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THE NEGATIVE TRANSMISSIBILITY ISSUE WHEN USING CVFEM IN PETROLEUM RESERVOIR SIMULATION – 1. THEORY

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Abstract: *Petroleum reservoir simulators were, until recently, developed using finite difference schemes in Cartesian grids. Seeking for generality and flexibility, curvilinear grids and unstructured grids started to be employed in the last decade. The Control Volume Finite Element Method-CVFEM is one of the technologies employed for unstructured grids of triangular and quadrilateral elements in 2D and tetrahedral and hexahedral elements in 3D. This procedure is a control volume method whose control volumes are created adding adjacent sub-control volumes of the elements surrounding a node. When deriving the discrete equations for multiphase flows, it is common to integrate the governing equations for a single flow and extending them to multiphase flow by introducing the mobility. This strategy, called herein CVFEM-S, although results in a scheme that facilitates the implementation into existing simulators, present serious implications which are discussed in this work. Starting the paper, a more rigorous approach, denoted by CVFEM-M is presented. The concept of transmissibility in structured and unstructured grids, using triangular and quadrilateral elements, is also discussed. It is shown that a physical meaning for the transmissibility only exists when the flux at the control volume interfaces can be calculated using only two grid-points. Nevertheless, in a number of situations, where the flux is calculated using three or even more grid-points the concept of transmissibility is used in a misleading way. It is also shown that when using CVFEM with triangular elements disobeying the angular restriction mentioned in the literature, the negative coefficients resulting from the discretization do have physical support, since they are not, in fact, "transmissibilities", as they are referred in the literature.*

Keywords: *reservoir simulation, petroleum, control-volume, finite volume method, finite element method, transmissibility.*

1. Introduction

The requirement of solving multiphase flows in petroleum reservoirs with complex geometries and, in general, with the presence of geological faults, increased the efforts dedicated to the development of methodologies employing unstructured grids. Several studies have demonstrated the advantages of using flexible grid in terms of results accuracy and computational time. Quandale (1993), for instance, compared the results obtained by different flexible grids in some reservoir simulators and concluded that these methods allow a significant computer time saving. The total number of grid nodes could be reduced by a factor of four or more with a flexible grid, while keeping the simulation results close to those obtained with regular grids.

The utilization of unstructured grids in conservative methods was proposed, in pioneering works in the area of computational fluid dynamics for solving the Navier-Stokes equations, by Baliga and Patankar (1983) using triangular elements and Schneider and Zedan (1983), using quadrilateral elements. In such a method the fluid flow properties are conserved in each control volume obtained assembling the sub-control volumes belonging to adjacent elements. Thus, the geometrical flexibility resembles the Finite Elements Method (FEM). It is named CVFEM (Control Volume Finite Element Method) because it employs the shape functions used in FEM and the assembling of the equations is equivalent. However, the denomination CVFEM is misleading and conveys the reader to view the methodology as being a finite element technique which uses control volumes for the integration of the equations. Actually, it is a finite volume methodology, whose only similarity with the finite element method is the use of elements for the domain geometrical representation and the shape functions for the variables interpolation. A better denomination would be Element-based Finite Volume Method (EbFVM), since it is simply a finite volume methodology that borrows from the finite element technique the concept of elements and its shape functions (Maliska 2004). In this paper one is keeping the CVFEM denomination.

Since the CVFEM-M, the procedure which obtains the discretized equations integrating the appropriate multiphase flow equations, has not yet considered in reservoir simulation, this paper begins with a shortly description of its characteristics and potentialities. After that, the CVFEM-S currently used in the petroleum literature is reviewed, as well as its equations deduced and discussed. Finally, the negative "transmissibility" which appears when obtuse triangles are used is also discussed and defined in new grounds.

2. The use of the CVFEM-M and its potentialities in reservoir simulation

In the CVFEM the elements (triangle and/or quadrilaterals for 2D) are formed by the information of the node definition (grid nodes) and the connectivity matrix, as in FEM. To obtain the approximate equations, CVFEM integrates the divergent form of the partial differential equation over non-overlapping control volumes, what is equivalent to make balance conservation on those volumes. Figure 1 shows an example of a grid used in this method, where it is depicted one triangular element (formed by nodes 5-3-2) and one quadrilateral element (formed by nodes 3-4-1-2). In this figure the control volumes formed around the nodes 3 and 4 are also shown, as well as the integration points (labeled by "*x*") located over its boundaries. This scheme of control volume construction belongs to the cell vertex category, since the center of the control volumes is a vertex of the element. Therefore, the resulting control volumes are formed by portions (sub-control volumes) of neighboring elements, and all fluxes at one specified integration point can be calculated using only data from the element where the integration point lies in.

