

Generalized Lagrangian Coordinates for Transport and Two-Phase Flows in Heterogeneous Anisotropic Porous Media

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Abstract. We show how Lagrangian coordinates provide an effective representation of how difficult non-linear, hyperbolic transport problems in porous media can be dealt with. Recalling Lagrangian description first, we then derive some basic but remarkable properties useful for the numerical computation of projected transport operators. We furthermore introduce new generalized Lagrangian coordinates with their application to the Darcy–Muskat two-phase flow models. We show how these generalized Lagrangian coordinates can be constructed from the global mass conservation, and that they are related to the existence of a *global* pressure previously defined in the literature about the subject. The whole representation is developed in two or three dimensions for numerical purposes, for isotropic or anisotropic heterogeneous porous media.

Key words: Lagrangian coordinates, global pressure, stream-line/tubes methods, Buckley–Leverett limit, hyperbolic flow.

Nomenclature

Bo	bond number.
Ca	capillary number.
\mathbf{e}_j or \mathbf{e}^j	covariant or contravariant form of base vector of the Lagrangian curvilinear coordinates.
$F(s_2) = \left(1 + \frac{kr_2\mu_1}{kr_1\mu_2}\right)^{-1}$	non linear fractional flow governing the saturation evolution of the Darcy–Muskat model.
\mathbf{g}	euclidean metric tensor.
g_{ij} and g^{ij}	covariant and contravariant form of the Euclidean metric tensor.
\mathbf{G} or \mathbf{g}	dimensional (in $\text{m}\cdot\text{s}^{-2}$) and non-dimensional gravity acceleration.
$G(s_2) = \bar{\mu} \left(\frac{\mu_1}{kr_1} + \frac{\mu_2}{kr_2}\right)^{-1}$	non linear function involved in the saturation evolution of the Darcy–Muskat model.
$-\frac{dp_c}{ds_2}$	
$\underline{\underline{\mathbf{K}}}$ or $\underline{\underline{\mathbf{k}}}$	dimensional (m^2) or non-dimensional permeability tensor fields.

$\tilde{\mathbf{k}}$	non-dimensional permeability tensor fields projected in Lagrangian curvilinear coordinates.
$kr_j, j = 1, 2$	relative permeability of phase j .
$\underline{\mathbf{kr}}$	relative permeability tensor.
$kr_+ = \bar{\mu} \left(\frac{kr_1}{\mu_1} + \frac{kr_2}{\mu_2} \right)$	composed averaged mobility.
$kr_- = \bar{\mu} \left(\frac{kr_2}{\mu_2} - \frac{kr_1}{\mu_1} \right)$	composed differential mobility.
ℓ	permeability correlation length.
μ	viscosity of a single phase fluid.
$\mu_j, j = 1, 2$	viscosity of fluid j .
$\bar{\mu} = \frac{1}{2}(\mu_1 + \mu_2)$	composed viscosity of two phase mixture.
P or p	dimensional (in N.m^{-1}) or non-dimensional pressure field of a single phase fluid flow.
P_j or $p_j, j = 1, 2$	dimensional (in N.m^{-1}) or non-dimensional pressure field associated with phase j .
$P_+ = P_1 + P_2$ or $p_+ = p_1 + p_2$	dimensional (in N.m^{-1}) or non-dimensional pressure sum.
P_+^* or p_+^*	dimensional (in N.m^{-1}) or non-dimensional global pressure.
$P_- = P_2 - P_1$ or $p_- = p_2 - p_1$	dimensional (in N.m^{-1}) or non-dimensional pressure difference.
$P_c(\mathbf{x}, s_2(\mathbf{x}))$ or $p_c(\mathbf{x}, s_2(\mathbf{x}))$	dimensional (in N.m^{-1}) or non-dimensional capillary pressure fields.
ϕ	rock porosity.
Ψ_1 or ψ_1	dimensional (in $\text{m}^2.\text{s}^{-1}$) or non-dimensional stream function in two dimensions.
Ψ_i or $\psi_i, i = 2, 3$	dimensional (in $\text{m}^2.\text{s}^{-1}$) or non dimensional stream functions in three dimensions.
ρ	fluid density (in kg.m^{-3}).
$\rho_+ = \rho_1 + \rho_2$	added fluid density (in kg.m^{-3}).
$\rho_- = \rho_2 - \rho_1$	differential fluid density (in kg.m^{-3}).
s	test scalar field.
$s_j, j = 1, 2$	saturation of phase j .
σ	surface tension between fluid 1 and 2 (in N.m^{-1}).
t	time (in s).
\mathbf{V}	fluid velocity (in m.s^{-1}).
$\mathbf{V}_j, j = 1, 2$	fluid velocity of phase j (in m.s^{-1}).
$\mathbf{V}_+ = \mathbf{V}_1 + \mathbf{V}_2$	global fluid velocity of phases 1 and 2 (in m.s^{-1}).

1. Introduction

As a rule natural geological or man-made industrial porous media are heterogeneous. Complex flows in such media, when involving a coupling between one-phase fluid flow and some scalar transport such as particle transport or thermal field are involved in a wide range of fundamental as well as applied problems. The present work propounds in its first section a detailed presentation of the classical Lagrangian representation, to be used in the computation of accurate transport processes in heterogeneous, anisotropic two or three dimensional porous media. The

main content of this first section is mainly didactic it aims at illustrating the well-known properties of Lagrangian coordinates. Nevertheless part of what is presented in the first section either is a new derivation of scattered current studies or presents by itself new, basic, but remarkable results.

Two-phase flows are also of great interest in the field of hydro-geology, geothermal and petroleum engineering. In these contexts, numerical simulations are increasingly used in forecasting and decision making. Today, the necessity of developing fast and effective numerical methods capable of tackling non-linear multi-phase flow problems of this kind is a growing concern (Mehrabi and Sahimi, 1997; Hansen *et al.*, 1997). Strong numerical difficulties remain extant in the computational simulation of non-linear behavior of two-phase front displacements in heterogeneous porous media (Wooding and Morrel-Seytoux (1976); Homsy (1987)). ‘Stream-line’ approaches were proposed several decades ago (Higgins and Leighton, 1962) to tackle the computation of such two phase flows. These methods, although limited regarding in several respects, have regained popularity in the recent literature (Gliman *et al.*, 1983; Blunt *et al.*, 1996; Bratvedt *et al.*, 1996; Garcia *et al.*, 1998), because of some important improvement in the computation speed, and distinctively small numerical diffusion. The aim of the second part of this study is to propose a unified and rigorous formalism on which these ‘stream-lines’ methods are based as well as to provide some new insights into their generalizations and their applications. We introduce, for the first time (to our knowledge), a generalised Lagrangian physical coordinate system in which the transport equations of the Darcy–Muskat model are rewritten. Then we can state easily the existence of a global pressure, previously introduced in the literature by Chavent (Verruijt and Barends, 1981; Chavent and Jaffré, 1986) with an integral formulation. The mathematical properties of the transport operators in the new system of coordinates are discussed as well as their relevance to numerical implementation. The paper is organized as follows. In the first section, we analyze the Lagrangian coordinate system properties for one-phase flows. The cases of isotropic and anisotropic permeabilities are then dealt with separately. Applications of the proposed formalism are discussed in the case of passive or active dispersion and for pressure diffusion in heterogeneous porous media. The second section of the paper addresses the question of two-phase flows in heterogeneous, anisotropic porous media in the frame of the Darcy–Muskat model. We introduce the global Lagrangian coordinates which extend the analysis of Chavent and Jaffré (1986) and Plouraboué (1998). Thus we can analyze the interesting properties of this coordinate system in the Buckley–Leverett limit where viscosity prevails over capillarity effects. These coordinates enable one to extend stream-lines methods (Higgins and Leighton, 1962; Blunt *et al.*, 1996) to three dimensional flows in the Buckley–Leverett limit. We shall later discuss the use of these coordinates when capillary effects are taken into account.

The methodology is presented formally for two- or three-dimensional media and illustrated numerically with simple examples.

2. One-Phase Flow and Convective Transport

In this section, we introduce and recall Lagrangian coordinates for flows through porous media. We illustrate the use of such coordinates on simple permeability fields solved numerically. Starting with this definition, we then show that the Darcy law imposes a relationship between the permeability field and the geometry of the Lagrangian coordinates through the Euclidean metric tensor. Hence, we illustrate some interesting applications of these coordinates in the case of active and passive transport.

