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On the Eulerian–Lagrangian Formulation of Balance Equations in Porous Media

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Received January 1, 1996; accepted February 6, 1997

The article presents a general approach to modeling the transport of extensive quantities in the case of flow of multiple multicomponent fluid phases in a deformable porous medium domain under nonisothermal conditions. The models are written in a modified Eulerian–Lagrangian formulation. In this modified formulation, the *material derivatives* are written in terms of *modified velocities*. These are the velocities at which the various phase and component variables propagate in the domain, along their respective characteristic curves. It is shown that these velocities depend on the heterogeneity of various solid matrix and fluid properties. The advantage of this formulation, with respect to the usually employed Eulerian one, is that *numerical dispersion*, associated with the advective fluxes of extensive quantities, are eliminated. The methodology presented in the article shows how the Eulerian–Lagrangian formulation is written in terms of the relatively small number of *primary* variables of a transport problem. © 1997 John Wiley & Sons, Inc. Numer Methods Partial Differential Eq **13:** 505–530, 1997

Keywords: Porous medium; modeling; transport phenomena; Eulerian–Lagrangian formulation; primary variables; reduced velocities

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Contract grant sponsors: Fund for the Promotion of Research at Technion AID/MERC EC/AVICENNE

CCC 0749-159X/97/050505-26

I. INTRODUCTION

In general, the balance equations that constitute the core of any model of transport of extensive quantities in a porous medium domain are presented in their Eulerian formulation. The same equations can also be presented in their Lagrangian formulation. In most cases, the reason for switching to the Lagrangian formulation stems from a problem associated with the numerical solution of the balance equation. It is well known that the term associated with the advective flux in such an equation produces *numerical dispersion*. On the other hand, numerical dispersion is avoided when the Lagrangian formulation is solved by the *method of characteristics*. Neuman and Sorek [1], Neuman [2], Sorek [3–7], Sorek and Braester [8–9], Konikow and Bredehoeft [10], Baptista [11], and Baptista *et al.* [12], among many others, have developed solutions of the Lagrangian formulation of the balance equation for the mass of a component of a fluid phase. In what follows, we shall extend this formulation to the general case of transport of any extensive quantity, and introduce the concept of an *apparent velocity*, or *modified velocity* of propagation of fluid variables.

A second reason for developing the (equivalent) Lagrangian formulation is that one can follow the evolution of a variable of a fluid phase, or a component of one (e.g., fluid mass density, pressure) along its *characteristic pathline*. The latter is associated with a *characteristic velocity* of the particle (e.g., mass weighted velocity for a mass particle). However, we shall see that the characteristic velocity of propagation of a variable can be obtained from the fluid velocity by taking into account heterogeneity in various solid matrix and fluid properties. By doing so, we obtain the reduced velocities that serve as *characteristic velocities* of propagation of these variables.

The entire discussion will be at the macroscopic level. No special symbol will be used to denote this fact.

II. GENERAL CASE

Consider the transport of an extensive quantity, E, of a fluid phase occupying part of the void space of a porous medium domain. Since we start by focusing attention on a single phase, we shall omit the symbol that denotes this phase. Let S and e denote the saturation of the phase and the density of E within it, respectively.

The Eulerian balance equation of E of a phase within a porous medium domain can be written in the form

$$\frac{\partial(\phi Se)}{\partial t} = -\nabla \cdot [\phi S(e\mathbf{V}^E + \mathbf{J}'^E)] - f^E_{\alpha\to\beta} + \phi S\rho\Gamma^E, \tag{1}$$

where ϕ denotes porosity, $\mathbf{V}^E$ denotes the velocity of the E-continuum, $\mathbf{J}'^E$ denotes the dispersive flux of E, due to variations in e and in $\mathbf{V}^E$ at the microscopic level, $f^E_{\alpha\to\beta}$ denotes the transfer of E from the considered α-phase to all other β-phases across common (microscopic) interphase boundaries, ρ is the mass density of the phase, and Γ^E denotes the rate of growth (= source) of E, per unit mass of the phase.