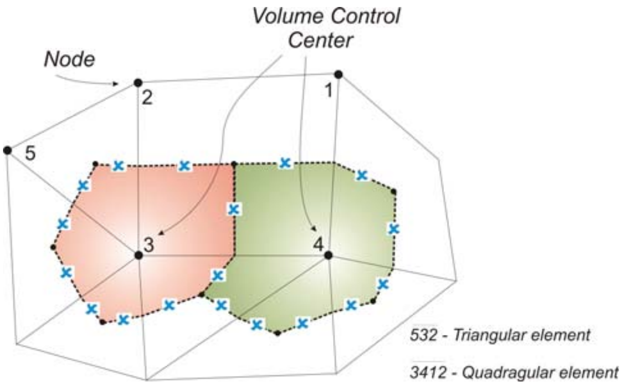


Figure 1. Example of a grid used in the CVFEM

In the procedure advanced in this paper the porous medium properties, like absolute permeability and porosity are stored in the center of the elements, differently from other CVFE approaches (Verma, 1997), which store the physical properties in the control volumes center. With this strategy, since the integration points lay inside the elements, there is no need of any type of averaging, when non-homogeneous media is considered, to calculate the permeability in these points, since the elements are homogeneous, i.e. each element has only one value of permeability. On the contrary, when properties are stored at the center of the control volumes, the integration point lies over a interface between two different media, requiring interpolation. The problems related to the internodal permeability evaluation shown in (Desbarats, 1987; Romeu and Noetinger, 1995; Cordazzo et al., 2003*a*), among others, do not exist in the method proposed in this paper. The porosity, by its turn, requires averaging in the transient term with the approach present herein.

There are at least two reasons why one can say that employing a mean value of porosity is not so troublesome as employing a mean value of permeability. First, often the range of variation of porosity values is lesser than the variation of permeabilities values in a field. Second, the permeability is a term appearing in Darcy Law, while porosity is not. We should remember that the Darcy law is the momentum equation for a porous media. These reasons justify the option for a numerical method that uses an average porosity value in the transient term, instead of an average permeability value for calculating mass fluxes. Cordazzo et al. (2002) proposed a weighted average porosity as a function of the volume of each sub-control volume.

Following, the CVFEM method is used integrating the two-phase governing equations, the right procedure to attain physical consistency.

2.1 The CVFEM-M equations

The two-phase governing partial differential equations to be integrated are given by

$$\frac{\partial\left(\phi S_m / B_m\right)}{\partial t} = \vec{\nabla}.\left(\lambda_m \overline{\overline{k}} \vec{\nabla} p\right) + q_m \tag{1}$$

where p is the pressure, λ is the mobility, ϕ is the porosity, S is the saturation, B is the volume formation factor, $\overline{\overline{k}}$ is the permeability tensor and q_m is the flow-rate per unit of volume, at reservoir conditions. For convenience, the gravity and capillary effects were neglected. The subscript indicating the phase ($m = w$ or o) is omitted from now on for the sake of simplicity.

The integration of Eq. 1 in time and over the elemental control volume reads

$$V_i \frac{\left(\phi S / B\right)_i^{n+1} - \left(\phi S / B\right)_i^n}{\Delta t} = \int_V \vec{\nabla}.\left(\lambda \overline{\overline{k}} \vec{\nabla} p\right) dV + q V_i \tag{2}$$

where V_i is the total volume of the control volume i formed by the sum of the sub-control volumes belonging to the elements surrounding node i.

Applying the Gauss divergence theorem to Eq. 2, one obtains

$$V_i \frac{\left(\phi S / B\right)_i^{n+1} - \left(\phi S / B\right)_i^n}{\Delta t} = \int_S \lambda \overline{\overline{k}} \vec{\nabla} p . d\vec{S} + q V_i \tag{3}$$

where the surface integral is over all the edges of a control volume.

Since in this method the pressure field is evaluated using the nodal values of each element (3 for triangles and 4 for quadrilaterals), the surface integral given in Eq. 3 will result in different discretized equations, depending on the type of element chosen. The differences arise on the shape function used, which is linear for triangular elements and bi-linear for quadrilateral elements. Despite these differences, there are no difficulties in working with these two kinds of elements in a same grid. In this work, however, only triangular elements are used because the discretized equations obtained here will be compared with those obtained with the CVFEM-S, which is a method that in reservoir simulation has been mostly applied with triangular elements. Nevertheless, the CVFEM-M discretized equations using quadrilateral elements can be seen in details elsewhere (Cordazzo et al., *2003b*; Hurtado et al., 2004).

Using the shape functions, the pressure inside the element is given by

$$p = \sum_{i=1}^{3} N_i(\xi, \eta) p_i \tag{4}$$

where N_i are the linear shape functions given by

$$N_1(\xi, \eta) = 1 - \xi - \eta \tag{5a}$$
$$N_2(\xi, \eta) = \xi \tag{5b}$$
$$N_3(\xi, \eta) = \eta \tag{5c}$$

where ξ and η are the local coordinates in the computational domain. The local coordinates allow each element to be treated identically, no matter how distorted the element may actually be in terms of the global coordinates. Figure 2 shows a triangular element in xy and in $\xi\eta$ spaces. In standard FEM this kind of element is called the "isoparametric" element (Hughes, 1987).

