_\Sigma \Delta t/\Delta x < 1$. The position of the gas front will be denoted by $x_\Sigma(t)$. The space interval will be divided into a finite number of equally spaced cells. Taking time t_n as starting time, a procedure for constructing the solution at time t_{n+1} will be developed. The index 'i' will be reserved to denote the cell containing the front at time t_{n+1} . Since $Cu < 1$ and $V_\Sigma < 0$, only two cases must be distinguished. Either, during the time interval (t_n, t_{n+1}) the gas front does not cross any inter-cell boundary (Case A); or it crosses one inter-cell boundary (Case B). Observe that in Case B the inter-cell boundary that is crossed is $x_{i+1/2}$.

Case A

A system of three space-time test functions, will be used in cell 'i' (i.e. $[x_{i-1/2}, x_{i+1/2}]$). It is:

$$w_1^o(x,t) \equiv 1 \tag{80}$$

$$w_2^o(x,t) = \begin{cases} 0, & x < x_\Sigma(t) \\ 1, & x > x_\Sigma(t) \end{cases} \tag{81}$$

for the oil and

$$w^g(x,t) = \begin{cases} 0, & x < x_\Sigma(t) \\ 1, & x > x_\Sigma(t) \end{cases} \tag{82}$$

for the gas. The resulting equations are:

$$\int_{t_n}^{t_{n+1}} \left(\lambda_o \frac{\partial p_o}{\partial x}\right)_{i+1/2} \mathrm{d}t + \int_{x_{i-1/2}}^{x_{i+1/2}} \left(\phi \frac{S_o}{B_o}\right)^n \mathrm{d}x = \int_{t_n}^{t_{n+1}} \left(\lambda_o \frac{\partial p_o}{\partial x}\right)_{i-1/2} \mathrm{d}t + \int_{x_{i-1/2}}^{x_{i+1/2}} \left(\phi \frac{S_o}{B_o}\right)^{n+1} \mathrm{d}x \tag{83}$$

$$\int_{t_n}^{t_{n+1}} \left(\lambda_o \frac{\partial p_o}{\partial x}\right)_{i+1/2} \mathrm{d}t + \int_{x_{\Sigma(t_n)}}^{x_{i+1/2}} \left(\phi \frac{S_o}{B_o}\right)^n \mathrm{d}x = \int_{t_n}^{t_{n+1}} \left(\lambda_o \frac{\partial p_o}{\partial x} + \phi \frac{S_o}{B_o} V_\Sigma\right)_{\Sigma(t)} \mathrm{d}t + \int_{x_{\Sigma(t_{n+1})}}^{x_{i+1/2}} \left(\phi \frac{S_o}{B_o}\right)^{n+1} \mathrm{d}x \tag{84}$$

$$\int_{t_n}^{t_{n+1}} \left\{R_s \lambda_o \frac{\partial p_o}{\partial x} + \lambda_g \frac{\partial p_g}{\partial x}\right\}_{i+1/2} \mathrm{d}t \int_{x_{\Sigma(t_n)}}^{x_{i+1/2}} \left\{\phi\left(R_s \frac{S_o}{B_o} + \frac{S_g}{B_g}\right)\right\}^n \mathrm{d}x = \int_{t_n}^{t_{n+1}} \left\{R_s \lambda_o \frac{\partial p_o}{\partial x} + \lambda_g \frac{\partial p_g}{\partial x} + \phi\left(R_s \frac{S_o}{B_o} + \frac{S_g}{B_g}\right) V_\Sigma\right\}_{\Sigma(t)} \mathrm{d}t + \int_{x_{\Sigma(t)^{n+1}}}^{x_{i+1/2}} \left\{\phi\left(R_s \frac{S_o}{B_o} + \frac{S_g}{B_g}\right)\right\}^{n+1} \mathrm{d}x \tag{85}$$

In these equations the usual notation for line integrals has been used. In particular $\mathrm{d}t = (1 + V_\Sigma^2)^{-1/2}\, \mathrm{d}\mathcal{S}$, where $\mathrm{d}\mathcal{S}$ is the length in space-time.

Equations (83)-(85) constitute a system of three equations for cell 'i', which must be coupled with the system of jump conditions (75) and (76) and the equations of the remaining cells (two for each cell, when a two-phase system is considered), to obtain a determined system. Assume, for the sake of definiteness, that we are solving for oil pressure and saturation of the gas. Cells, other than cell 'i', can be treated in a standard manner, solving for oil pressure and gas saturation at the center of the cells. However, cell 'i' must be treated in a special manner. We have available a system of five equations, constituted by eqns (75),(76) and (83)-(85). A possible choice (and this one was used in the present study) of the corresponding five unknowns is: the jump and average of the pressure gradient ($\mathcal{S}^{n+1}$ and $\mathcal{M}^{n+1}$, respectively), the velocity v_Σ^{n+1} of the gas front, the gas saturation at the gas front $S_{g\Sigma}^{n+1}$ (these four unknowns defined on $\Sigma(t)$) and the oil pressure p_{oi}^{n+1} at the center of cell 'i'. In this manner a determined system is achieved. A special feature of this procedure is that one does not solve for saturation at the center of cell 'i'.