2.1. LAGRANGIAN COORDINATES IN ONE PHASE FLOWS

The Darcy law relating the pressure gradient ∇P to the velocity \mathbf{V} reads:

$$\mathbf{V}(\mathbf{x}) = -\frac{1}{\mu} \underline{\underline{\mathbf{K}}}(\mathbf{x}) \nabla P(\mathbf{x}), \quad (1)$$

where μ is the fluid viscosity and $\underline{\underline{\mathbf{K}}}$ the intrinsic porous media permeability tensor. For the sake of simplicity in the following, the viscosity μ will be fixed to 1. In two dimensions, the velocity field is related to the curl of the stream function $\Psi_1 = (0, 0, \Psi_1)$ by $\mathbf{V}(\mathbf{x}) = \nabla \times \Psi_1$. In three dimensions (Matanga (1993)) the velocity field is related to two orthogonal scalar stream-functions Ψ_2 and Ψ_3 : $\mathbf{V}(\mathbf{x}) = \nabla \Psi_2(\mathbf{x}) \times \nabla \Psi_3(\mathbf{x})$. Hereafter, permeability, pressure, velocity and stream-functions are non-dimensionalized by $\Sigma_{ij} \langle K_{ij} \rangle$, $\langle P \rangle$, $\langle \|\mathbf{V}\| \rangle$ and $\langle \|\Psi_i\| \rangle$ ($i = 1, 2, 3$) respectively where $\langle f \rangle = (1/\Omega) \int_{\Omega} f d\Omega$ and Ω is the volume of the porous medium. In what follows, capital letters refer to non-dimensional variables whereas lower case variables refer to dimensionless variables. Thus p and ψ_i will refer to dimensionless pressure and stream functions.

We deal separately with the case in which the medium is isotropic and with the case in which it is anisotropic.

2.1.1. Isotropic Heterogeneous Permeability

In a heterogeneous isotropic medium, $\underline{\underline{\mathbf{k}}}(\mathbf{x}) = k(\mathbf{x}) \underline{\underline{\mathbf{I}}}$ where $\underline{\underline{\mathbf{I}}}$ is the identity tensor. Due to Darcy's law (1) the mass conservation and incompressibility of the fluid imposes the following relation for the pressure and stream-functions in two dimensions:

$$\operatorname{div} \left(\frac{1}{k} \nabla \psi_1 \right) = \operatorname{div} (k \nabla p) = 0. \quad (2)$$

Stream functions are also determined by similar equations in three dimensions (Zijl, 1986; Matanga, 1993). Different boundary conditions can be applied in order to pose the problem properly (2). As an example, in a square domain, the pressure can be imposed along two opposite sidewalls and be periodic in the other direction. The boundary conditions on stream-function depend on the pressure

field. Hence, the Darcy law has to be applied at the domain frontier. This can be done by imposing a Neumann boundary condition for the stream-function along every wall. Such boundary conditions are illustrated on Figure 1 with a simple one-mode spatial heterogeneity of the permeability field. We numerically compute the pressure p and stream-function ψ_1 and represent their isovalues on a square domain. Comparing Figure 1(a) and 1(b), one can see how the heterogeneity contrast has a drastic influence on the flow field structure. Lagrangian coordinates are thus directly related to the permeability field. Figure 1(c) illustrates the fact that an up-scaled description of a heterogeneous isotropic porous media necessitates a tensorial up-scaled permeability field to describe the coupling between the mean vertical pressure gradient and the mean horizontal flow. Tensorial permeabilities are thus an important issue that we will consider in the following section. As displayed in Figure 1, the iso-pressure lines and stream-lines are orthogonal for isotropic porous media. This orthogonality results from the Darcy relation (1)

$$\nabla \psi_i \cdot \nabla p = 0 \quad \text{for } i = 1, 2, 3. \quad (3)$$

Consequently, (p, ψ_1) and (p, ψ_2, ψ_3) define an orthogonal curvilinear system of coordinates which follows trajectories of passive tracers that would be injected into the flow. It thus defines a Lagrangian system of coordinates which can be built in two or three dimensions. This coordinate system has been numerically computed in Figure 2(a) and 2(b), for the pressure and stream-function fields displayed in Figure 1(a) and 1(b). This computation requires the inversion of the non-linear relation $(p(\mathbf{x}), \psi_1(\mathbf{x}))$, to $(x(p, \psi_1), y(p, \psi_1))$.

Because of the orthogonality of the Lagrangian coordinate system, the associated Euclidean metric tensor $\underline{\underline{\mathbf{g}}}$ is diagonal in the case of isotropic permeability fields. Its contravariant form $\underline{\underline{\mathbf{g}}}^{ij}$ (conventionally with upper suffix) in two dimensions reads

$$g^{11} = \|\nabla p\|^2, \quad g^{22} = \|\nabla \psi_1\|^2, \quad (4)$$

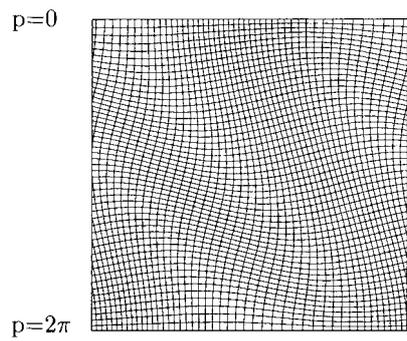
where the first coordinate suffix 1 refers to the pressure coordinate p , and the second suffix 2 to the stream-function ψ_1 . In three dimensions the contravariant Euclidean metric tensor form reads

$$g^{11} = \|\nabla p\|^2, \quad g^{22} = \|\nabla \psi_2\|^2, \quad g^{33} = \|\nabla \psi_3\|^2, \quad (5)$$

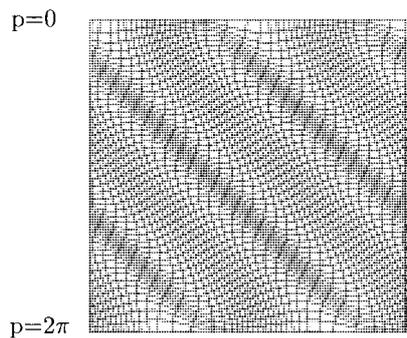
where the first coordinate suffix 1 refers to the pressure p , the second 2 to the stream-function ψ_2 , and the third 3 to ψ_3 . The covariant form of $\underline{\underline{\mathbf{g}}}$ verifies relation

$$g^{ij} g_{jk} = \delta_k^i, \quad (6)$$

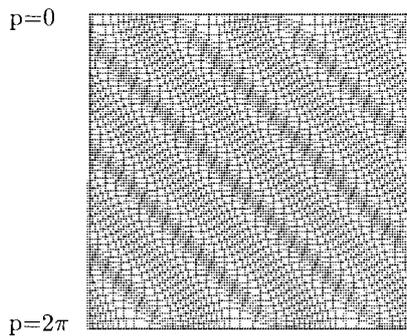
where the conventional sum of repeated indices is used. Using the previous definitions, we next project some interesting transport operators on the Lagrangian coordinates. We first bring out the relationship between the permeability field and



(a)

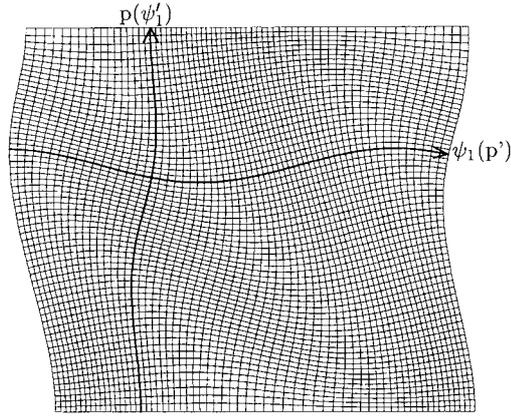


(b)

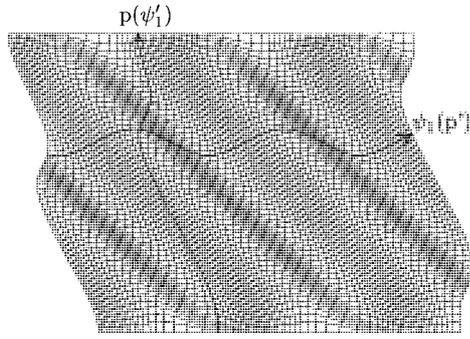


(c)

Figure 1. (a) Isovalues of the numerical solution of the pressure and stream-function in the case of a mono-mode permeability field $k(x, y) = 2.1 + \cos(x + y)$ on two period in each directions. The boundary condition for the pressure is of Diriclet type on the lower and upper walls, equal respectively to 2π and 0 , and periodic on the two other opposite side walls. The boundary conditions are of Neumann type for the stream-function ψ_1 . (b) Same conventions as (a), but for the permeability field $k(x, y) = 1.2 + \cos(x + y)$. (c) Same computation as (a) represented over three periods.