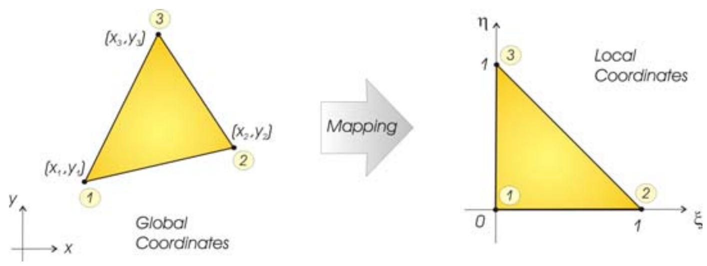


Figure 2 – Triangular element in xy and in $\xi\eta$ spaces

The coordinates of any point within the element can be also expressed in function of the element nodal values, as done with the pressure (Eq. 4). In order to determine the pressure gradient it is necessary to calculate the shape functions derivatives, $\partial N_i / \partial x$ and $\partial N_i / \partial y$. Using the chain rule

$$\frac{\partial N_i}{\partial \xi} = \frac{\partial N_i}{\partial x}\frac{\partial x}{\partial \xi} + \frac{\partial N_i}{\partial y}\frac{\partial y}{\partial \xi} \tag{6a}$$

$$\frac{\partial N_i}{\partial \eta} = \frac{\partial N_i}{\partial x}\frac{\partial x}{\partial \eta} + \frac{\partial N_i}{\partial y}\frac{\partial y}{\partial \eta} \tag{6b}$$

one obtains a system of two equations and two unknowns, where only the derivatives of N_i in relation to x and y are unknowns. Solving this system, one gets

$$\vec{\nabla} p = \left[\frac{(p_2 - p_1)(y_3 - y_1) - (p_3 - p_1)(y_2 - y_1)}{\det(J)}\right]\hat{i} + \left[\frac{(p_3 - p_1)(x_2 - x_1) - (p_2 - p_1)(x_3 - x_1)}{\det(J)}\right]\hat{j} \tag{7}$$

where the subscripts 1, 2 and 3 are the nodes shown in Fig. 2, and $\det(J)$ is the Jacobian of transformation, given by

$$\det(J) = (x_2 - x_1)(y_3 - y_1) - (x_3 - x_1)(y_2 - y_1) \tag{8}$$

To simplify and facilitate the comparison with the equations available in the literature (Fung et al., 1991), the following change of variables is set

$$a_1 = x_3 - x_2 \qquad a_2 = x_1 - x_3 \qquad a_3 = x_2 - x_1 \tag{9a}$$

$$b_1 = y_2 - y_3 \qquad b_2 = y_3 - y_1 \qquad b_3 = y_1 - y_2 \tag{9b}$$

Rewriting the Eq. 7, one can show that

$$\vec{\nabla} p = \frac{1}{2A}\sum_{i=1}^{3}\left(b_i\hat{i} + a_i\hat{j}\right)p_i \tag{10}$$

where the Jacobian was replaced by twice the triangle area, A, for convenience.

Substituting Eq. 10 into 3, one obtains

$$\int_V \vec{\nabla}.\left(\lambda \bar{\bar{k}}\vec{\nabla} p\right)dV = \frac{1}{2A}\int_S \sum_{i=1}^{3}\left(b_i\hat{i} + a_i\hat{j}\right)p_i\,\lambda\bar{\bar{k}}.d\vec{S} \tag{11}$$

The permeability tensor $\bar{\bar{k}}$ and the area vector are given, respectively, as

$$\bar{\bar{k}} = \begin{bmatrix} k_{xx} & k_{xy} \\ k_{yx} & k_{yy} \end{bmatrix} \tag{12}$$

and

$$d\vec{S} = dy\hat{i} - dx\hat{j} = \left(\frac{\partial y}{\partial \xi}d\xi + \frac{\partial y}{\partial \eta}d\eta\right)\hat{i} - \left(\frac{\partial x}{\partial \xi}d\xi + \frac{\partial x}{\partial \eta}d\eta\right)\hat{j} \tag{13}$$

and after replacing them in Eq. 11, one obtains

$$\int_V \vec{\nabla}.\left(\lambda \bar{\bar{k}} \vec{\nabla} p\right) dV = \int_S \left[\lambda k_{xx}\left(b_1 p_1 + b_2 p_2 + b_3 p_3\right)\left(b_2 d\eta - b_3 d\xi\right) + \lambda k_{xy}\left(a_1 p_1 + a_2 p_2 + a_3 p_3\right)\left(b_2 d\eta - b_3 d\xi\right) + \right.$$
$$\left. -\lambda k_{yx}\left(b_1 p_1 + b_2 p_2 + b_3 p_3\right)\left(a_3 d\xi - a_2 d\eta\right) - \lambda k_{yy}\left(a_1 p_1 + a_2 p_2 + a_3 p_3\right)\left(a_3 d\xi - a_2 d\eta\right)\right] \tag{14}$$

One can note that all terms in the right side of Eq. 14, except the mobility λ, are constant inside the elements, since either they depend on nodal values only or they are defined by elements, such as the absolute permeability. The mobility, of course, is calculated using the nodal values also, but considering the upwind direction. So, the mobility, instead of other terms, cannot be simply put outside the integral. As already stated, this integral is evaluated over all the edges of the control volumes, where the integration of all terms, including the mobility, can be approximated as the product of the mean value and the area at every edge.