Case B

The system of space-time weights to be used in cell 'i' (i.e. $[x_{i-1/2}, x_{i+1/2}]$), is:

$$w_1^o(x,t) \equiv 1 \tag{86}$$

for the oil and

$$w_1^g(x,t) = \begin{cases} 0, & x < x_\Sigma(t) \\ 1 & x > x_\Sigma(t) \end{cases} \tag{87}$$

for the gas. The system of space-time weights to be used in cell 'i+1' (i.e. $[x_{i+1/2}, x_{i+3/2}]$), is:

$$w_2^o(x,t) \equiv 1 \tag{88}$$

for the oil and

$$w_2^g(x,t) = \begin{cases} 0, & x < x_\Sigma(t) \\ 1 & x > x_\Sigma(t) \end{cases} \tag{89}$$

for the gas. In addition, a space-time weight with support in the union of cells 'i' and 'i+1', is applied to the oil equation. It is defined by

$$w_3^o(x,t) = \begin{cases} 0, & x < x_\Sigma(t) \\ 1 & x > x_\Sigma(t) \end{cases} \tag{90}$$

Corresponding to these five weighting functions, five equations are derived for the union of cells 'i' and 'i+1'. Putting them together with the jump conditions (eqns (75) and (76)) a system of seven equations is obtained. The corresponding seven unknowns selected for the applications in the present paper were: the jump and average of the pressure gradient at the gas front at time t_{n+1}, the velocity of the advancing front v_Σ, the values p_{oi}^{n+1} and p_{oi+1}^{n+1}, of the oil pressure at cells 'i' and 'i+1', respectively, and the saturations of the gas S_{gi+1}^{n+1} and $S_{g\Sigma}^{n+1}$ at the center of cell 'i+1' and at the gas front, respectively. Again, as in Case A, a special feature of the procedure is that one does not solve for the saturation at the center of cell 'i'.

8 Finite differences for discontinuous functions

For the construction of an Eulerian-Lagrangian approach to shock modeling it is essential to apply finite difference formulas to functions with jump discontinuities. Since the use of such formulas is non-standard, in this Section we present an example, to illustrate the procedure.

Consider an interval of the real line and a uniform partition in it, as shown in Fig.2, where a notation usual in applications of the cells method has been adopted. Thus, the 'nodes' will be the centers of the subintervals of the partition. The ith subinterval (cell) of the partition will be $[x_{i-1/2}, x_{i+1/2}]$, whose center is x_i, and it is limited by the interelement boundary points $x_{i-1/2}$ and $x_{i+1/2}$. In Fig. 2, we have illustrated three neighboring cells (cells 'i-1', 'i' and 'i+1'). Assume the first derivative of the oil pressure p_o , has a jump discontinuity at x_Σ and $x_{i-1/2} \leq x_\Sigma \leq x_{i+1/2}$, p_o itself being continuous. Our purpose is to construct a second order approximation to $\left(\frac{\partial p_o}{\partial x}\right)_{i-1/2}$. If $x_i \leq x_\Sigma$ one can apply the usual centered finite difference formula:

$$\left(\frac{\partial p_o}{\partial x}\right)_{i-1/2} = \frac{p_{oi} - p_{oi-1}}{h} + O(h^2) \tag{91}$$

However, when $x_\Sigma < x_i$, eqn (91) is not applicable and a modified formula, accounting for the discontinuity, is needed.

In what follows the notation

$$\left[\frac{\partial p_o}{\partial x}\right]_\Sigma = \mathcal{S} \quad ; \quad \left[\frac{\partial^2 p_o}{\partial x^2}\right]_\Sigma = \mathcal{R} \tag{92}$$

is adopted and an auxiliary function $\hat{p}_o$, defined by:

$$\hat{p}_o = \begin{cases} p_o - \frac{1}{2}\mathcal{S}(x - x_\Sigma) - \frac{1}{4}\mathcal{R}(x - x_\Sigma)^2, & if\ x_\Sigma \le x \\ p_o + \frac{1}{2}\mathcal{S}(x - x_\Sigma) + \frac{1}{4}\mathcal{R}(x - x_\Sigma)^2, & if\ x \le x_\Sigma \end{cases} \tag{93}$$

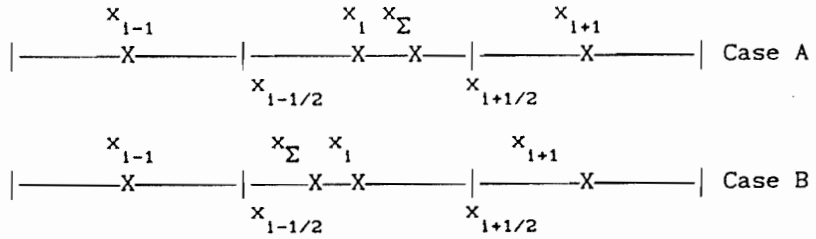


Figure 2.