The Lagrangian form of the same balance is

$$\frac{D_{\mathbf{V}^E}}{Dt}(\phi Se) = -\phi Se\nabla \cdot \mathbf{V}^E + \nabla \cdot \phi S\mathbf{J}'^E - f^E_{\alpha\to\beta} + \phi S\rho\Gamma^E, \tag{2}$$

or

$$\frac{1}{\phi}\frac{D_{\mathbf{v}^E}\phi}{Dt}+\frac{1}{S}\frac{D_{\mathbf{v}^E}S}{Dt}+\frac{1}{e}\frac{D_{\mathbf{v}^E}e}{Dt}=-\nabla\cdot\mathbf{V}^E+\frac{1}{\phi Se}\nabla\cdot\phi S\mathbf{J}'^E-\frac{1}{\phi Se}f^E_{\alpha\to\beta}+\frac{\rho}{e}\Gamma^E, \quad (3)$$

where

$$\frac{D_{\mathbf{v}}(..)}{Dt}\equiv\frac{\partial(..)}{\partial t}+\mathbf{V}\cdot\nabla(..)$$

denotes the *material derivative* of (..) of a particle moving at a velocity $\mathbf{V}$. The material derivative is a way of expressing processes in a continuum. The material derivative of $(..)^E$ of an E-continuum expresses the variation of $(..)^E$ in time as observed by following *fixed* particles of this continuum, identified by their *material coordinates*, say, their points of origin. A description of a process that makes use of the material derivative is also referred to as a *Lagrangian description.*

Since ϕSe expresses the quantity of E per unit volume of porous medium, the l.h.s. of (2) describes how this quantity varies along the curve that describes the movement of the particle that travels at a velocity $\mathbf{V}^E$. This curve is called the *characteristic curve* of the considered particle. Similar interpretations can be given to the terms on the l.h.s. of (3).

Instead of employing the velocity $\mathbf{V}^E$ of the E-continuum, let us express the balances of E, making use of the mass weighted velocity of the phase, $\mathbf{V}$. The difference between the two gives rise to the diffusive flux of E, relative to that of the mass of the phase. At the microscopic level, we define the diffusive flux of E by $\mathbf{j}^E=e(\mathbf{V}^E-\mathbf{V})$. At the macroscopic (averaged) level, we define the *diffusive flux* of E, relative to the (averaged) movement of the mass of the phase, as

$$\mathbf{J}^E=e(\mathbf{V}^E-\mathbf{V}).$$

Note that we have referred to the microscopic and macroscopic levels of description, but have not employed special symbols to distinguish between the two.

Thus, another form of (1) is

$$\frac{\partial}{\partial t}(\phi Se)=-\nabla\cdot[\phi S(e\mathbf{V}+\mathbf{J}^{*E}+\mathbf{J}^E)]-f^E_{\alpha\to\beta}+\phi S\rho\Gamma^E, \quad (4)$$

where $\mathbf{J}^{*E}$ denotes the dispersive flux of E due to variations in e and in $\mathbf{V}$ at the microscopic level, and $\mathbf{J}^E$ denotes the diffusive flux of E, relative to the mass averaged velocity. We often combine the dispersive and diffusive fluxes by introducing the hydrodynamic dispersive flux, $\mathbf{J}^E_h(=\mathbf{J}^{*E}+\mathbf{J}^E)$.

Let us assume, as indeed we find in many cases, that the flux of hydrodynamic dispersion of E can be expressed as a *Fickian-type* expression, i.e., a linear relation to the gradient of e. For example, here

$$\mathbf{J}^{*E}_h=-\mathbf{D}^E_h\cdot\nabla e,\ \text{with}\ \mathbf{D}^E_h=\mathbf{D}^E+\mathcal{D}^E, \quad (5)$$

in which $\mathbf{D}^E$ is the coefficient of dispersion of E, and $\mathcal{D}^E$ is the coefficient of diffusion of E (in a porous medium). We can then rewrite (4) in the form

$$\frac{\partial}{\partial t}(\phi Se)=-\nabla\cdot[\phi S(e\mathbf{V}-\mathbf{D}^E_h\cdot\nabla e)]-f^E_{\alpha\to\beta}+\phi S\rho\Gamma^E. \quad (6)$$