(a)



(b)

Figure 2. (a) Lagrangian coordinates computed from the pressure/stream-function solution of Figure 1(a). We represent in bold two particular sets of coordinates $p(\psi_1')$ and $\psi_1(p')$ which intersect at point $(x(p', \psi_1'), y(p', \psi_1'))$ (b) same convection as (a) from Figure 1(b).

the flow field structure, and thus the Euclidean metric, coming from the Darcy law. The local gradient variations of pressure and stream-functions are directly related to the permeability field heterogeneity. The more heterogeneous the permeability is, the more heterogeneous the lines of constant pressure and stream-function are. This observation has a simple mathematical formulation.

Let us first examine the transformation of the permeability tensor in the Lagrangian coordinates. For isotropic problems, the permeability tensor $\underline{\underline{\tilde{\mathbf{k}}}}$, written in orthogonal Lagrangian coordinates does not change

$$\underline{\underline{\tilde{\mathbf{k}}}} = \underline{\underline{\tilde{\mathbf{k}}}} = \underline{\underline{\mathbf{k}}}. \quad (7)$$

From Darcy's Equation (1), it follows that in two dimensions we have

$$\tilde{k} = k = \frac{\|\nabla\psi_1\|}{\|\nabla p\|} = \sqrt{\frac{g^{22}}{g^{11}}}, \quad (8)$$

and in three dimensions:

$$\tilde{k} = k = \frac{\|\nabla\psi_2\| \|\nabla\psi_3\|}{\|\nabla p\|} = \sqrt{\frac{g^{22}g^{33}}{g^{11}}}. \quad (9)$$

Thus relation (8) is the Darcy law rewritten in the Lagrangian coordinates illustrated on Figures 2(a) and 2(b).

In the case of curvilinear orthogonal systems of coordinates, differential operators such as gradient and divergence can still be used without a tensorial representation. In the case of transport processes in which convection prevails, it is interesting to examine the Lagrangian convective operator D/Dt of a transported quantity s :

$$\frac{Ds}{Dt} = \frac{\partial s}{\partial t} + \mathbf{v} \cdot \nabla s. \quad (10)$$

Because this operator is hyperbolic, it is a source of numerical difficulties (Aziz and Settari, 1979). When it is expressed in the Lagrangian coordinates, the convection transport operator is much more simple. In two dimensions, it reads

$$\frac{Ds}{Dt} = \frac{\partial s}{\partial t} + \|\nabla p\| \|\nabla\psi_1\| \frac{\partial s}{\partial p}, \quad (11)$$

and in three dimensions:

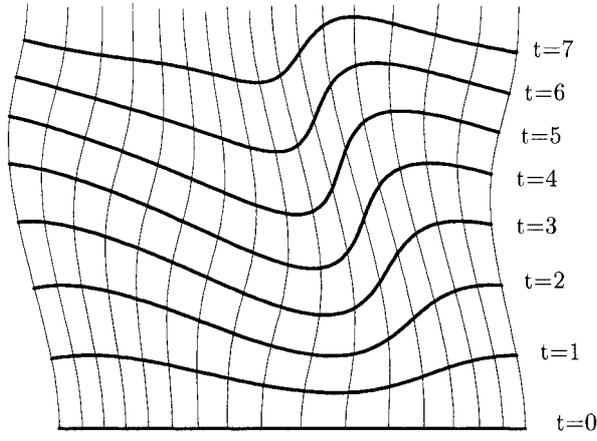
$$\frac{Ds}{Dt} = \frac{\partial s}{\partial t} + \|\nabla p\| \|\nabla\psi_2\| \|\nabla\psi_3\| \frac{\partial s}{\partial p}. \quad (12)$$

We can see that in the two- and three-dimensional cases, this operator is one dimensional in the Lagrangian coordinates, as expected from the construction of the coordinates. To illustrate this basic property, we compute the front position of a purely convected tracer in Figure 3 from the integration of the velocity field along the stream-lines obtained on Figure 2. The front roughness is directly linked with the velocity fluctuations, and hence the permeability field heterogeneities.

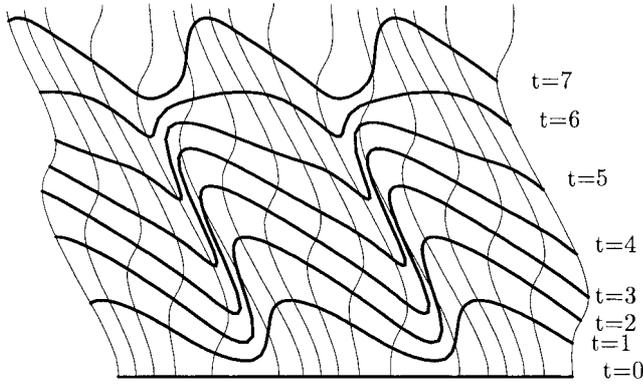
Let us now express the transport operator (2) in the Lagrangian coordinates. In the case of a scalar permeability, it is easy to show that in two dimensions, for any scalar field s we have

$$\text{div}(\tilde{k}\nabla s) = \sqrt{g} \left(\frac{\partial^2 s}{\partial p^2} + \frac{\partial}{\partial \psi_1} \left(\left[\frac{\|\nabla\psi_1\|}{\|\nabla p\|} \right]^2 \frac{\partial s}{\partial \psi_1} \right) \right), \quad (13)$$

$$\text{div} \left(\frac{1}{\tilde{k}} \nabla s \right) = \sqrt{g} \left(\frac{\partial}{\partial p} \left(\left[\frac{\|\nabla p\|}{\|\nabla\psi_1\|} \right]^2 \frac{\partial s}{\partial p} \right) + \frac{\partial^2 s}{\partial \psi_1^2} \right), \quad (14)$$



(a)



(b)

Figure 3. (a) Convection at infinite Péclet number of a tracer front from an horizontal line on the below wall through the heterogeneous permeability field of Figure 1(a). The tracer fronts are displayed with bold lines at different equally spaced times, while stream-lines are represented with thin line. (b) Same convection as (a) from Figure 1(b).

where g is the determinant of the contravariant metric tensor: $g = \det \underline{\underline{\mathbf{g}}}^{ij} = \|\nabla p\|^2 \|\nabla \psi_1\|^2$. Note that these transport operators are homogeneous in one direction. This property is called a partial tensorisation of the transport operator (2) in Lagrangian coordinates. This property remains for the three-dimensional version of the first operator (13)

$$\operatorname{div}(\tilde{k}\nabla s) = \sqrt{g} \left(\frac{\partial^2 s}{\partial p^2} + \frac{\partial}{\partial \psi_2} \left(\left[\frac{\|\nabla \psi_2\|}{\|\nabla p\|} \right]^2 \frac{\partial s}{\partial \psi_2} \right) + \frac{\partial}{\partial \psi_3} \left(\left[\frac{\|\nabla \psi_3\|}{\|\nabla p\|} \right]^2 \frac{\partial s}{\partial \psi_3} \right) \right), \quad (15)$$

where $g = \det \underline{\underline{\mathbf{g}}}^{ij} = \|\nabla p\|^2 \|\nabla \psi_2\|^2 \|\nabla \psi_3\|^2$. However, the three-dimensional version of the operator (14) is not homogeneous and reads

$$\begin{aligned} \operatorname{div} \left(\frac{1}{k} \nabla s \right) &= \sqrt{g} \left(\frac{\partial}{\partial p} \left(\left[\frac{\|\nabla \psi_2\| \|\nabla \psi_3\|}{\|\nabla p\|} \right]^2 \frac{\partial s}{\partial p} \right) + \right. \\ &\quad \left. + \frac{\partial}{\partial \psi_2} \left(\|\nabla \psi_3\|^2 \frac{\partial s}{\partial \psi_2} \right) + \frac{\partial}{\partial \psi_3} \left(\|\nabla \psi_2\|^2 \frac{\partial s}{\partial \psi_3} \right) \right). \end{aligned} \quad (16)$$

To our knowledge, results (13)–(16) are not documented in the literature. Although basic, they are however remarkable, because of their potential numerical and theoretical interest. We discuss in Section 2.2 the use of these properties on the efficiency of numerical computations.