This function is $\mathcal{C}^2$. Therefore, writing $\Delta x = h$, one has:

$$\begin{aligned} \left(\frac{\partial \bar{p}_o}{\partial x}\right)_{i-1/2} &= \frac{\hat{p}_{oi} - \hat{p}_{oi-1}}{h} + O(h^2) \\ &= \frac{p_{oi} - p_{oi-1}}{h} + \frac{\mathcal{S}}{2}(\xi + 1) - \frac{\mathcal{R}h}{8}\{\xi^2 + 2(\xi + 1)\} + O(h^2) \end{aligned} \tag{94}$$

with $\xi = (x_\Sigma - x_i)/(h/2)$. Here, the assumption that the partition is uniform, has been used. On the other hand

$$\left(\frac{\partial \hat{p}_o}{\partial x}\right)_{i-1/2} = \left(\frac{\partial p_o}{\partial x}\right)_{i-1/2} + \frac{\mathcal{S}}{2} - \frac{\mathcal{R}h}{4}(\xi + 1) + O(h^2) \tag{95}$$

Combining (94) and (95), it is obtained:

$$\left(\frac{\partial p_o}{\partial x}\right)_{i-1/2} = \frac{p_{oi} - p_{oi-1}}{h} + \frac{\mathcal{S}}{2}\xi - \frac{\mathcal{R}h}{8}\xi^2 + 0(h^2) \tag{96}$$

The jump '$\mathcal{R}$', of the second derivative is not known and in applications of formula (96) to partial differential equations, it is necessary to eliminate it. The second derivative of $\hat{p}_o$ will be computed in two alternative forms:

(a) - Firstly, the standard centered difference formula is applied to $\hat{p}_o$. For our purposes it is only necessary to consider the case when $x_\Sigma \leq x_i$. Using eqn (93) it is seen that

$$\hat{p}_{oi-1} = p_{oi-1} - \frac{h}{4}\mathcal{S}(\xi+2) + \frac{h^2}{16}\mathcal{R}(\xi+2)^2 \tag{97}$$

$$\hat{p}_{oi+1} = p_{oi+1} + \frac{h}{4}\mathcal{S}(\xi-2) - \frac{h^2}{16}\mathcal{R}(\xi-2)^2 \tag{98}$$

$$\hat{p}_{oi} = p_{oi} + \frac{h}{4}\mathcal{S}\xi - \frac{h^2}{16}\mathcal{R}\xi^2 \tag{99}$$

Therefore

$$\hat{p}_{oi-1} + \hat{p}_{oi+1} - 2\hat{p}_{oi} = p_{oi-1} + p_{oi+1} - 2p_{oi} - \frac{h}{2}\mathcal{S}(\xi+2) + \frac{h^2}{8}\mathcal{R}(\xi^2+4\xi) \tag{100}$$

and

$$\left(\frac{\partial^2 \hat{p}_o}{\partial x^2}\right)_i = \frac{p_{oi-1} + P_{oi+1} - 2p_{oi}}{h^2} - \frac{\mathcal{S}}{2h}(\xi+2) + \frac{\mathcal{R}}{8}(\xi^2+4\xi) + O(h^2) \tag{101}$$

(b) - Secondly, the first derivative of $\hat{p}_o$ *is differentiated.* Thus,

$$\left(\frac{\partial^2 \hat{p}_o}{\partial x^2}\right)_i = \frac{\left(\frac{\partial \hat{p}_o}{\partial x}\right)_{i+1/2} - \left(\frac{\partial \hat{p}_o}{\partial x}\right)_{\Sigma+}}{x_{i+1/2} - x_\Sigma} + O(h)$$

which can also be written as

$$\left(\frac{\partial^2 \hat{p}_o}{\partial x^2}\right)_i = \frac{\left(\frac{\partial \hat{p}_o}{\partial x}\right)_{i+1/2} - \left(\frac{\partial \hat{p}_o}{\partial x}\right)_{\Sigma+}}{h(1-\xi)/2} + O(h) \tag{102}$$

Taking the derivative of eqn (93)

$$\left(\frac{\partial \hat{p}_o}{\partial x}\right)_{\Sigma+} = \left(\frac{\partial p_o}{\partial x}\right)_{\Sigma+} - \frac{\mathcal{S}}{2} \tag{103}$$

and

$$\left(\frac{\partial \hat{p}_o}{\partial x}\right)_{i+1/2} = \left(\frac{\partial p_o}{\partial x}\right)_{i+1/2} - \frac{\mathcal{S}}{2} - \frac{\mathcal{R}}{2}(x_{i+1/2} - x_\Sigma)$$

