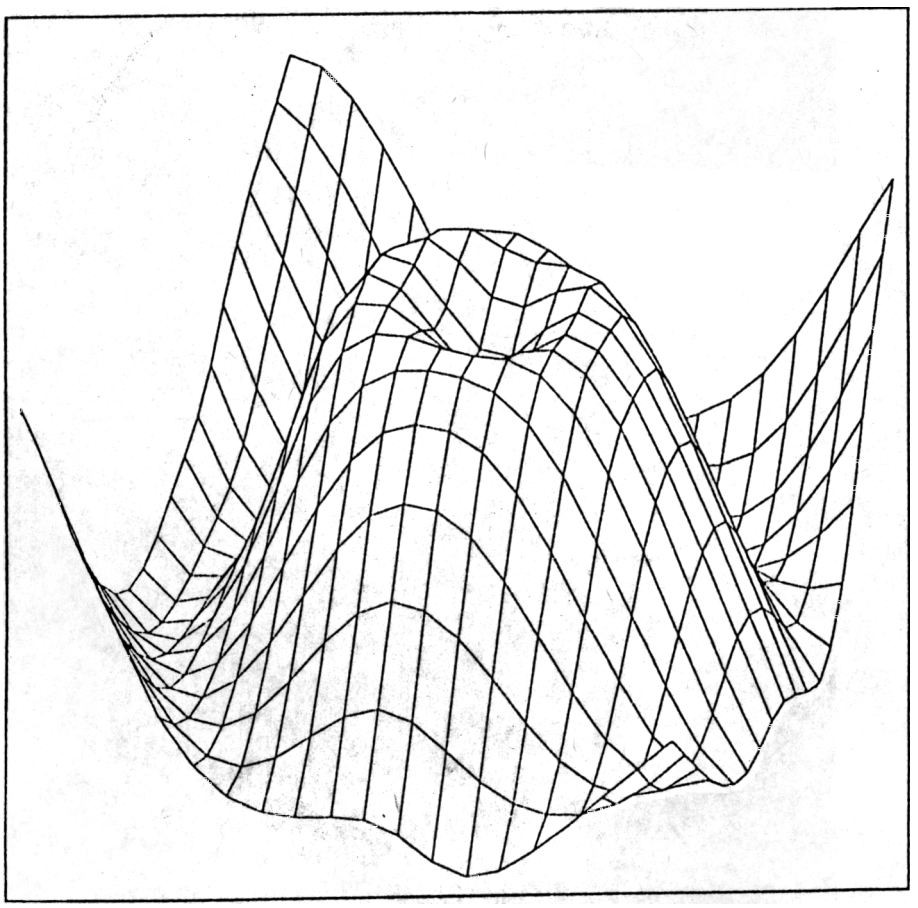
ADVANCES IN COMPUTER METHODS FOR PARTIAL DIFFERENTIAL EQUATIONS - VII



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EULERIAN-LAGRANGIAN APPROACH TO THE MODELING OF SHOCKS IN PETROLEUM RESERVOIRS

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1. INTRODUCTION

Apparently, in Petroleum Engineering the first studies of discontinuous fronts or shocks, are contained in the papers that originated the classical Buckley-Leverett Theory [1,2]. In reservoir studies, this theory has been used mainly in the form presented by Welge [3] (see also [4]). Later on, Cardwell and Sheldon et al. in a couple of papers [5,6], discussed shock formation using the method of characteristics, throwing additional light on Buckley-Leverett theory and in the method of Welge.

However, a more general theory of discontinuities in oil production is possible and it would be useful. Buckley-Leverett theory applies when the fluids and the rocks can be treated as incompressible and effects of capillary pressure can be neglected. The work by Sheldon et al. [6] opened the door to some generalizations, such as the incorporation of compressibility and gravity segregation. Kale [7] proposed a two-dimensional extension of Buckley-Leverett theory using a linear approximation of the fractional flow function. An important contribution in this direction was made by Glimm et al. [8], who proposed a front tracking method for petroleum reservoir simulation in which the formulation of shock conditions, is based on "hyperbolic conservation laws" and this approach has been applied recently by Bratvedt et al. [9], to develop a front tracking method for reservoir simulation, which also approximates the fractional flow function by piecewise linear functions. However, in these latter papers, attention was centered mainly on the computational aspects. It must also be mentioned, that fundamental blocks in Glimm's construction are the solutions of local Riemann problems.