2.1.2. Anisotropic Heterogeneous Permeability

In a case of anisotropic heterogeneous permeability, the pressure and stream-function obey the following partial differential equations in two dimensions

$$\operatorname{div}(\underline{\underline{\mathbf{k}}}^{-1} \nabla \psi_1) = \operatorname{div}(\underline{\underline{\mathbf{k}}} \nabla p) = 0. \quad (17)$$

Similar equations for stream-functions in three dimensions can be found (Zijl, 1986). These equations with the proper boundary conditions define a curvilinear non-orthogonal system of coordinates. There is nevertheless an orthogonality property between the stream-functions gradient and the flux (sometimes called k -orthogonality)

$$\nabla \psi_i \cdot \underline{\underline{\mathbf{k}}} \nabla p = 0 \quad \text{for } i = 1, 2, 3. \quad (18)$$

This relation is less simple than in the isotropic case. Figure 4 displays two examples of pressure/stream-function solutions for a fully tensorial permeability field. The gradients of pressure p and stream-function ψ_1 are not orthogonal as can be observed in the computed Lagrangian coordinates of Figure 5. Another important difference with the isotropic case concerns the permeability tensor $\underline{\underline{\tilde{\mathbf{k}}}}$ in the Lagrangian coordinates which is different from its original expression $\underline{\underline{\mathbf{k}}}$. Note first that its expression can be simplified because $\underline{\underline{\mathbf{k}}}$ is symmetric: $\underline{\underline{\mathbf{k}}}^T = \underline{\underline{\mathbf{k}}}$. Consequently, the transformed tensor $\underline{\underline{\tilde{\mathbf{k}}}}$ is symmetric $\underline{\underline{\tilde{\mathbf{k}}}}^T = \underline{\underline{\tilde{\mathbf{k}}}}$. Moreover, it is easy to show that $\underline{\underline{\tilde{\mathbf{k}}}}$ is diagonal. Let us prove this important property in two dimensions, the extension to the three-dimensional case being obvious.

The non-diagonal coefficients of the permeability tensor are obtained by using the metric tensor of the coordinate change

$$\tilde{k}^{12} = \frac{\partial p}{\partial x} \frac{\partial \psi_1}{\partial x} k^{11} + \frac{\partial p}{\partial y} \frac{\partial \psi_1}{\partial y} k^{22} + k^{12} \left(\frac{\partial p}{\partial x} \frac{\partial \psi_1}{\partial y} + \frac{\partial p}{\partial y} \frac{\partial \psi_1}{\partial x} \right). \quad (19)$$

The right hand side of this relation is exactly identical to relation (18) in two dimensions so that $\tilde{k}^{12} = 0$ and $\tilde{k}^{21} = 0$. The covariant form of the permeability

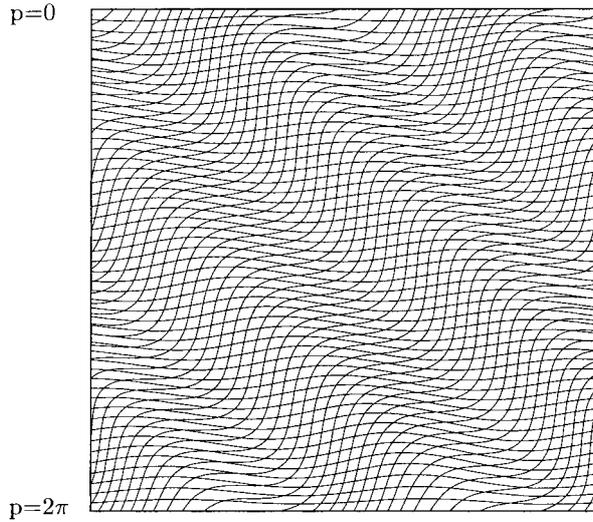


Figure 4. Same computation as Figure 1 but in the case of a full tensorial permeability field, $k^{11}(x, y) = 2.1 + \cos(x + y)$, $k^{12} = 1 = k^{21}$, $k^{22}(x, y) = 2.1 + \cos(2(x + y))$. One can clearly observe the non-orthogonality of the pressure and stream-function.

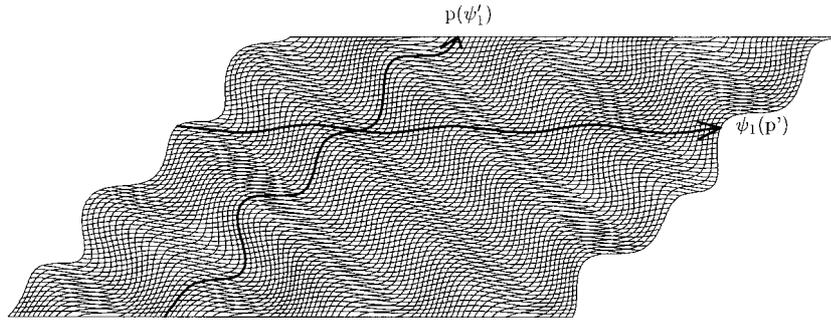


Figure 5. Lagrangian coordinates computed from Figure 4.

tensor is thus diagonal and reads

$$\begin{aligned}\tilde{k}^{11} &= \left(\frac{\partial p}{\partial x}\right)^2 k^{11} + \left(\frac{\partial p}{\partial y}\right)^2 k^{22} + 2\frac{\partial p}{\partial x}\frac{\partial p}{\partial y}k^{12}, \\ \tilde{k}^{22} &= \left(\frac{\partial \psi_1}{\partial x}\right)^2 k^{11} + \left(\frac{\partial \psi_1}{\partial y}\right)^2 k^{22} + 2\frac{\partial \psi_1}{\partial x}\frac{\partial \psi_1}{\partial y}k^{12}.\end{aligned}\quad (20)$$

This remarkable property holds in the three-dimensional case provided that $\underline{\mathbf{k}}$ is symmetrical. This result was already differently derived in (Edwards *et al.*, 1998) in two dimensions.

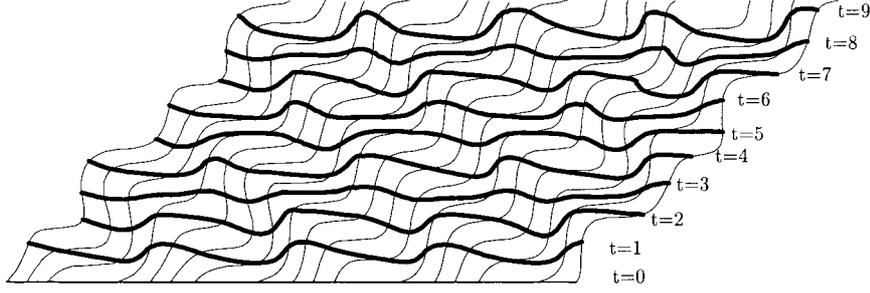


Figure 6. Same computation as in Figure 3 for convection at infinite Péclet number in the full tensorial permeability field of Figure 4 on Lagrangian coordinates computed in Figure 5.