This latter equation can be transformed into

$$\left(\frac{\partial \hat{p}_o}{\partial x}\right)_{i+1/2} = \frac{p_{oi} - p_{oi-1}}{h} - \frac{\mathcal{S}}{2} - \frac{\mathcal{R}h}{4}(1-\xi) \tag{104}$$

because

$$\left(\frac{\partial p_o}{\partial x}\right)_{i+1/2} = \frac{p_{oi+1} - p_{oi}}{h} + O(h^2)$$

Therefore

$$\left(\frac{\partial^2 \hat{p}_o}{\partial x^2}\right)_i = \frac{2}{h(1-\xi)}\left\{\frac{p_{oi+1}-p_{oi}}{h} - d_{o\Sigma+}\right\} - \frac{\mathcal{R}}{2} + O(h) \tag{105}$$

where the notation

$$d_{o\Sigma} = \left(\frac{\partial p_o}{\partial x}\right)_\Sigma \tag{106}$$

is understood. Using the relation $d_{o\Sigma+} = d_{o\Sigma} + \mathcal{S}/2$, combining eqns (101) and (105), and clearing for $\mathcal{R}$, one gets

$$\mathcal{R} = \frac{w^-}{h}\left\{\frac{(\xi+1)p_{oi+1} + (\xi-1)p_{oi-1} - 2\xi p_{oi}}{h} - 2\dot{d}_{o\Sigma} - \mathcal{S}\right\} + \frac{4\mathcal{S}}{h(\xi+2)} + O(h) \tag{107}$$

where $w^- = -8/(\xi+2)^2(\xi-1)$. This equation case is applied when $x_\Sigma \in [x_{i-1/2}, x_i]$. Similarly, when $x_\Sigma \in [x_i, x_{i+1/2}]$, one has

$$\mathcal{R} = \frac{w^+}{h}\left\{\frac{(\xi+1)p_{oi+1} + (\xi-1)p_{oi-1} - 2\xi p_{oi}}{h} - 2\dot{d}_{o\Sigma} + \mathcal{S}\right\} + \frac{4\mathcal{S}}{h(\xi-2)} + O(h) \tag{108}$$

where $w^+ = 8/(\xi-2)^2(\xi+1)$.

9 Numerical results

In this Section, some numerical results that were obtained[1] using the Eulerian-Lagrangian procedure for modelling shocks, together with a finite difference black oil simulator, neglecting capillary pressure, are presented.

A linear reservoir is considered, producing at a constant oil rate of 800 m /day at the left boundary, and a no flow boundary at the right end (L = 550 meters) . This reservoir is composed of two zones, a left undersaturated oil zone and a right saturated zone, where the oil and gas phases coexist. Initially, the pressure is the same for all positions, $S_g = 0.7$ in the saturated zone, and the front is located at x= 275 meters.

The PVT properties for the oil phase consist of constant viscosity and two values of B_o and R_s , one at the left side of the front and another at the right side, respectively. For the gas phase the PVT properties used, are typical in the oil industry. Straight line relationships are used for the relative permeabilities.

In order to check the validity of the simulator results, we have considered two cases: firstly, the undersaturated zone was taken as incompressible, and secondly, a non-zero value was given to the rock compressibility.

The analytical solution for the first case in the undersaturated zone dictates a constant pressure gradient. Figure 3, shows a comparison of pressure profiles at different times for this case. Two kinds of profiles are presented. The solid lines correspond to the solution obtained when the proposed formulation is included, and the dashed lines correspond to the traditional formulation in which jumps are not considered. As already mentioned, the pressure gradient is constant in the incompressible zone.

To correlate the transient (one phase) solution for a slightly compressible liquid