Other related approaches, are based on the method of characteristics [10–14] and more recently, in combining the method of characteristics with Localized Adjoint Method (ELLAM) [15,16]. This approach was first proposed for multiphase problems of reservoir Engineering by Herrera and Ewing [17]. However, these methods although suited to deal with abrupt continuous fronts, do not include the treatment of shocks and are usually limited to miscible flow problems.

In this paper we present an approach to treat discontinuous fronts or shocks, recently proposed by Herrera et al. [17,18]. We would like to call attention to the following aspects of our presentation:

a) A systematic formulation of "jump conditions" of general applicability to multi-phase systems;

b) Introduction of finite difference schemes for discontinuous functions;

c) An Eulerian-Lagrangian approach to front tracking; and

d) A rigorous mathematical setting is given for more general problems.

Regarding the generality of the "jump conditions" here derived, it must be mentioned that they are based on the fundamental "balance laws" of Continuum Mechanics. These are the fundamental physical laws in which models of macroscopic physical systems are based, and have complete generality. Indeed, they are applicable to any kind of multiphase problem with shocks, occurring in Petroleum Engineering.

Another interesting point is the use of "finite difference formulas" for functions with jump discontinuities. Standard applications of such formulas require that the functions be differentiable. However, at present Herrera [20] has been developing finite difference formulas which are applicable to fully discontinuous functions and numerical results that have been obtained using them, for some problems of petroleum reservoir simulation, have been reported [18]. In Petroleum Engineering, one important advantage of using finite differences for front tracking is that numerical schemes that are obtained are easily incorporated in the software available for reservoir simulation, since this is most frequently based on finite difference approximations.

The advantages of using an Eulerian-Lagrangian approach to front tracking, instead of using a moving frame of reference, has been recognized in applications of the method of characteristics [10–16] and has been the motivation for the development of the Modified Method of Characteristics. The combined use of finite difference formulas for functions with jumps and an Eulerian-Lagrangian approach is very fruitful, since these two methodologies match very well [11].

In this paper our procedure is briefly explained and as an illustration it is applied to treat the shocks which occur when a gas front invades a region of undersaturated liquid oil. The case of an advancing front of gas into undersaturated liquid oil has been treated previously [21–23], but to our knowledge, jumps were incorporated in the model for the first time in [18], and the numerical results obtained were quite satisfactory.

2. Jump Conditions

To give to our developments a sound physical and mathematical basis, we start from first principles. The basis of the fundamental equations that govern the flow and transport of fluids in a reservoir are the balance equations of Continuum Mechanics. The synthesis of this theory that has been given by Allen, Herrera, and Pinder [24], and by Herrera and Allen [25], are very convenient for our purposes. In the case of multi-phase systems, each phase α moves with its own velocity $\underline{v}^\alpha$. Here, $\alpha = 1,\ldots,N$, 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 the intensive property ψ^α associated with component α, are:

$$\psi^\alpha_t + \nabla\cdot(\psi^\alpha \underline{v}^\alpha) - \nabla\cdot\underline{\tau}^\alpha = g^\alpha \tag{1a}$$

and

$$[\psi^\alpha(\underline{v}^\alpha - \underline{v}_\Sigma) - \underline{\tau}^\alpha]\cdot\underline{n} = g^\alpha_\Sigma \tag{1b}$$

Here, the vector $\underline{\tau}^\alpha$, is the *flux* of ψ^α across surfaces in space, while the quantities g^α and g^α_Σ represent *external supply* of ψ^α [23,24], per unit volume and unit time, in the case of g^α, while g^α_Σ represents *external supply* of ψ^α through the discontinuity, per unit area and unit time.

Equation (1*a*) is the "general differential balance law", to be satisfied at every point of the space occupied by the continuous system. Equation (1*b*), 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 (generally, space-time) of discontinuity Σ, which moves with velocity $\underline{v}_\Sigma$ and in which the physical variables may have jump discontinuities. In addition, the square brackets are defined as the "jumps" across 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, the positive side of Σ is defined to be that one towards which the vector $\underline{n}$ points to. The sense of this latter vector, however, is chosen arbitrarily. Finally, it must be mentioned that in the form presented here, Eq. (1*b*) is slightly more general than that presented in [24] and [25], because the possibility of non-vanishing external supply through the discontinuity, has been included.