The sub-control volumes (*Scv*), in xy and $\xi\eta$ spaces, are presented in Fig. 3. The integration points ("x") are located in their inner surfaces, where the integral in Eq. 14 is approximated. The surface integral over the element boundaries, in contrast, will not be regarded, because it vanishes when the global matrix is assembled as the fluxes across the element boundaries cancel one another.

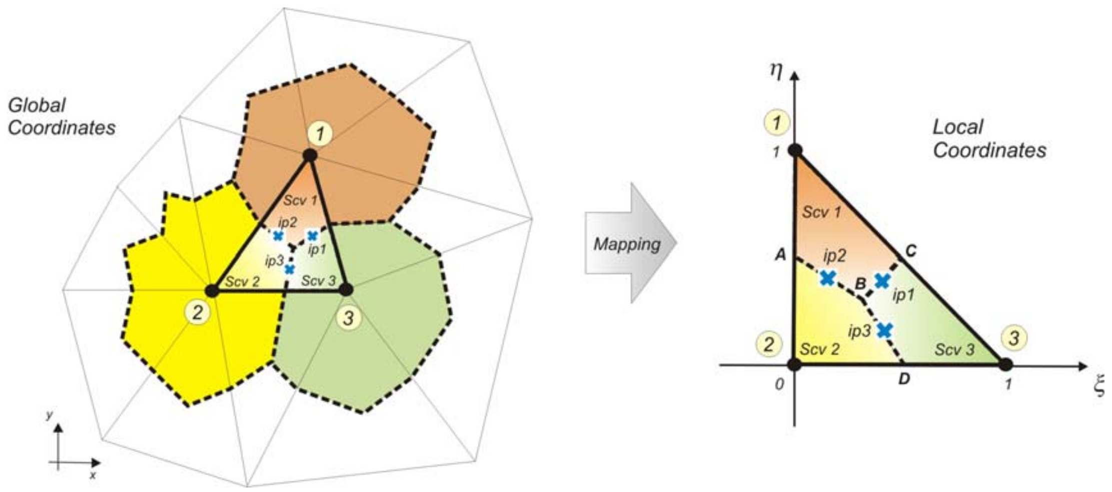


Figure 3 – Triangular element, showing its sub-control volumes (*Scv*) and the integration points (*ip*)

Thus, in order to obtain the discretized balance equation of *Scv*1 (in the triangular element of Fig. 3), for instance, the integration of Eq. 14 is approximated over the surface of this sub-control volume, where the integration points 1 and 2 (*ip1* and *ip2*) lie. One can note that the mobility in each integration point multiplies the three nodal values of pressure according to Eq. 14, which rewritten compactly for this sub-control volume results in

$$\int_{scv1} \vec{\nabla}.\left(\lambda \bar{\bar{k}} \vec{\nabla} p\right) dV = Q_1 = \lambda_{12}\left[\tau^{12}_{AB\,scv1}\left(p_2 - p_1\right) + \tau^{13}_{AB\,scv1}\left(p_3 - p_1\right)\right] + \lambda_{13}\left[\tau^{12}_{BC\,scv1}\left(p_2 - p_1\right) + \tau^{13}_{BC\,scv1}\left(p_3 - p_1\right)\right] \tag{15}$$

where λ_{12} is the mobility of surface *AB* in Fig. 3 that separates the control volumes 1 and 2, and so on. The terms τ are coefficients containing all geometrical and absolute permeability information of the interface. Their superscripts 12 and 13 are utilized to indicate that they are multiplying the terms $(p_2 - p_1)$ and $(p_3 - p_1)$, respectively, while the subscripts *AB* and *BC* indicate that the term is resulted of the flux balance at the interface of sub-control volumes "1 and 2" and "1 and 3", respectively. Furthermore, it is needed to utilize the subscript *Scv1* in the Eq. 15, because the terms τ are not symmetrical inside the elements, for instance the term τ^{13}_{BC} calculated by mass balance in the *Scv1* can be different from the term τ^{13}_{BC} resulted of the mass balance in the *Scv3*.