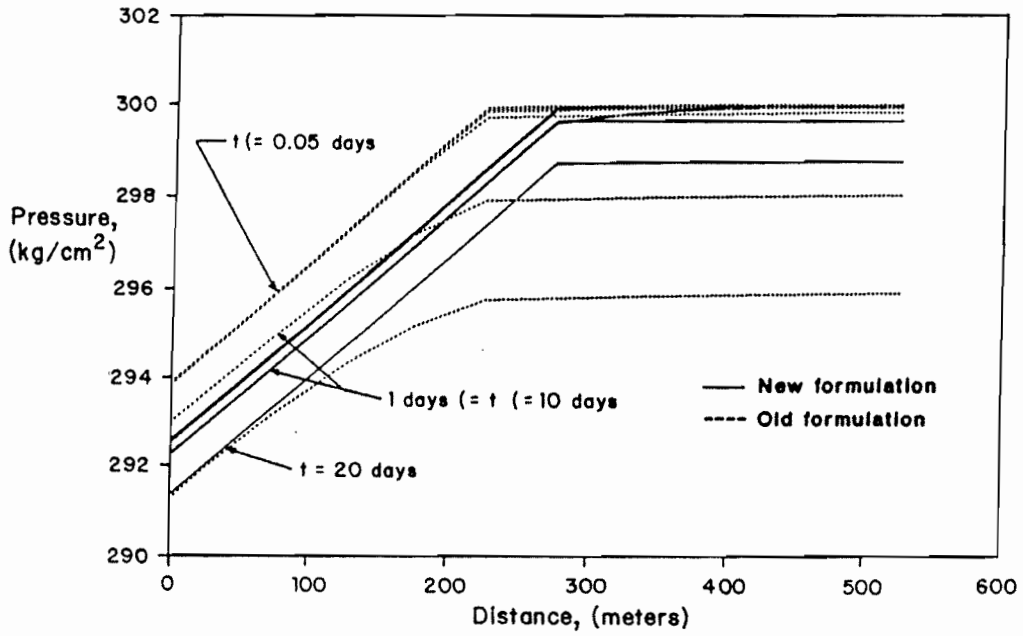
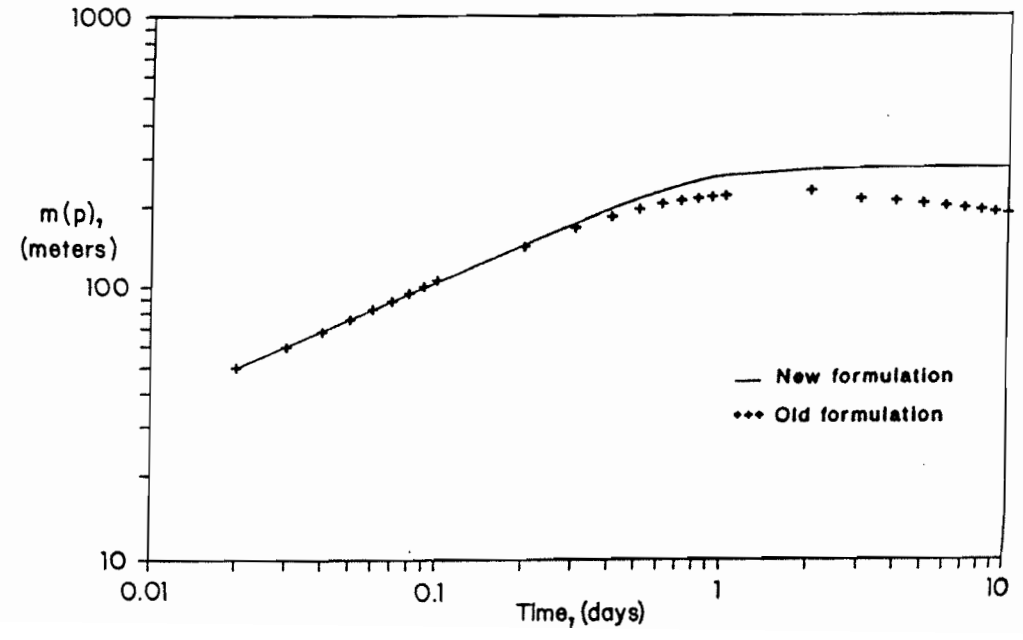


Figure 3: Comparison of pressure profiles for new and old formulation, incompressible case.