To illustrate the use of Eqs. (1), 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 non-volatile oil. This implies that the total number of components are four and that $\underline{v}^\alpha$, in Eqs. (1*b*), 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:

$$\psi^{w} = \phi S_w \rho_w, \qquad \bar{\psi}^{o} = \phi S_o \bar{\rho}_o, \qquad \bar{\psi}^{dg} = \phi S_0 \bar{\rho}_{dg}, \qquad \psi^{g} = \phi S_g \rho_g \tag{2}$$

for the intensive properties associated with water, non-volatile oil, dissolved gas and gas in the gas phase, respectively. The notations: $\bar{\rho}_o$ and $\bar{\rho}_{dg}$ are used for the effective densities of non-volatile oil and dissolved gas, respectively. Also, the *flux* τ corresponding to each one of these intensive properties vanishes identically, since no physical diffusion is present. Applying Equation (1*a*) to each one of these intensive properties one gets, in a straight forward manner, the familiar system of equations of black oil models (see details in [18]):

$$\nabla \cdot [\lambda_w(\nabla p_w - \gamma_w \nabla z)] = \frac{\partial}{\partial t}\left(\frac{\phi S_w}{B_w}\right)$$

$$\nabla \cdot [\lambda_o(\nabla p_o - \gamma_o \nabla z)] = \frac{\partial}{\partial t}\left(\frac{\phi S_o}{B_o}\right)$$

$$\nabla \cdot [R_s \lambda_o(\nabla p_o - \gamma_o \nabla z) + \lambda_g(\nabla p_g - \gamma_g \nabla z)] = \frac{\partial}{\partial t}\left[\phi\left(R_s \frac{S_o}{B_o} + \frac{S_g}{B_g}\right)\right] \tag{3c}$$

where

$$\lambda_l = \frac{k_{rl}}{\mu_l B_l}\underline{\underline{k}} \qquad (l = w, o, g) \tag{4}$$

are the mobilities.

In a similar fashion, applying Equation (1*b*) to each one of the four intensive properties, it is obtained:

$$[\phi \rho_w S_w(\underline{v}^{w} - \underline{v}_\Sigma)] \cdot \underline{n} = 0,$$

$$[\phi \bar{\rho}_o S_o(\underline{v}^{o} - \underline{v}_\Sigma)] \cdot \underline{n} = 0,$$

$$[\phi \bar{\rho}_{dg} S_o(\underline{v}^{o} - \underline{v}_\Sigma)] \cdot \underline{n} = g^{o}_{\Sigma g},$$

$$[\phi \rho_g S_g(\underline{v}^{g} - \underline{v}_\Sigma)] \cdot \underline{n} = g^{g}_{\Sigma o}.$$

In addition, Darcy's Law requires:

$$[p_l] = 0; \qquad l = w, o, g \tag{7}$$

Finally, the quantities $g^{o}_{\Sigma g}$ and $g^{g}_{\Sigma o}$ stand for the exchange of mass between the gaseous and liquid phases. Mass conservation requires that:

$$g^{o}_{\Sigma g} + g^{g}_{\Sigma o} = 0 \tag{8}$$

So that, adding up Eqs (6), it is obtained:

$$[\phi \bar{\rho}_{dg} S_o \underline{v}^{o} + \phi \rho_g S_g \underline{v}^{g}] \cdot \underline{n} - [\phi \bar{\rho}_{dg} S_o + \phi \rho_g S_g]\underline{v}_\Sigma \cdot \underline{n} = 0 \tag{9}$$

Continuity of the pressures of the different phases implies the continuity of ρ_w. In addition, it is assumed that the porosity ϕ, is continuous. This allows canceling the factors ϕ and ρ_w in Equations (5) and (9), and writing them as:

$$[S_w(\underline{v}^{w} - \underline{v}_\Sigma)] \cdot \underline{n} = 0, \tag{10a}$$

$$\left[\left(\frac{S_o}{B_o}\right)(\underline{v}^{o} - \underline{v}_\Sigma)\right] \cdot \underline{n} = 0, \tag{10b}$$

$$\left[\left(\frac{R_s S_o}{B_o}\right)(\underline{v}^{o} - \underline{v}_\Sigma) + \left(\frac{S_g}{B_g}\right)(\underline{v}^{g} - \underline{v}_\Sigma)\right] \cdot \underline{n} = 0, \tag{10c}$$

when the volume factors, are introduced. Equations (10), together with (7), constitute the desired system of jump conditions for the three-phase (four component) oil reservoir. They relate the jumps of the physical variables with the velocity $\underline{v}_\Sigma$ 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 both of them, B_o and R_s, may change with the bubble point.