The last equation can be rewritten in an Euler–Lagrange formulation, in the form

$$\frac{1}{\phi}\frac{D_{\mathbf{v}}\phi}{Dt}+\frac{1}{S}\frac{D_{\mathbf{v}}S}{Dt}+\frac{1}{e}\frac{D_{\tilde{\mathbf{v}}}e}{Dt}=-\nabla\cdot\mathbf{V}+\frac{\mathbf{D}^E_h}{e}:(\nabla\nabla e)-\frac{1}{\phi Se}f^E_{\alpha\to\beta}+\frac{\rho}{e}\Gamma^E, \quad (7)$$

where

$$\tilde{\mathbf{V}} = \mathbf{V} - \frac{1}{\phi S}\nabla(\phi S \mathbf{D}_h^E) \tag{8}$$

is a *modified velocity*, due to spatial variations in ϕ, S, and $\mathbf{D}_h^E$, which serves as the *characteristic velocity* for the propagation of e [12], in conjunction with a dispersion gradient, also recognized an ''apparent advective velocity,'' which is sometimes refereed to as ''an additional source term.''

III. MOTIVATION

The Eulerian form of (6) is, usually, rewritten in the Eulerian–Lagrangian (EL) form

$$\frac{D_{\mathbf{v}}}{Dt}(\phi S e) = -\nabla \cdot \mathbf{V} + \frac{1}{\phi S e}\nabla \cdot (\phi S \mathbf{D}_h^E \cdot \nabla e) - \frac{1}{\phi S e} f_{\alpha\to\beta}^E + \frac{\rho}{e}\Gamma^E. \tag{9}$$

The motivation for introducing the modified form (7), which we shall henceforth refer to as a *Modified Eulerian–Lagrangian* form (MEL), is to highlight the role played by the modified velocity, $\tilde{\mathbf{V}}$, defined in (8).

The EL formulation is reported to be effective in overcoming *numerical dispersion* phenomena, when simulating problems that are dominated by advection. In view of (8), it is argued that the second term on the r.h.s. of (8) can play an important role in dictating whether a situation will be advection dominant or not. Note that this influence may occur for governing equations with no reference to $\mathbf{V}$, or even when $\mathbf{V} = 0$. We, thus, suggest that it may be preferable to simulate advection dominated problems by the MEL-formulation, (7), rather than by the EL-formulation, (9).

Moreover, we often implement the EL-formulation on the basis of presuming that advection fluxes are dominant. Such an assumption, however, may not always be justified. It is, therefore, preferable to implement the MEL scheme instead.

IV. PARTICULAR CASES

In order to gain some insight into the meaning of a *modified velocity*, (7), let us consider two examples.

Example 1: Saturated flow in a porous medium domain.

We assume that:

1. Isothermal conditions prevail.
2. The fluid is compressible, with $\rho = \rho(p)$. The fluid's compressibility, β_p^ρ, is defined by

$$\beta_p^\rho = \frac{1}{\rho}\frac{d\rho}{dp}, \beta_p^\rho = \text{ constant.}$$

3. The solid is slightly compressible, so that $\phi = \phi(p)$, with (e.g., [13]) a solid matrix compressibility defined by

$$\alpha = \frac{1}{1-\phi}\frac{d\phi}{dp}, \alpha = \text{ constant.}$$

However, we shall assume that the solid's velocity is much smaller than that of the fluid, i.e., $|\mathbf{V}| \gg |\mathbf{V}_s|$.