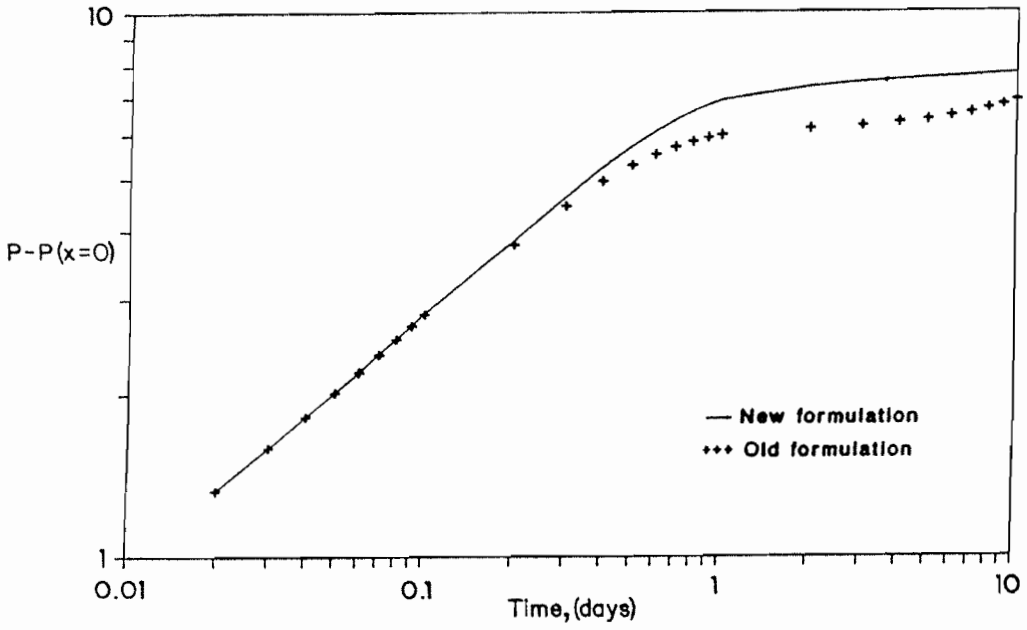


Figure 5: Comparison on pressure drop behavior for new and old formualations.

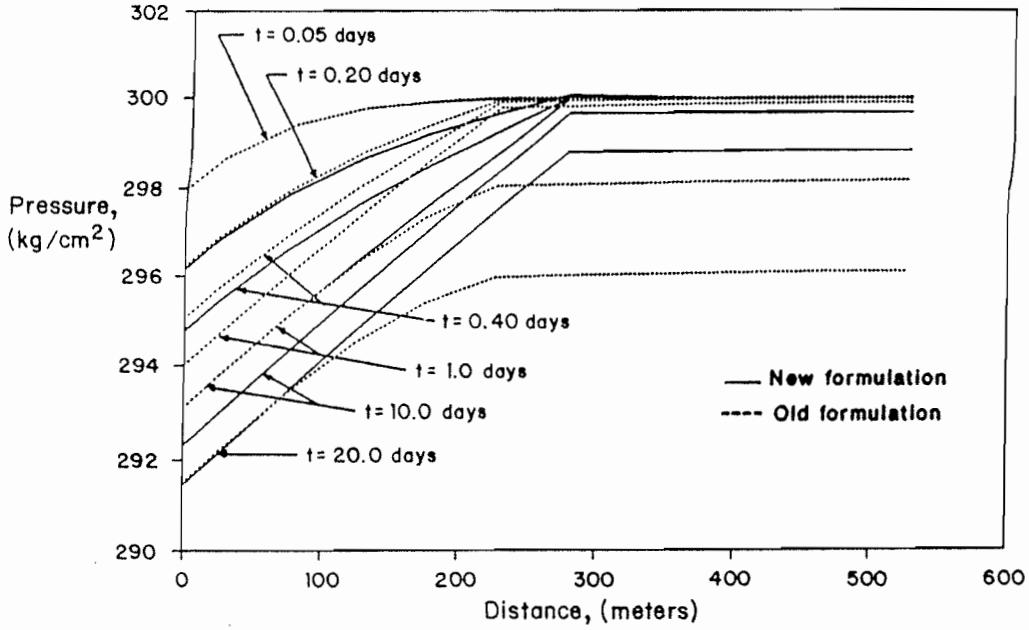


Figure 6: Comparison of pressure profiles for new and old formulations, compressible case.

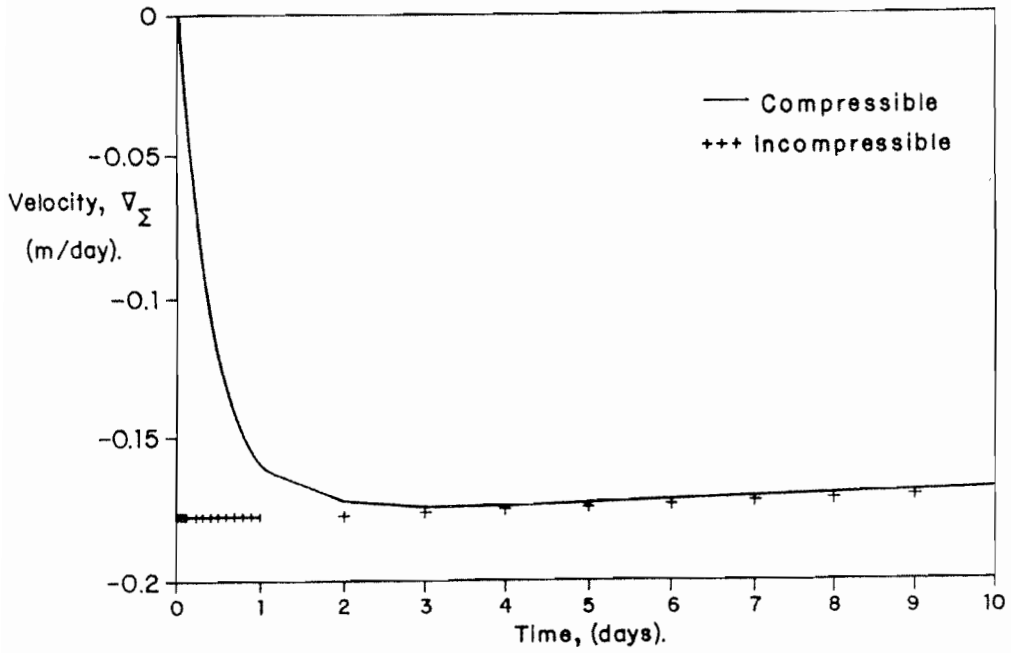


Figure 7: Velocity of the advancing front for the compressible and incompressible case.