3. The Velocity of the Advancing Front

Thus far the discussion has been completely general. 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 extensively used by Herrera in his "Algebraic Theory of Boundary Value Problems" [26–30], will be applied. This is:

$$[rs] = \dot{r}[s] + \dot{r}[r] \tag{11}$$

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

$$\dot{r} = (r_+ + r_-)/2 \tag{12}$$

To treat the case of a front of gas advancing into a non-saturated liquid oil, the unit normal $\underline{n}$ to the gas front Σ, will be taken with its sense opposite to $\underline{v}^g$ (i.e. $\underline{v}^g \cdot \underline{n} \leq 0$), 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 defined in 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:

$$\underline{v}_\Sigma \cdot \underline{n} = \eta \underline{v}^g \cdot \underline{n} \qquad \underline{v}_o \cdot \underline{n} = \zeta \underline{v}^g \cdot \underline{n} \tag{13}$$

and

$$\omega = \frac{S_o B_g}{B_o S_g} \tag{14}$$

Then, equations (10*b*) and (10*c*), can be written as:

$$[\omega(\zeta - \eta)] = 0, \tag{15a}$$

$$[R_s \omega(\zeta - \eta)] + 1 - \eta = 0. \tag{15b}$$

Using formula (11), Eq. (15*a*) can be transformed into:

$$\dot{\zeta}[\omega] + \dot{\omega}[\zeta] = \eta[\omega] \tag{16}$$

from which it follows that

$$\dot{\zeta} = \eta - \dot{\omega}\frac{[\zeta]}{[\omega]}. \tag{17}$$

On the other hand, Eq. (15*b*), when use is made of the identity (11) and after simplifying by means of Eq. (15*a*), can be written as:

$$[R_s]\overline{\omega(\zeta - \eta)} + 1 - \eta = 0. \tag{18}$$

Here, as in what follows, use is made of a bar to indicate that the average refers to the whole expression covered by the bar. From (18), it follows that

$$[R_s]\left(\overline{\omega\zeta} - \dot{\omega}\eta\right) + 1 - \eta = 0 \tag{19}$$

which can be further simplified by means of an algebraic identity closely related with (11); this is: $\overline{\omega\zeta} = [\omega][\zeta]/4 + \dot{\omega}\dot{\zeta}$. Applying this identity and combining the resulting equation with Eq. (17), one gets:

$$\eta = 1 - [R_s]\frac{[\zeta]}{[\omega]}\omega_+\omega_- \tag{20}$$

Equations (13), (17) and (20), determine the velocity of the advancing front, but as they stand, they look cryptic. 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:

$$\left(\underline{v}_\Sigma - \underline{v}_+^o\right) \cdot \underline{n} = \epsilon\left(\underline{v}^g - \underline{v}_+^o\right) \cdot \underline{n} \tag{21}$$

Using Eqs. (13), it can be seen that

$$\epsilon = \frac{\eta - \zeta_+}{1 - \zeta_+}. \tag{22}$$

When the auxiliary relations:

$$\eta - \zeta_+ = \frac{[\zeta]}{[\omega]}\omega_-; \qquad 1 - \zeta_+ = \left\{1 + [R_s]\omega_+\right\}\frac{[\zeta]}{[\omega]}\omega_- \tag{23}$$

which are implied by Eqs. (17) and (20), after some algebraic manipulations, are used in Eq. (22), the expression

$$\epsilon = \frac{1}{1 + [R_s]\omega_+} = \frac{1}{1 + [R_s]\dfrac{B_g S_{o+}}{S_g B_{o+}}} \tag{24}$$

for the retardation factor ϵ, is obtained. Equation (24), together with (21), yield the velocity of the advancing gas front. Observe that $R_{s+} \geq R_{s-}$, so that $\epsilon \leq 1$.

4. Numerical Formulation of Jump Conditions

Equation (24) is informative and permits acquiring insight on the manner in which the advance of the gas front takes place. However, for numerical applications we have preferred to start from Eqs. (10) and transform them in the manner explained in [18].