Another way of presenting Eq. 15, which will be used further, is

$$Q_1 = \Im_{12_{Svc1}}\left(p_2 - p_1\right) + \Im_{13_{Svc1}}\left(p_3 - p_1\right) \tag{16}$$

where

$$\Im_{12_{Svc1}} = \lambda_{12}\tau^{12}_{AB\,Svc1} + \lambda_{13}\tau^{12}_{BC\,Svc1} \tag{17a}$$

$$\Im_{13_{Svc1}} = \lambda_{12}\tau^{13}_{AB_{Svc1}} + \lambda_{13}\tau^{13}_{BC_{Svc1}} \tag{17b}$$

3. Considerations about the CVFEM-S procedure

As already mentioned, the CVFEM-S is the application of the general CVFEM ideas to integrate the equations for single phase flows. The same equations are then expanded to treat multiphase flows by simply adding the mobility term (Forsyth, 1990; Fung et al., 1991; Gottardi and Dall´Olio, 1992). These CVFEM-S methods are already available and implemented in some commercial simulators, employing triangular grids (e.g. Quandalle, 1993; Stars User's Guide, 2002). The CVFEM-M, on the other hand, integrates the multiphase flow equations, as already stated. The discretized equations using CVFEM-S are now developed.

The flux term of the transport equation for the single-phase problem is given by

$$\int_V \vec{\nabla}.\left(\overline{\overline{k}}\,\vec{\nabla}p\right)dV = \int_S \overline{\overline{k}}\,\vec{\nabla}p.d\vec{S} \tag{18}$$

where the pressure gradient can be obtained by Eq. 10.

Substituting the expression of $\overline{\overline{k}}$ (Eq. 12), $d\vec{S}$ (Eq. 13), and the gradient of p (Eq. 10) into Eq. (18), this equation becomes

$$\begin{aligned}\int_V \vec{\nabla}.\left(\overline{\overline{k}}\,\vec{\nabla}p\right)dV = {} & \frac{1}{2A}\left[k_{xx}\left(b_1p_1+b_2p_2+b_3p_3\right)+k_{xy}\left(a_1p_1+a_2p_2+a_3p_3\right)\right]\left[b_2\int_S d\eta - b_3\int_S d\xi\right]+ \\ & +\frac{1}{2A}\left[-k_{yx}\left(b_1p_1+b_2p_2+b_3p_3\right)-k_{yy}\left(a_1p_1+a_2p_2+a_3p_3\right)\right]\left[a_3\int_S d\xi - a_2\int_S d\eta\right]\end{aligned} \tag{19}$$

Hence, the discretized balance equation for the sub-control volume 1 in Fig. 3, for example, is given by

$$\int_{Scv1} \vec{\nabla}.\left(\overline{\overline{k}}\,\vec{\nabla}p\right)dV = \frac{1}{4A}\left\{\sum_{i=1}^{3}\left(k_{xx}b_ip_i+k_{xy}a_ip_i\right)\left(b_2+b_3\right)-\sum_{i=1}^{3}\left(k_{yx}b_ip_i+k_{yy}a_ip_i\right)\left(-a_2-a_3\right)\right\} \tag{20}$$

Using the definition of variable a and b given in Eq. 9, one can show that

$$b_1 = -\left(b_2+b_3\right) \qquad \text{and} \qquad a_1 = -\left(a_2+a_3\right) \tag{21}$$

that, when introduced in Eq. 20, results in

$$Q_1 = -\frac{1}{4A}\left\{\sum_{i=1}^{3}\left(k_{xx}b_ip_i+k_{xy}a_ip_i\right)\left(b_1\right)+\sum_{i=1}^{3}\left(k_{yx}b_ip_i+k_{yy}a_ip_i\right)\left(a_1\right)\right\} \tag{22}$$

The above equation can be conveniently written if the same substitution of variables used in Eq. 9 and 10 is performed

$$\begin{aligned}Q_1 = {} & -\frac{1}{4A}\left\{k_{xx}\left[\left(p_2-p_1\right)b_2+\left(p_3-p_1\right)b_3\right]+k_{xy}\left[\left(p_2-p_1\right)a_2+\left(p_3-p_1\right)a_3\right]\right\}b_1+ \\ & -\frac{1}{4A}\left\{k_{yx}\left[\left(p_2-p_1\right)b_2+\left(p_3-p_1\right)b_3\right]+k_{yy}\left[\left(p_2-p_1\right)a_2+\left(p_3-p_1\right)a_3\right]\right\}a_1\end{aligned} \tag{23}$$

and, after collecting terms, we can obtain the equation written in the desired form, namely

$$Q_1 = T_{12}\left(p_2 - p_1\right) + T_{13}\left(p_3 - p_1\right) \tag{24}$$

where

$$T_{ij} = -\left(\frac{k_{xx}\, b_i b_j + k_{xy}\, a_i b_j + k_{yx}\, b_i a_j + k_{yy}\, a_i a_j}{4A}\right) \tag{25}$$

in which the subscripts *i* assumes values 1 and *j* the values 2 and 3, resulting in the coefficients T_{12} and T_{13}, respectively. These terms are often called "transmissibilities" in the literature, denomination considered not appropriated as we shall see in section 5. However, since this denomination is familiar to the readers, it will be still used in this paper.