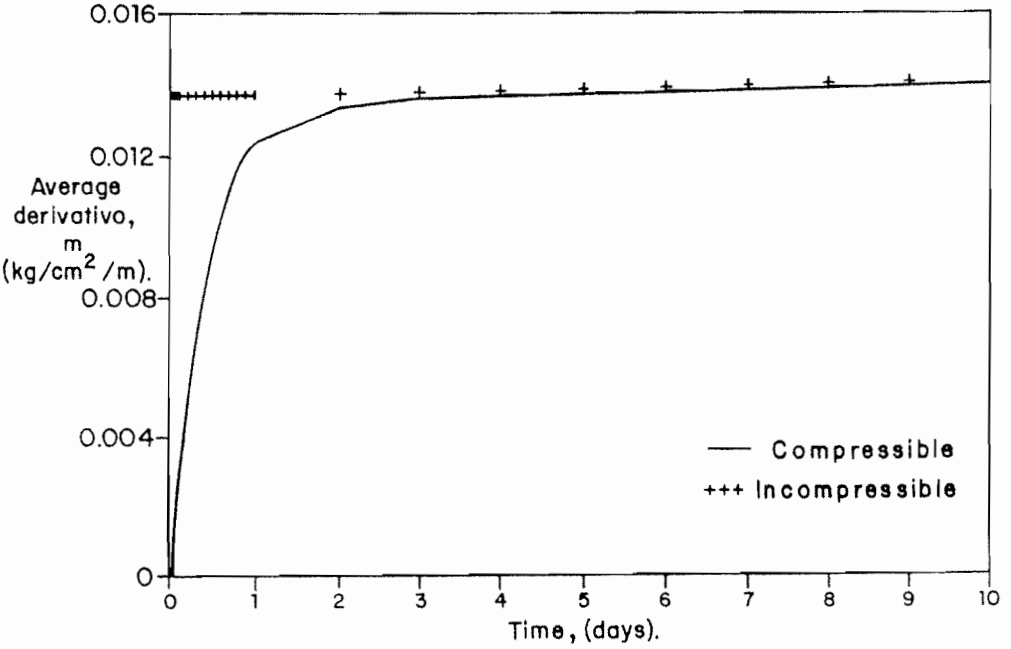


Figure 8: Average of the pressure gradient at the front for the compressible and incompressible cases.

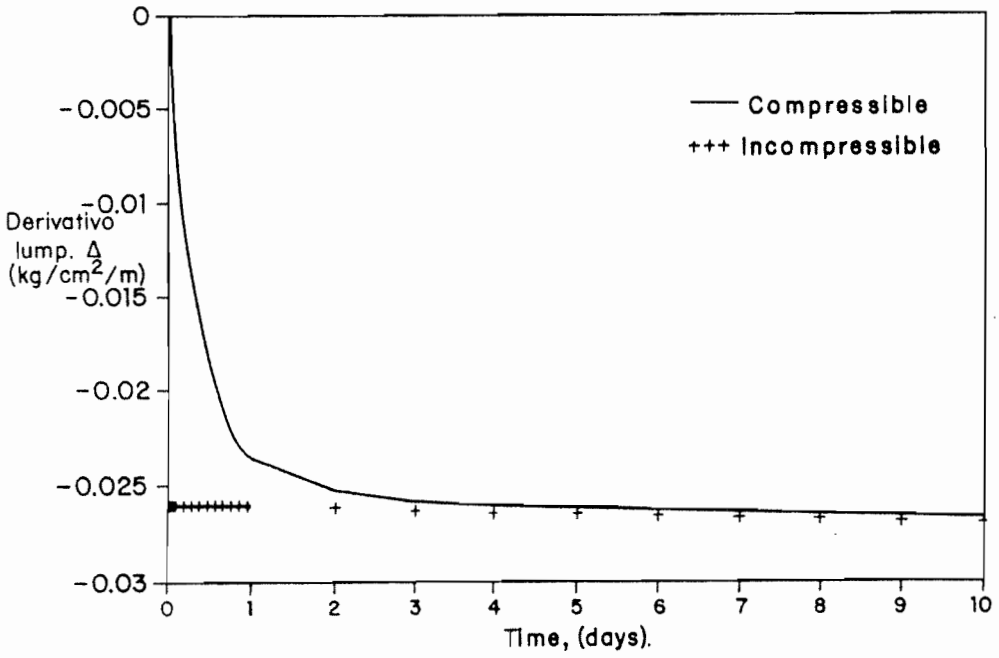


Figure 9: Jump in pressure gradient at the front for the compressible and incompressible cases.