Recall that in the isotropic case, the metric is diagonal. This does not hold in the anisotropic case where in two dimensions the contravariant form of the metric tensor reads

$$\underline{\underline{g}}^{ij} \equiv \begin{pmatrix} \nabla p^2 & \nabla p \cdot \nabla \psi_1 \\ \nabla p \cdot \nabla \psi_1 & \nabla \psi_1^2 \end{pmatrix}. \quad (21)$$

In three dimensions, the stream-function gradients can be chosen orthogonal and the covariant form of the metric tensor becomes

$$\underline{\underline{g}}^{ij} \equiv \begin{pmatrix} \nabla p^2 & \nabla p \cdot \nabla \psi_2 & \nabla p \cdot \nabla \psi_3 \\ \nabla p \cdot \nabla \psi_2 & \nabla \psi_2^2 & 0 \\ \nabla p \cdot \nabla \psi_3 & 0 & \nabla \psi_3^2 \end{pmatrix}. \quad (22)$$

The Lagrangian coordinate system is defined by two sets of mutually orthogonal vectors (\mathbf{e}_i) and (\mathbf{e}^i): ($\mathbf{e}_i \cdot \mathbf{e}^j$) = δ_i^j . The contravariant bases are defined by ($\mathbf{e}^1 = \nabla p$, $\mathbf{e}^2 = \nabla \psi_1$) and ($\mathbf{e}^1 = \nabla p$, $\mathbf{e}^2 = \nabla \psi_2$, $\mathbf{e}^3 = \nabla \psi_3$) in two and three dimensions, respectively. As we did when dealing with the isotropic case, we turn to the expression of the convective transport operator (10) in the Lagrangian coordinates. Using the tensorial notation, it reads

$$\frac{Ds}{Dt} = \frac{\partial s}{\partial t} + \mathbf{v} \cdot (\underline{\underline{g}}^{ij} \partial_j s) = \frac{\partial s}{\partial t} + \mathbf{v} \cdot (\mathbf{e}^i \partial_i s). \quad (23)$$

In two dimensions the velocity is orthogonal to the stream-function gradient: $\mathbf{v} = \mathbf{e}^1$ ($\|\mathbf{e}^2\|/\|\mathbf{e}^1\|$) so that Equation (23) becomes

$$\frac{Ds}{Dt} = \frac{\partial s}{\partial t} + \frac{\|\nabla \psi_1\|}{\sqrt{g_{11}}} \frac{\partial s}{\partial p}. \quad (24)$$

This property has a simple physical interpretation, since, even if isobar lines are no more orthogonal with stream-lines, stream-lines remain the convection trajectory by definition. This is illustrated in Figure 6 in the case of two fully tensorial permeability fields.

In three dimensions we have: $\mathbf{v} = \mathbf{e}^2 \times \mathbf{e}^3 = \mathbf{e}_1(\|\mathbf{e}^2\|\|\mathbf{e}^3\|/\|\mathbf{e}_1\|)$. Equation (23) becomes

$$\frac{Ds}{Dt} = \frac{\partial s}{\partial t} + \frac{\|\nabla\psi_2\|\|\nabla\psi_3\|}{\sqrt{g_{11}}} \frac{\partial s}{\partial p}. \quad (25)$$

An important advantage of the coordinate change is that in both the two- and three-dimensional cases, the convection operator is one dimensional. Moreover the transport tensorial Equation (13) reads in two dimensions

$$\sqrt{g}\partial_l(\underline{\underline{\tilde{\mathbf{k}}}}^{li}\partial_{i}s) = \sqrt{g}\left(\frac{\partial}{\partial p}\left(\frac{\tilde{k}^{11}}{\sqrt{g}}\frac{\partial s}{\partial p}\right) + \frac{\partial}{\partial\psi_1}\left(\frac{\tilde{k}^{22}}{\sqrt{g}}\frac{\partial s}{\partial\psi_1}\right)\right), \quad (26)$$

where g is the determinant of the contravariant metric tensor: $g = \det\underline{\underline{\mathbf{g}}}^{ij}$. In three dimensions it becomes

$$\begin{aligned} \sqrt{g}\partial_l(\underline{\underline{\tilde{\mathbf{k}}}}^{li}\partial_{i}s) = & \sqrt{g}\left(\frac{\partial}{\partial p}\left(\frac{\tilde{k}^{11}}{\sqrt{g}}\frac{\partial s}{\partial p}\right) + \frac{\partial}{\partial\psi_2}\left(\frac{\tilde{k}^{22}}{\sqrt{g}}\frac{\partial s}{\partial\psi_2}\right) + \right. \\ & \left. + \frac{\partial}{\partial\psi_3}\left(\frac{\tilde{k}^{33}}{\sqrt{g}}\frac{\partial s}{\partial\psi_3}\right)\right). \end{aligned} \quad (27)$$

Thus $\underline{\underline{\tilde{\mathbf{k}}}}^{ij}$ acts as an effective diagonal permeability tensor for the heterogeneous transport equations written in the Lagrangian coordinates. This important property, may be exploited in the numerical computation of transport with a tensorial permeability (Edwards *et al.*, 1998) as will be discussed in the next section.

2.2. APPLICATION TO PASSIVE OR ACTIVE TRANSPORT PROCESSES

In the case of passive scalar transport, diffusion and convection play antagonist roles according to the permeability heterogeneity. Convection enhances heterogeneity by a non-local integration of the velocity field fluctuations, while diffusion tends to erase the specific permeability field structure. When convection prevails over diffusion, the specific structure of the permeability field can thus influence transport.

As indicated in the last subsection, the convection operator (10) is one dimensional in the Lagrangian coordinates for both isotropic and anisotropic media. In the limit of infinite Péclet numbers, this property enables one to compute the dispersion curves in an efficient and accurate way and a straightforward parallelization of the dispersion convective process can be applied. Figure 3(a) shows the tracer front computed from the Lagrangian coordinates of Figure 2(a). In the non-infinite Péclet number limit, the coordinate system can be effectively used to solve the hyperbolic transport equation, which is a source of numerical difficulties in heterogeneous media (Saad *et al.*, 1990).

Active transport can also be very precisely and effectively computed in the Lagrangian coordinates (Cirpka and Kitanidis, 2000). Particles deposited or re-convected

depending on the local values of the velocity field are of interest in numerous applications (Gruesbeck and Collins, 1982; Dowel-Boyer *et al.*, 1986). The typical size of these particles is generally large enough to make their diffusion weak so that the Péclet number is large. Hence, the particle motion is governed by a convection equation of type (10) which makes the Lagrangian coordinate projection useful. The local permeability $k(\mathbf{x}, \mathbf{t})$ is an autonomous function on the time t and depends on the concentration of particles: $k(\mathbf{x}, \mathbf{t}) \equiv k(\mathbf{x}, s(\mathbf{x}, \mathbf{t}))$. Such formulation although commonly used in practical applications — for example in crystallization process (Yeum *et al.*, 1989; Beckermann *et al.* 1988) or dissolution (Fredd *et al.*, 1998) — is not obvious. The chosen function $k(\mathbf{x}, s(\mathbf{x}, \mathbf{t}))$ describes phenomenologically the complex micro-structural coupling between geometry modification and mass flow, particles or solute, at the pore scale. Nevertheless, this modification occurs at a time scale much larger than the typical convection through a pore. In this context of time decoupling, such formulation can be theoretically justified and some explicit computation can be done on particular geometries, for example, in the context of solidification in mushy zones (Goyeau, 1999). Hence in the quasi-steady-state limit commonly used (Gruesbeck, 1982; Dowell-Boyer, *et al.*, 1986), the transport Equation (2) is time dependent through the concentration $s(t)$ which depends on the Darcy flux \mathbf{v} . In this situation, we may take advantage of the projection of the transport equation onto the Lagrangian coordinates in order to solve the problem numerically.