Similarly, for the other sub-control volumes of Fig. 3,

$$Q_2 = T_{12}\left(p_1 - p_2\right) + T_{23}\left(p_3 - p_2\right) \tag{26}$$

$$Q_3 = T_{13}\left(p_1 - p_3\right) + T_{23}\left(p_2 - p_3\right) \tag{27}$$

After adding the contribution of all triangles that share the same node, the equation for each control volume can be written as

$$V_i \frac{\left(\phi S / B\right)_i^{n+1} - \left(\phi S / B\right)_i^{n}}{\Delta t} = \sum_{j \in \xi_i} T_{ij}^{\,g}\left(p_j - p_i\right) + qV_i \tag{28}$$

where $T_{ij}^{\,g}$ is the global transmissibility between the nodes *i* and *j*, and it represents the contributions of the two elements sharing the same side. When at least one control volume of *i* or *j* is on the external boundary, the global transmissibility is only the transmissibility T_{ij} of the element composed of these nodes. The total control volume *i*, V_i, in turn, was already defined in Eq. 2.

The usual way employed in petroleum reservoir simulation techniques to obtain the discretized equations for multiphase flows is just to use Eq. 28, derived for single phase flows, multiplied by the phase mobility λ_{ij}, evaluated at upstream conditions. The resulting equations are given by

$$Q_1 = \lambda_{12} T_{12}\left(p_2 - p_1\right) + \lambda_{13} T_{13}\left(p_3 - p_1\right) \tag{29}$$

which are correct only for locally orthogonal grids, where the fluxes can be correctly calculated using two grid points. For triangular grids, however, this procedure is not physically supported, since in these grids the fluxes can be correctly calculated only if three nodal values are used (cf Eq. 15), each one being multiplied by two values of mobility. This conclusion was already pointed out by other investigators (Palagi, 1992; Heinemann et al. 2001). Most probably the equations for multiphase flows were obtained in this way to keep the computer code simpler.

4. Comparison between the CVFEM-S and CVFEM-M equations

This section is devoted for pointing out the difference in the equations obtained using the CVFEM-S and CVFEM-M methodologies. The transport equation for the sub-control volume 1 in Fig. 3 is used as example.

Equation 29 represents the mass balance for the sub-control volume 1 according to CVFEM-S. This equation will be compared with Eq. 16, deduced using CVFEM-M for the same sub-control volume. The clear difference between these formulations is that in the CVFEM-S equation there is only one value of mobility multiplying the pressure differences, while in the CVFEM-M, each pressure difference is multiplied by two parameters, as can be seen in the equations below.

$$\text{CVFEM-S:} \qquad Q_1 = \lambda_{12} T_{12} (p_2 - p_1) + \lambda_{13} T_{13} (p_3 - p_1) \tag{30}$$

$$\text{CVFEM-M:} \qquad Q_1 = \left(\lambda_{12} \tau^{12}_{AB\,Svc1} + \lambda_{13} \tau^{12}_{BC\,Svc1}\right)(p_2 - p_1) + \left(\lambda_{12} \tau^{13}_{AB\,Svc1} + \lambda_{13} \tau^{13}_{BC\,Svc1}\right)(p_3 - p_1) \tag{31}$$

However, it is easy to show that

$$T_{12} = \tau^{13}_{AB\,Svc1} + \tau^{13}_{BC\,Svc1} \qquad \text{and} \qquad T_{13} = \tau^{12}_{AB\,Svc1} + \tau^{12}_{BC\,Svc1} \tag{32}$$

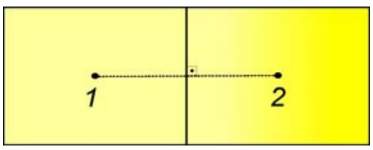
Therefore, if in Eq. 31, the mobility λ_{13}, multiplying $(p_2 - p_1)$, is replaced by the mobility λ_{12}, and if the mobility λ_{12} multiplying $(p_3 - p_1)$ is replaced by the mobility λ_{13}, Eq. 30, is recovered, but requiring $\lambda_{12} = \lambda_{13}$, which only applicable to single phase flows. Therefore, Eq. 30 is not correct for multiphase flows. In some types of problems the results of these two methods may give almost the same results, but there are others where the use of Eq. 30 for multiphase flows increases severely the grid orientation effects. The impact of these differences on practical problems is demonstrated in a companion paper (Cordazzo et al., 2004).

5. Considerations about the negative transmissibilities in CVFEM

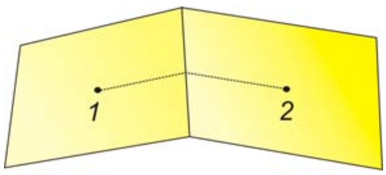
It is often claimed in the literature (Fung et al*.*, 1993; Sonier et al., 1993) that negative transmissibilities arise when triangles with angles greater than 90º are used in the grid. In such cases it is said that this negative transmissibility has no physical meaning and it is recommended not to use a grid with those characteristics. To obey the angular restriction reduces enormously the flexibility of the grid generators and, therefore, is undesirable. It is demonstrated in this work that the negative coefficients which appear in this situation do have physical meaning and, what is more relevant, they no longer can be viewed as transmissibilities. In order to put this issue in clear grounds, some important concepts related to the transmissibilities need to be reviewed. To reach this goal, the transmissibilities in triangular grids are analyzed.