For simplicity, in what follows only two phases will be considered. For that case, the jump conditions can be transformed into [18]:

$$\dot{\lambda} s + \left[\frac{\phi S_o}{B_o}\right] v_\Sigma + [\lambda_o] m = 0, \tag{25a}$$

$$\left(2\overline{R_s \lambda_o} + \lambda_{g+}\right) s + 2\left[\phi\left(R_s \frac{S_o}{B_o} + \frac{S_g}{B_g}\right)\right] v_\Sigma + 2\left(\lambda_{g+} + [R_s \lambda_o]\right) m = 0. \tag{25b}$$

Here, the notation $s = [\partial p_o / \partial x]$ and $m = \overline{\partial p_o / \partial x}$, is understood and capillary pressure has been neglected. For the numerical treatment, in [18], Eqs. (25) were used as a system of equations for the unknowns s, v_Σ and 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 (3) in a suitable manner, as it is explained in the next Section.

5. The Weighted Equations

The one-dimensional version of Equations (3*b* and *c*), is:

$$\frac{\partial}{\partial x}\left(\lambda_o \frac{\partial p_o}{\partial x}\right) - \frac{\partial}{\partial t}\left(\frac{\phi S_o}{B_o}\right) = 0, \tag{26a}$$

$$\frac{\partial}{\partial x}\left(R_s \lambda_o \frac{\partial p_o}{\partial x} + \lambda_g \frac{\partial p_g}{\partial x}\right) - \frac{\partial}{\partial t}\left\{\phi\left(R_s \frac{S_o}{B_o} + \frac{S_g}{B_g}\right)\right\} = 0. \tag{26b}$$

In this Section these equations will 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 (or control volume) method.

As an illustration, the procedure is explained for the case $Cu = -(V_\Sigma \Delta t / \Delta x) < 1$. 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}. When $Cu < 1$ 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: The system of space-time weights to be used in cell i (i.e.; $[x_{i-1/2}, x_{i+1/2}]$), is:

$$w_1^\circ(x,t) \equiv 1 \tag{27a}$$

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

for the oil and

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

for the gas.

The resulting equations, constitute a system of three equations for cell i, which must be coupled with the system of jump conditions 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 pressure and saturation of the gas. Cells, other than cell i, can be treated in a standard manner, solving for example, for oil pressure and gas saturation at the center of the cell. However, cell i must be treated in a special manner. We have available the system of five equations The five unknowns that were chosen in [18] were: the jump and average of the pressure gradient (s and m, respectively), the velocity v_Σ of the gas front (these three unknown functions defined on $\Sigma(t)$), the saturation and the pressure. Then, the resulting system of equations was solved for the value p_{oi}^{n+1} at the center of cell i and the value $S_{g\Sigma}^{n+1}$ of gas saturation at the gas front, together with s^{n+1}, m^{n+1} and v_Σ^{n+1}. A special feature of this procedure is that one does not solve for saturation at the center of cell i.

Case B: The treatment is similar, except that the system of space-time weights to be used in cell i (i.e.; $[x_{i-1/2}, x_{i+1/2}]$), is:

$$w_1^o(x,t) \equiv 1$$

for the oil and

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

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:

$$w_2^o(x,t) \equiv 1$$

for the oil and

$$w_2^g(x,t) = \begin{cases} 0, & x < x_\Sigma(t) \\ 1, & x > x_\Sigma(t) \end{cases} \tag{28d}$$

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

$$w_3^o(x,t) = \begin{cases} 0, & x < x_\Sigma(t) \\ 1, & x > x_\Sigma(t) \end{cases} \tag{28e}$$

For additional details of the numerical treatment, the reader is referred to [18].

6. Finite Differences for Discontinuous Functions

For the construction of an Eulerian-Lagrangian approach to front tracking, it is essential to apply finite difference formulas to functions with jump discontinuities. Such formulas are being developed by Herrera [20] and they have been used in the numerical applications of the method presented here. Since the use of such formulas is not 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. 1. A notation which is usual in applications of the cells method has been adopted. Thus, the "nodes" will be the centers of the subintervals of the partition. The i–th 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 Figure 1, we have illustrated cells $i-1$, i and $i+1$. Assume the first