The numerical procedure implies computing the pressure and the stream function at instant t using $k(\mathbf{x}, s(\mathbf{x}, \mathbf{t}))$ and then to integrate the transport equation along the obtained streamlines to get $s(t + \Delta t)$. The easy computation of the convective part of this problem, is not the only advantage of Lagrangian coordinates. The new Lagrangian coordinates at instant $t + \Delta t$ has to be found. One straightforward method is to compute the new Lagrangian coordinates by means of an iterative linear solver, since $(p(t + \Delta t), \psi(t + \Delta t))$ are close to $(p(t), \psi(t))$. An alternative method consists in using the fact that the operators (13) and (15,16) are tensorized in the p direction. To be more precise, the operator (2) at instant $t + \Delta t$ can be approached by using a Taylor expansion of the same operator at the instant t :

$$\begin{aligned}
& \text{div}(k(t + \Delta t)\nabla p(t + \Delta t)) \\
&= \text{div}(k(t)\nabla p(t + \Delta t)) + \text{div}(\delta k \nabla F^l[p(t)]) + O(\Delta t^{l+1}) \\
&= \sqrt{g} \left(\frac{\partial^2 p(t + \Delta t)}{\partial p(t)^2} + \frac{\partial}{\partial \psi_1(t)} \left(\left[\frac{\|\nabla \psi_1(t)\|}{\|\nabla p(t)\|} \right]^2 \frac{\partial p(t + \Delta t)}{\partial \psi_1} \right) \right) + \\
& \quad + \text{div}(\delta k \nabla F^l[p(t)]) + O(\Delta t^{l+1}), \tag{28}
\end{aligned}$$

where $\delta k = k(t + \Delta t) - k(t)$ and $F^l[p(t)]$ is l th order Taylor expansion of $p(t + \Delta t)$. Hence, the pressure and stream-functions coordinates at instant $t + \Delta t$ are solved on the coordinate system made of the Lagrangian coordinates at instant t . Due to the fact that the dependence of the pressure $p(t + \Delta t)$ on $p(t)$ is dissociated from its dependence on $\psi(t)$, the computation of $p(t + \Delta t)$ can be achieved by means of a

partial diagonalization method (Higgins and Leighton, 1962; Haidvogel and Zang, 1979) in the p direction. The main interest of this method is that it does not require the computation and inversion of a matrix whose size would be $N_p \times N_{\psi_1}$ in two-dimensions where N_p and N_{ψ_1} are the numbers of unknowns in each directions. Such a method should be particularly effective in three dimensions (Higgins and Leighton, 1962).

The same method can be set forth in the case of other complex transports such as dissolution and re-precipitation (Cussler, 1982). Another interesting application of the effective solving scheme (28) is the Theis formulation of the pressure diffusion problem. The pressure measurement in well tests is a powerful and popular tool in the characterization of well logs permeability field (de Swaan, 1976). The measure of the pressure variations δp in time around an imposed pressure reference P_{ref} provides information on the effective permeability field. When linearizing the compressible effects of the fluid filling the porous media, the pressure evolution can be described by the following equation:

$$\alpha_{P_{\text{ref}}} \frac{\partial P}{\partial t} = -\text{div}(k \nabla p), \quad (29)$$

where $\alpha_{P_{\text{ref}}} = 1/\rho[\partial\rho\phi/\partial P]_{P_{\text{ref}}}$ involves the derivatives of the fluid density ρ and porosity ϕ product $\rho\phi$ evaluated at the pressure reference P_{ref} . The transformation of the right hand side of equation (29) in the Lagrangian coordinates operator (13) can thus be applied to the resolution of equation (29) with a efficient partially diagonalization method.

In the case of anisotropic media, the transport operators (17) are heterogeneous in all directions. Nevertheless, the transformed permeability tensor is diagonal in the Lagrangian coordinates. *A priori* this property cannot be used in order to improve the numerical procedure but can be helpful to overcome numerical difficulties encountered in the calculus of pressure field in a full tensorial permeability field (Yanosik and McCracken, 1979; Durlofsky, 1991; Edwards and Rogers, 1994). Tensorial permeability field permits, with finite volume discretization, to gain much precision in the numerical calculus. Hence in Lagrangian coordinates, scheme order can be lowered with the same accuracy as the Cartesian resolution (Edwards *et al.*, 1998). This property could prove to be very useful in the numerical computation of flows in complex anisotropic reservoirs.

3. Two-Phase Flow

Two-phase flows in porous media averaged over the pore scale are described by the generalized Darcy relation

$$\mathbf{V}_j(\mathbf{x}) = -\frac{\underline{\underline{\mathbf{K}}}(\mathbf{x})kr_j}{\mu_j}(\nabla P_j(\mathbf{x}) - \rho_j\mathbf{G}), \quad \text{with } j = 1, 2, \quad (30)$$

where P_j , \mathbf{V}_j and μ_j are the pressure, velocity and viscosity of the phase j respectively and \mathbf{G} is the gravity field. $\underline{\underline{\mathbf{K}}}$ is the intrinsic porous media permeability tensor,

k_{rj} and ρ_j are relative permeability and density of the phase j . In agreement with Muskat (1948), we have

$$kr_j \equiv kr_j(s_j), \quad (31)$$

where s_j is the saturation of the phase j , with $s_1 + s_2 = 1$ and kr_j are the diagonal components of the relative permeability tensor. In what follows we will consider, to simplify the issue, the second phase saturation s_2 . We will refer to Equations (30) and (31) as the Darcy–Muskat (DM) model for two phase flows in porous media. Over the last decades, many authors have proposed (and sometimes demonstrated) a full tensorial extension of the relative permeability concept (De Gennes, 1983; S. Whitaker, 1986; Kalaydjian and Legait, 1988; Bear and Bachmat, 1991; Liang and Lohrenz, 1994; Dullien and Dong, 1996; Lasseux *et al.*, 1996).

In the present section, we first introduce the main hypothesis and the dimensionless variables. Next we examine the diagonal generalized two-phase flow model (30) in which there is no direct coupling between the pressure gradient and the flux of each phase. Finally we turn to the case of a full tensorial relative permeability which will prove to be an easy generalization of the diagonal case.

3.1. DIMENSIONLESS VARIABLES

On a geological scale, intrinsic permeability as well as wettability heterogeneities of porous rocks on the scale of the elementary representative volume are crucial parameters which influence the macroscopic properties. The coupling between the phase saturation and the pressure difference between the phases is described by the phenomenological capillary pressure curve

$$P_-(\mathbf{x}, s_2(\mathbf{x})) = P_2(\mathbf{x}) - P_1(\mathbf{x}) = P_c(\mathbf{x}, s_2(\mathbf{x})). \quad (32)$$

Although this relation is history-dependent, we assume (as is usually done in many applications) that the pressure difference between the phases is a single valued function of the saturation. This assumption is correct for a single run along the hysteresis curve such as single drainage or imbibition process. In the context of reservoir simulations, such approximations are commonly used (Aziz and Settari, 1979; Chavent and Jaffré, 1986).

The (DM) model can be formulated in condensed form by means of the *global stream-function* (Higgins and Leighton, 1962; Glimm *et al.*, 1983; Blunt *et al.*, 1996). Since the total flux is divergence free for incompressible flows, a global stream-function can be defined in two dimensions as $\mathbf{V}_+(\mathbf{x}) = \mathbf{V}_1 + \mathbf{V}_2 = \nabla \times \Psi_{1+}(\mathbf{x})$. The three dimensional version of this definition is $\mathbf{V}_+ = \nabla \Psi_{2+} \times \nabla \Psi_{3+}$. The global velocity \mathbf{V}_+ , stream-functions Ψ_{i+} ($i = 1, 2, 3$), the pressure sum $P_+ = P_1 + P_2$ and the gravity are non-dimensionalized by $\langle \|\mathbf{V}_+\| \rangle$, $\langle \Psi_{i+} \rangle$, $\langle P_+ \rangle$ and $|\mathbf{G}|$, respectively. For our purpose, we also define the viscosity mean $\bar{\mu} = (\mu_1 + \mu_2)/2$, the composed densities $\rho_+ = \rho_1 + \rho_2$ and $\rho_- = \rho_2 - \rho_1$ and the non-dimensionalized composed mobilities

$$kr_+ = \bar{\mu} \left(\frac{kr_1}{\mu_1} + \frac{kr_2}{\mu_2} \right) \quad \text{and} \quad kr_- = \bar{\mu} \left(\frac{kr_2}{\mu_2} - \frac{kr_1}{\mu_1} \right).$$

Following Leverett (Leverett, 1940; Bear and Bachmat, 1991), we introduce the dimensionless capillary pressure $p_-(\mathbf{x}, s_2) = \sqrt{\langle K \rangle} P_-(\mathbf{x}, s_2) / \sigma$ where σ is the interfacial tension between the phases and $\langle K \rangle$ the averaged permeability. We define a capillary number $\text{Ca} = (\bar{\mu} \langle V_+ \rangle / \sigma) (\ell / \sqrt{\langle K \rangle})$ constructed from the averaged Darcy flux $\langle \|\mathbf{V}_+\| \rangle$, the mean viscosity $\bar{\mu}$, the ratio between the typical correlation length of the heterogeneity ℓ and at typical pore size $\sqrt{\langle K \rangle}$. This dimensionless number is a measure of the capillary forces on the scale of one elementary representative volume. The Bond number $\text{Bo} = \rho_- G \langle K \rangle^2 / \sigma$ estimates the ratio between gravity and capillarity forces.