5.1 The interblock transmissibilities

The transmissibility between two blocks 1 and 2, T_{12}, is a widely used concept and its origin can be found in the calculation of the fluxes through the control surfaces in orthogonal structured grids (Heinemann and Brand, 1989; Maliska et al., 2001; Cordazzo et al., 2002), as shown in Fig. 4*a*. By definition, T_{12}, when multiplied by a physical parameter at the interface and by the pressure difference of these two control volumes, gives the total mass flux crossing that interface. As a consequence of the definition, transmissibility is only defined for locally orthogonal grids, as shown in Fig. 4*a*. Nevertheless, this concept is also used even when the total flux through a surface requires the calculation of the gradient in two directions, as in locally non-orthogonal grids, as depicted in Fig. 4*b*. In this case, to use the concept, one of the gradients must be neglected. The remaining term now fits the definition, but the flux calculated is, of course, not the correct one.



(a)



(b)

Figure 4 – Orthogonal *(a)* and *(b)* non-orthogonal control volumes

Most reservoir simulation models use two-point flux approximation for any grid and, therefore they use the concept of transmissibility. Again, it should be stressed that the fluxes are not correctly calculated. In the other hand, using only two grid points in the flux calculation avoids complex stencils and reduces the computational effort, at the expenses of precision, when the grid is not locally orthogonal.

In these schemes, the mass flow-rate of a component between two adjacent grid-blocks *i* and *j* in the discrete form of the conservation equations is given by

$$Q_{ij} = \sum_{p=1}^{P} \left(\lambda_p\right)_{ij} \left(\frac{kA}{h}\right)_{ij} \left(\Phi_j - \Phi_i\right)_P \tag{33}$$

where λ_p is the mobility of phase p, P is the number of phases; k is the absolute permeability; Φ is the phase potential, A_{ij} and h_{ij} are, respectively, an area where the mass flows through and a suitable length for the gradient determination in the surface, both of them determined by the rules of grid construction employed. In Eq. 33, the terms independent of pressure and saturation can be grouped in the form

$$Q_{ij} = T_{ij} \sum_{p=1}^{P} \left(\lambda_p\right)_{ij} \left(\Phi_j - \Phi_i\right)_P \tag{34}$$

where T_{ij} is called transmissibility which is, therefore, defined as

$$\boxed{T_{ij} = k_{ij} \frac{A_{ij}}{h_{ij}}} \tag{35}$$

The transmissibilities depend only on block geometry and permeability, being therefore independent of either pressure, or saturation, or any other variable. They need to be calculated only in the beginning of a simulation if the grid is fixed. Their utilization in field scale problems has several advantages, like the easy numerical representation of geologic faults. For instance, a sealing fault can be modeled simply setting the transmissibility between the two blocks separated by the fault to zero value. Sealing fault constitutes an impermeable linear barrier that will prevent the fluid from flowing in reservoir. The transmissibility concept has been also used in different fields of engineering, for instance the heat transfer (Bejan, 1993).

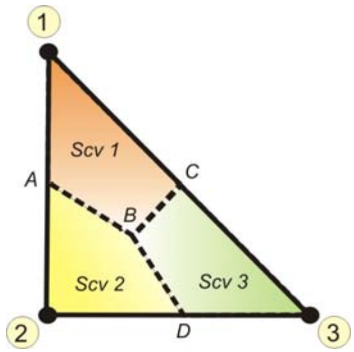


Figure 5 – Triangular element composed of three sub-control volumes (*Scv*)

5.2 The transmissibilities in triangular grids

As already stated, the transmissibility applies when two-point flux approximation schemes are used. For triangular elements, as in non-orthogonal grids, the flow-rate must be calculated using the gradients in two directions (involving three grid points), as discussed in section 2.1. For instance, the mass flow- rate in the interface between the sub-control volumes *1* and *2* in Fig. 5, is given by

$$\underbrace{Q_{12} = \lambda_{12}\left[\tau_{AB\,scv1}^{12}\left(p_2 - p_1\right) + \tau_{AB\,scv1}^{13}\left(p_3 - p_1\right)\right]}_{\text{Mass flow-rate through the face } AB} \tag{36}$$

and the mass flow-rate between the sub-control volumes *1* and *3* is given by

$$Q_{13} = \underbrace{\lambda_{13}\left[\tau^{13}_{BC\,scv1}\left(p_3 - p_1\right) + \tau^{12}_{BC\,scv1}\left(p_2 - p_1\right)\right]}_{\boxed{\text{Mass flow-rate through the face } BC}} \tag{37}$$

Hence, the mass flow-rate through the face *AB* cannot be calculated using only the grid-nodes 1 and 2 and, therefore, τ^{12}_{AB} and τ^{13}_{AB} in Eq. 36, and τ^{13}_{BC} and τ^{12}_{BC} in Eq. 37 are not transmissibilities. If τ^{13}_{AB} in Eq. 36 is neglected, τ^{12}_{AB} may be viewed as a transmissibility but, as in non-orthogonal grids, the mass flow is not correctly calculated. Opposed as to what happens in non-orthogonal grids, in which quasi-orthogonal situations may occur, allowing neglect the cross-derivative term, in regular triangular grid the two terms in Eq. 36 and 37 are always very similar.