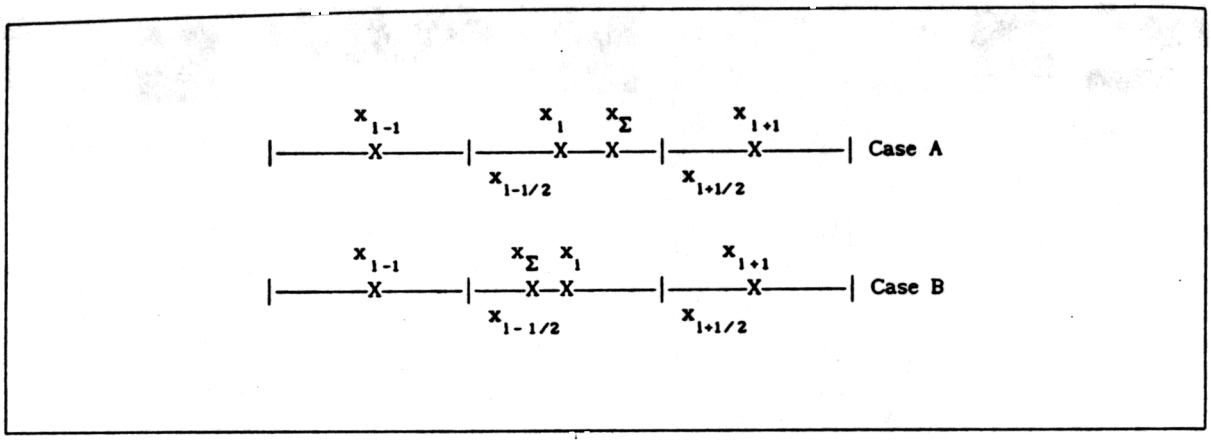

FIGURE 1.

derivative of the oil pressure p_o, has a jump discontinuity at x_Σ and $x_{i-1/2} \le x_\Sigma \le x_{i+1/2}$, 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 $x_i \le x_\Sigma$ one can apply the usual centered differences formula:

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

However, when $x_\Sigma < x_i$, Eq. (29) is not applicable and a modified formula, accounting for the discontinuity, is needed.

In what follows the notation

$$\left[\frac{\partial p_o}{\partial x}\right]_\Sigma = s \qquad \left[\frac{\partial^2 p_o}{\partial x^2}\right]_\Sigma = r \tag{30}$$

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

$$\hat{p}_o = \begin{cases} p_o - \frac{1}{2}s(x - x_\Sigma) - \frac{1}{4}r(x - x_\Sigma)^2 & \text{if } x_\Sigma \le x, \\ p_o + \frac{1}{2}s(x - x_\Sigma) + \frac{1}{4}r(x - x_\Sigma)^2 & \text{if } x \le x_\Sigma. \end{cases}$$

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

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

$$= \frac{p_{oi} - p_{oi-1}}{h} + \frac{s}{2}(\xi + 1) - \frac{rh}{8}\{\xi^2 + 2(\xi + 1)\} + O(h^2) \tag{32}$$

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

$$\left(\frac{\partial \hat{p}_o}{\partial x}\right)_{i-1/2} = \left(\frac{\partial p_o}{\partial x}\right)_{i-1/2} + \frac{s}{2} - \frac{rh}{4}(\xi + 1) + O(h^2). \tag{33}$$

Combining (32) and (33), it is obtained:

$$\left(\frac{\partial p_o}{\partial x}\right)_{i-1/2} = \frac{p_{oi} - p_{oi-1}}{h} + \frac{s}{2}\xi - \frac{rh}{8}\xi^2 + O(h^2) \tag{34}$$

The jump r of the second derivative is not known and in applications of formula (34) to partial differential equations, it is necessary to eliminate it. To this end, the second derivative of $\hat{p}_o$ is computed in two alternative forms:

a) Firstly, the standard centered difference formula is applied to $\hat{p}_o$.

b) Secondly, the first derivative of $\hat{p}_o$ is differented.

Here, we skip the details and only the final results are given. They are:

$$r = \frac{w^-}{h}\left\{\frac{(\xi+1)p_{oi+1}+(\xi-1)p_{oi-1}-2\xi p_{oi}}{h} - 2\dot{d}_{o\Sigma} - s\right\} + \frac{4s}{h(\xi+2)} + O(h) \tag{35a}$$

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

$$r = \frac{w^+}{h}\left\{\frac{(\xi+1)p_{oi+1}+(\xi-1)p_{oi-1}-2\xi p_{oi}}{h} - 2\dot{d}_{o\Sigma} + s\right\} + \frac{4s}{h(\xi-2)} + O(h)$$

where $w^+ \doteq 8/(\xi-2)^2(\xi+1)$. Here, the notation $d_{o\Sigma} = (\partial p_o/\partial x)_\Sigma$ is understood.

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