3.2. DARCY–MUSKAT MODEL WITH SCALAR PERMEABILITY $\underline{\mathbf{k}} = k \underline{\mathbf{I}}$

Relation (30) can be rewritten with the previously defined variables

$$\frac{1}{K(\mathbf{x})kr_+} \mathbf{V}_+(\mathbf{x}) = -\frac{1}{2\bar{\mu}} \left(\nabla P_+(\mathbf{x}) + \frac{kr_-}{kr_+} \nabla P_-(\mathbf{x}, s_2) - \left(\rho_+ + \rho_- \frac{kr_-}{kr_+} \right) \mathbf{G} \right). \quad (33)$$

We define the global pressure ∇P_+^* (Verruijt and Barends, 1981; Chavent and Jaffré, 1986; Plouraboué, 1998) by

$$\nabla P_+^* = \frac{1}{2} \left(\nabla P_+(\mathbf{x}) + \frac{kr_-}{kr_+} (s_2) (\nabla P_-(\mathbf{x}) - \nabla_x P_c(\mathbf{x}, s_2)) - \rho_+ \mathbf{G} \right), \quad (34)$$

where

$$\nabla P_- = \nabla_x P_c + \frac{\partial P}{\partial s_2} \nabla s_2. \quad (35)$$

The global pressure P_+^* has to be defined from relation (34) with a gauge condition. The curl of a vectorial field has to be chosen and can be defined from the boundary conditions. Equation (33) can be rewritten in a form similar to that of the Darcy equation between the global stream-function and the global pressure. Inserting the global pressure into Equation (33), the dimensionless version of the resulting equation is

$$\frac{1}{k(\mathbf{x})kr_+} \mathbf{v}_+ + \nabla p_+^* = -\frac{1}{\text{Ca}} \frac{kr_-}{2kr_+} (\nabla_x p_c(\mathbf{x}, s_2) - \text{Bo} \mathbf{g}). \quad (36)$$

The global pressure was first introduced mathematically (Chavent and Jaffré, 1986) to provide a unique variable which takes into account the coupling between the saturation field and the pressure fields. His definition was rather different from the one given here, integrating relation (34) and choosing a specific boundary condition to fix the gauge. The Darcy like structure of relation (36) shows that this variable is

the dual variable of the *global* stream-function, on a *global* Lagrangian coordinates (p_+^*, ψ_{1+}) in two dimensions and $(p_+^*, \psi_{2+}, \psi_{3+})$ in three dimensions. Because the right hand side of relation (36) is not zero, these *global* Lagrangian coordinates are not orthogonal. This new interpretation sheds new light on the existence of a global pressure for two-phase flows, which is the direct consequence of the existence of a global stream-function, coming from the divergence free of the global flux. The evolution of the saturation is governed by a non-linear convection-diffusion equation which is usually (Wooding and Morrel-Seytoux, 1976; Homsy, 1987) written as

$$\frac{\phi}{v_+} \frac{\partial s_2}{\partial t} + \mathbf{v}_+ \cdot \nabla F(s_2) = \frac{1}{\text{Ca}} \text{div} (G(s_2) \nabla s_2), \quad (37)$$

where v_+ is the norm of the velocity, ϕ is the rock porosity and $F(s_2)$, $G(s_2)$ are two dimensionless non-linear functions of the saturation s_2 given by

$$F(s_2) = \frac{1}{\left(1 + \frac{kr_2 \mu_1}{kr_1 \mu_2}\right)}, \quad G(s_2) = \frac{\bar{\mu}}{\left(\frac{\mu_1}{kr_1} + \frac{\mu_2}{kr_2}\right)} \frac{dp_c}{ds_2}. \quad (38)$$

Following the analysis of Section 2.1, Equation (34) implies a coupling between the global stream-functions ψ_{i+} and the saturation. Relation (30) joined to the conservation of mass gives for $i = 1, 2, 3$:

$$\text{div} \left(\frac{\nabla \psi_{1+}(\mathbf{x})}{k(\mathbf{x})kr_+} \right) = -\frac{1}{2\text{Ca}} (\nabla_x p_-(\mathbf{x}, s_2) - \text{Bo} \mathbf{g}) \times \nabla_{s_2}(\mathbf{x}) \frac{d(kr_-/kr_+)}{ds_2}, \quad (39)$$

and:

$$\text{div} (k(\mathbf{x})kr_+ \nabla p_+^*) = -\frac{1}{2\text{Ca}} \text{div} (k(\mathbf{x})kr_- (\nabla_x p_-(\mathbf{x}, s_2) - \text{Bo} \mathbf{g})). \quad (40)$$

Situations in which $\text{Ca} \gg 1$ are realistic at a larger scale than the pore scale. Viscosity effects prevail over the capillary effects, at this scale. Relation (36) shows that the global pressure/stream-functions are not orthogonal. Nevertheless in the high capillary number limit, there is a quasi-orthogonal relation between $\nabla \psi_{i+}$ and ∇p_+^* :

$$\nabla \psi_{i+} \cdot \nabla p_+^* \propto \frac{1}{\text{Ca}} \ll 1 \quad \text{for } i = 1, 2, 3. \quad (41)$$

Now we wish to examine the limit where $\text{Ca} \rightarrow \infty$ which is the Buckley-Leverett limit of the two-phase flow Darcy–Muskat model. This limit constitutes a large scale approximation of the Darcy–Muskat model where the viscous forces prevails over all other forces. It constitutes a convective limit of the two-phase flow equations which is widely used in petroleum engineering. We next introduce an appropriate orthogonal system of coordinates onto which the convective limit of the above transport equations will be projected.

3.3. THE BUCKLEY–LEVERETT LIMIT OF THE (DM) EQUATIONS

In such situations, many numerical analyses have used the stream-function coordinate to study the Darcy–Muskat model in two dimensions (Garcia *et al.*, 1998; Edwards *et al.*, 1998). Some extensions of these methods have been carried out in isotropic three dimensional permeability fields, without an explicit computation of the stream-functions, but using a random walk Lagrangian reconstruction of the stream-lines (Blunt *et al.*, 1996).

In the present section, we show how the formalism presented in Section 2.1 can be used in the study of two-phase flows in porous media in the Buckley–Leverett limit. The orthogonal system of coordinates and the formal analogy between the equations make it possible to do so.

We note with a superscript 0 variables which are solutions of the (DM) model in the limit $\text{Ca} \rightarrow \infty$. We define the dimensionless variables using the notations introduced in the preceding subsection. We thus define the velocity \mathbf{v}_+^0 , stream-functions ψ_{i+}^0 with $i = 1, 2, 3$ and global pressure p_+^{*0} so that equation (36) reads

$$\mathbf{v}_+^0(\mathbf{x}) = -k(\mathbf{x})k_{r+}(s_2^0)\nabla p_+^{*0}(\mathbf{x}), \quad (42)$$

with $\mathbf{v}_+^0 = \nabla \times \psi_{1+}^0$ in two dimensions and $\mathbf{v}_+^0 = \nabla \psi_{2+}^0 \times \nabla \psi_{3+}^0$ in three dimensions. From Equation (42) and the incompressibility constraint of each phase, we have

$$\text{div} \left(\frac{1}{kk_{r+}(s_2^0)} \nabla \psi_{i+}^0 \right) = \text{div} (kk_{r+}(s_2^0) \nabla p_+^{*0}) = 0 \quad \text{for } i = 1, 2, 3. \quad (43)$$

As was previously mentioned, Equation (42) indicates that the global stream functions $\nabla \psi_{i+}^0$ and the global pressure ∇p_+^{*0} are orthogonal. In this limit we can define the associated saturation s_2^0 whose evolution is described by a purely convective equation

$$\frac{\phi}{v_+} \frac{\partial s_2^0}{\partial t} + \mathbf{v}_+^0 \cdot \nabla F(s_2^0) = 0. \quad (44)$$

As already observed in Section 2.1, in the coordinates (p_+^{*0}, ψ_{i+}^0) the non-linear convective operator is one-dimensional. This simplification is one of the major reasons for the popularity of streamlines methods (Blunt *et al.*, 1996). Nevertheless even when one dimensional, the integration of equation (44) requires a specific numerical treatment with high order numerical schemes (Aziz and Settari, 1979; Douglas and Yrang, 1984; Saad *et al.*, 1990). According to what has been stated in Section 2.1, the transport operator (43) can be rewritten in the Buckley–Leverett coordinates (p_+^{*0}, ψ_{i+}^0) where it is homogeneous in the p_+^{*0} direction. This property can be exploited to simplify the numerical computation of three dimensional problems as mentioned in Section 2.2. In the next subsection, we focus on the influence of finite capillary numbers.