The total mass flow-rate through the inner interfaces of the sub-control volume 1 in Fig. 5 can be obtained by summing Eq. 36 and 37. Since the mass fluxes in the areas AB and BC both depend on $(p_2 - p_1)$ and $(p_3 - p_1)$, one can write the total mass flux as

$$Q_1 = \underbrace{\Im_{12_{Svc1}}\left(p_2 - p_1\right)}_{\boxed{\text{This is \textbf{NOT} the mass flow-rate through the face } AB}} + \underbrace{\Im_{13_{Svc1}}\left(p_3 - p_1\right)}_{\boxed{\text{This is \textbf{NOT} the mass flow-rate through the face } BC}} \tag{38}$$

where

$$\Im_{12_{Svc1}} = \lambda_{12}\,\tau^{12}_{AB_{Svc1}} + \lambda_{13}\tau^{12}_{BC_{Svc1}} \qquad \text{and} \qquad \Im_{13_{Svc1}} = \lambda_{12}\,\tau^{13}_{AB_{Svc1}} + \lambda_{13}\,\tau^{13}_{BC_{Svc1}} \tag{39}$$

Writing the total mass flow-rate as in Eq. (38) may lead to the interpretation that the right hand terms are the mass flow rate through face AB and BC, respectively. This induces the definition of transmissibilities $\Im_{12_{Svc1}}$ and $\Im_{13_{Svc1}}$ but, in fact each term mixes up portions of these fluxes in each face. Therefore:

$$\underbrace{\underbrace{\Im_{13_{Svc1}}} \quad \text{and} \quad \underbrace{\Im_{12_{Svc1}}}}_{\boxed{\text{are \textbf{NOT} \textbf{TRANSMISSIBILIDADES !}}}}$$

It is important to note that the above conclusion applies for single as well as multiphase flow, since even in a single-phase case, when the mobility is reduces to unity in Eq. 36 and 37, the fluxes can be correctly calculated only using three grid-points. Therefore, there is no physical impediment for the coefficients in Eq. 38 to be negative. Actually, when using triangles disobeying the angular restriction mentioned claimed in the literature, these negative terms must appear (Cordazzo et al., 2004). The true transmissibility factor, when it applies, is always a positive number. As already mentioned it is not corrected to interpret these negative coefficients as transmissibilities.

After these considerations, therefore, it is clear that the process of deriving the discretized equations based on the single-phase equations and then extending them to multiphase formulations, as done by the CVFEM-S, is wrong. The procedure of adding the mobilities in the discretized equations is not correct because the terms $T_{12}\left(p_2-p_1\right)$ and $T_{13}\left(p_3-p_1\right)$ are not fluxes between the volumes '1 and 2' and '1 and 3', respectively, as already shown.

In order to illustrate the conclusions obtained here, some practical problems are solved in the companion paper (Cordazzo et al., 2004).

3. Conclusions

In this paper several aspects related to the conservative approach of discretizating the equations using triangular grids were addressed. Initially, the process of discretizing the CVFEM-M equations for triangular elements was performed, which consists on the integration of the conservative differential equations considering the existence of more than one phase. Even though the equations for quadrilateral grids are not deduced here, the process of obtaining them is quite similar. It was also shown that this method has several advantages, the most important being the no requirement of any permeability averaging properties, since they are storaged in the center of the elements and the variables in the center of control volumes.

These equations were compared with the ones deduced for the Control Volume Finite Element Method (CVFEM) as it is found in the petroleum literature, called here CVFEM-S. Based on an analysis of the differences between the two methods, we conclude that the procedure used in CVFEM-S is physically not suitable for unstructured grids, though this procedure results in straightforward equations that are easily implemented in existing simulators. The impact of utilizing each one of these methods in several practical cases is discussed elsewhere (Cordazzo et al., 2004).Finally, the concept of transmissibility in structured and unstructured grids was also discussed. It was shown that a physical meaning for the transmissibility only exists when the flux in the volume interfaces is calculated using only two grid-points values. Nevertheless, the transmissibility is, in a number of situations, used in a misleading way, since in that cases the flux is calculated using three or more grid-points values. It was shown that when using triangles disobeying the angular restriction mentioned in the literature, the negative coefficients resulting from the discretization do have physical support, once they are not, in fact, "transmissibilities", as they are often referred.

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