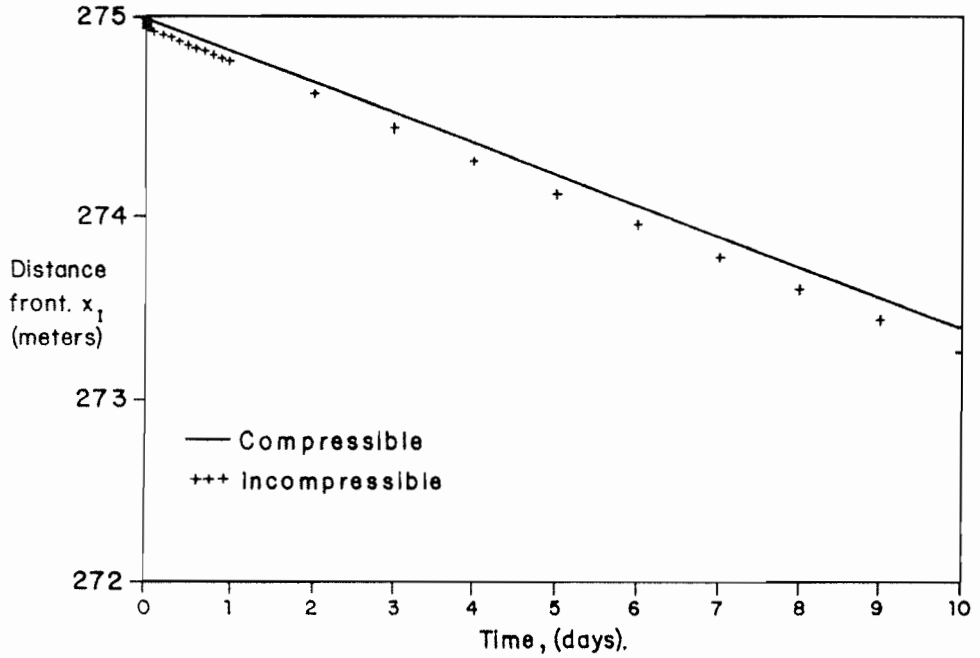


Figure 10: Position of the front for the compressible and incompressible cases.

with a multiphase flow solution, Raghavan & Camacho,[35–37] have proposed the use of a function of pressure and saturation, called pseudopressure, which is defined as follows:

$$m(p) = \frac{k\,h\,W}{q}\int_{x=0}^{x=L}\left[\frac{k_{ro}}{\mu_o\,B_o}\frac{\partial P}{\partial x}\right]\,\mathrm{d}x \tag{109}$$

For a linear system containing a slightly compressible liquid, Nabor & Barham[38] have shown that the pressure drop behaves linearly with time in a log-log plot, with a slope of one-half during the transient period. Once the outer boundary is manifested in the response, the solution deviates from a straight line moving up for a closed outer boundary and achieving a constant value, when a constant pressure in the outer boundary is prescribed. When, as in the traditional approach, the jumps are not considered in the formulation, the pseudopressure will deviate below the straight line for a closed outer boundary, after the transient period. To overcome this limitation, Camacho & Raghavan[36,37] suggested to include an additional integral in the right hand side of eqn (109). In this manner, variations in the average properties are taken into account.

For a constant pressure (constant saturation) outer boundary, eqn (109) yields a constant value, equal to the position of this boundary, after the transient period has ended. Figure 4 shows the behavior of the pseudopressure for the compressible case. The solid line corresponds to the solution obtained when the jumps are included, and the dots correspond to the traditional formulation. It can be observed the presence of a straight line with one-half slope during the transient period, for both formulations. Observe that when the jumps are considered in the formulation, the pseudopressure is equal to the position of the front, since this has a similar effect to an outer boundary of constant pressure. For the formulation without jumps, the pseudopressure falls below because of the reason explained before.

The behavior of pressure at $x = 0$ is shown in Fig. 5. In Fig. 6 it is presented a comparison of pressure profiles at different times. The results of Figs 5 and 6 correspond to those of Fig. 4. The solid lines represent the proposed formulation and the dots the traditional formulation.

Figures 7 to 10 show the behavior of v_Σ, m, $\mathcal{S}$, and, x_Σ versus time, respectively, for both compressible and incompressible inner zone cases. The solid lines represent the compressible case and the dots the incompressible one.

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