3.4. GENERAL (DM) MODEL WITH LARGE CAPILLARY NUMBERS

Global Lagrangian coordinates can be extended to the general resolution of Equations (37), (39) and (40) in the presence of capillary forces at large capillary numbers. The idea of this section is to compute the real global pressure/stream-function with an iterative procedure, starting from the zero order of the Buckley–Leverett solution. Such an iterative scheme can also be used to take into account some gravity effects coming from a density difference between phases. We illustrate such a procedure on the first correction terms to show explicitly the generalization in the case of non-zero capillarity pressure. We expand the fields in power series of the $1/\text{Ca}$

$$\begin{aligned} \mathbf{v}_+ &= \mathbf{v}_+^0 + \frac{1}{\text{Ca}} \mathbf{v}_+^1 + \dots, \\ s_2 &= s_2^0 + \frac{1}{\text{Ca}} s_2^1 + \dots, \\ p_+^* &= p_+^{*0} + \frac{1}{\text{Ca}} p_+^{*1} + \dots, \\ \psi_{i+} &= \psi_{i+}^0 + \frac{1}{\text{Ca}} \psi_{i+}^1 + \dots \quad \text{for } i = 1, 2, 3. \end{aligned} \quad (45)$$

From Equation (45) we write the equation for the perturbation of the saturation s_2^1

$$\frac{\phi}{v_+} \frac{\partial s_2^1}{\partial t} + \mathbf{v}_+^0 \cdot \nabla s_2^1 F''(s_2^0) = -\mathbf{v}_+^1 \cdot \nabla F(s_2^0) + \text{div}(G(s_2^0) \nabla s_2^0), \quad (46)$$

where F'' denotes the second derivative of F relative to s_2 . The left-hand side of Expression (46) is the operator acting on s_2^1 . The right-hand side of Equation (46) does not depend on s_2^1 . Note also that the left-hand side of Equation (46) is one dimensional when it is rewritten in the Buckley–Leverett coordinates (p_+^{*0}, ψ_{i+}^0) . Hence the transport Equation (46) of the saturation correction s_2^1 can be transformed into an hyperbolic one-dimensional equation. The same simplification holds for the first order perturbation of the pressure which verifies:

$$\begin{aligned} \text{div}(k(\mathbf{x})k r_+(s_2^0) \nabla p_+^{*1}) &= -\text{div}(k(\mathbf{x})k r_-(s_2^0) (\nabla_x p_-(\mathbf{x}, s_2^0) + \text{Bo} \mathbf{g})) \\ &\quad -\text{div}(s_2^1 k(\mathbf{x})k r'_+(s_2^0) \nabla p_+^{*0}). \end{aligned} \quad (47)$$

Again, the left-hand side is a transport operator acting on p_+^{*1} and the right-hand side does not depend on p_+^{*1} . The transport operator can be rewritten in the (p_+^{*0}, ψ_{i+}^0) coordinates where it becomes homogeneous in the p_+^{*0} direction. Again, this property can be used to increase the efficiency of the computation of the global pressure correction. The same method can be applied to higher order corrections of pressure and stream-functions.

3.5. TENSOR PERMEABILITY $\underline{\mathbf{k}}$ AND NON DIAGONAL RELATIVE PERMEABILITY $\underline{\mathbf{kr}}$

We are now turning to the case in which the permeability is a tensor, while the relative permeability is a diagonal tensor. Equations (36), (39) and (40) can be easily extended to a tensorial permeability field \mathbf{k} as in Section 2.1

$$\mathbf{k}^{-1}(\mathbf{x})kr_+^{-1}\mathbf{v}_+ = -\nabla p_+^* - \frac{1}{2\text{Ca}} \frac{kr_-}{kr_+} (\nabla_x p_c(\mathbf{x}, s_2) + \text{Bo } \mathbf{g}), \quad (48)$$

and for $i = 1, 2, 3$

$$\begin{aligned} & \text{div}(\mathbf{k}^{-1}(\mathbf{x})kr_+^{-1}\nabla\psi_{i+}(\mathbf{x})) \\ &= -\frac{1}{2\text{Ca}} (\nabla_x p_-(\mathbf{x}, s_2) + \text{Bo } \mathbf{g}) \times \nabla s_2(\mathbf{x}) \frac{d(kr_-/kr_+)}{ds_2}. \end{aligned} \quad (49)$$

In this case, the global Lagrangian coordinates are not orthogonal even in the Buckley–Leverett limit. Instead, at finite capillary numbers, we find

$$\nabla\psi_i \cdot \mathbf{k}kr_+\nabla p_+^* \propto \frac{1}{\text{Ca}} \quad \text{for } i = 1, 2, 3, \quad (50)$$

and in the Buckley–Leverett limit

$$\nabla\psi_i^0 \cdot \mathbf{k}kr_+\nabla p_+^{*0} = 0 \quad \text{for } i = 1, 2, 3. \quad (51)$$

As was previously mentioned, the convection operator is one dimensional in the Buckley–Leverett limit even in the case of anisotropic permeability fields when it is expressed in the Buckley–Leverett Lagrangian coordinates in two or three dimensions. Hence the whole analysis can be used to simplify the numerical computation of the time integration of the hyperbolic equation. The Buckley–Leverett Lagrangian coordinates are also useful for computing the capillary correction to the purely viscous case.

The case of tensorial relative permeability can also be of interest at least from a theoretical point of view. It is difficult to assess its practical interest owing to the lack of experimental results concerning the values of the non-diagonal components of the relative permeability. However the generalization of the above method can be applied with minor changes in the definition of kr_+ and kr_- :

$$\begin{aligned} kr_+ &= \bar{\mu} \left(\frac{kr_1}{\mu_1} + \frac{kr_2}{\mu_1} + \frac{kr_{12}}{\mu_2} + \frac{kr_{21}}{\mu_1} \right), \\ kr_- &= \bar{\mu} \left(-\frac{kr_1}{\mu_1} + \frac{kr_2}{\mu_1} - \frac{kr_{12}}{\mu_2} + \frac{kr_{21}}{\mu_1} \right), \end{aligned} \quad (52)$$

where $\underline{\mathbf{kr}}$ is defined by

$$\underline{\mathbf{kr}} \equiv \begin{pmatrix} kr_{11} & kr_{12} \\ kr_{21} & kr_{22} \end{pmatrix}. \quad (53)$$

4. Conclusion

In this paper, we have presented a systematic examination of the properties of Lagrangian coordinates and their potential usefulness for numerical computation in porous media flows. This formulation, which applies, for the most general heterogeneous porous media in two or three dimensions, has been described in detail in the case of different one-phase flow transport processes, and in the case of the two-phase flow Darcy–Muskat model.

For one-phase flows we have discussed the significance of these coordinates for active transport, which involves a coupling of convection with some complex processes. We also showed the interest of Lagrangian coordinates for the computation of pressure diffusion problems due to a partial tensorisation of transport operator. In the case of an anisotropic symmetric permeability tensor, we showed that the permeability tensor is diagonal in the Lagrangian coordinates system.

For two-phase flows, we have extended the results obtained in (Plouraboué, 1998) to anisotropic permeability fields and to three dimensions. General *global* Lagrangian coordinate provide a new interpretation for the existence of a global pressure for two-phase flows. These coordinates give a rigorous and formal background to ‘stream-line’ methods as well as some new insights into their generalization. In the limit of infinite capillary numbers (Buckley–Leverett limit), the generalized *global* Lagrangian coordinates system is orthogonal. The hyperbolic non-linear convection of the phase saturation is one dimensional along the *global* pressure coordinate. At finite capillary numbers or when it exists a density gradient between phases, the orthogonality does not hold any more. We have proposed a generalization of ‘stream-line’ method via an iterative scheme for finite Capillary numbers and/or with non-zero Bond number. We illustrated such an iterative procedure that takes into account capillary effects.

We hope that these results will provide a new framework for future improvements of Lagrangian numerical simulations in porous media flows.

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