4. We neglect the dispersive flux of the total mass of the fluid phase.
5. No mass sources are present.

For this conceptual model, the mass balance equation may be written in the Eulerian-formulation as

$$\frac{\partial \phi\rho}{\partial t} = -\nabla \cdot \phi\rho\mathbf{V}, \tag{10}$$

or in the EL-formulation as

$$\frac{1}{\phi}\frac{D_{\mathbf{v}}\phi}{Dt} + \frac{1}{\rho}\frac{D_{\mathbf{v}}\rho}{Dt} = -\nabla \cdot \mathbf{V}, \tag{11}$$

or, in view of the assumptions listed above, as

$$\frac{D_{\mathbf{v}}p}{Dt} = -\frac{\phi}{S_0}\nabla \cdot \mathbf{V}, \tag{12}$$

where

$$S_0 = \phi\beta_p^\rho + (1-\phi)\alpha$$

is the *specific storativity* of the porous medium. We shall assume that S_0 is constant.

At this point, we focus our attention on the r.h.s. of (11). We continue to assume that, although we are considering a deformable porous medium, $|\mathbf{V}| \gg |\mathbf{V}_s|$, so that Darcy's law takes the form

$$\mathbf{V} = -\frac{\mathbf{k}}{\mu\phi} \cdot (\nabla p + \rho g \nabla z), \tag{13}$$

in which the fluid's dynamic viscosity, μ, is assumed constant, and $\mathbf{k}$ is the permeability.

We can rewrite the r.h.s. of (12) in the form

$$\begin{aligned} -\frac{\phi}{S_0}\nabla \cdot \mathbf{V} &= \frac{\phi}{S_0}\nabla \cdot \left[\frac{\mathbf{k}}{\mu\phi} \cdot (\nabla p + \rho g \nabla z)\right] \\ &= \frac{1}{\mu S_0}[\nabla \mathbf{k} + \rho g \beta_p^\rho (\mathbf{k} \cdot \nabla z)] \cdot \nabla p + \frac{\rho g}{\mu S_0}(\nabla \mathbf{k} \cdot \nabla z) + \frac{1}{\mu S_0}\mathbf{k} : \nabla\nabla p, \end{aligned} \tag{14}$$

in which we have assumed that $|\phi\nabla\mathbf{k}| \gg |\mathbf{k}\nabla\phi|$.

We may, thus, rewrite the mass balance equation in terms of pressure only, in the form

$$\frac{D_{\tilde{\mathbf{v}}}p}{Dt} = \frac{\rho g}{\mu S_0}(\nabla \mathbf{k} \cdot \nabla z) + \frac{1}{\mu S_0}\mathbf{k} : \nabla\nabla p, \tag{15}$$

where

$$\tilde{\mathbf{V}} \equiv \mathbf{V} - \frac{1}{\mu S_0}(\nabla \mathbf{k} + \rho g \beta_p^\rho \mathbf{k} \cdot \nabla z) \tag{16}$$

is the characteristic (= reduced) velocity for changes in fluid pressure. We note that the reduction in velocity is due to the fluid's compressibility, and to the spatial variations in permeability.

Finally, before leaving this example, let us assume that the deformation is such that the solid's velocity cannot be neglected. We note that Darcy's law actually gives the velocity of the fluid relative to the solid, viz.,

$$\mathbf{V} - \mathbf{V}_s \equiv \mathbf{V}_r = -\frac{\mathbf{k}}{\mu\phi} \cdot (\nabla p + \rho g \nabla z). \tag{17}$$

Then, the mass balance equation for the fluid, (10), becomes

$$\begin{aligned}\frac{\partial \phi\rho}{\partial t} &= -\nabla\cdot\phi\rho\mathbf{V} = -\nabla\cdot\phi\rho\mathbf{V}_r - \nabla\cdot\phi\rho\mathbf{V}_s \\ &= -\mathbf{V}\cdot\nabla\phi\rho - \phi\rho\nabla\cdot\mathbf{V}_r - \phi\rho\nabla\cdot\mathbf{V}_s.\end{aligned} \tag{18}$$

From the mass balance of the solid matrix, assuming that ρ_s is constant, we obtain

$$\nabla\cdot\mathbf{V}_s = -\frac{1}{1-\phi}\frac{D_{\mathbf{v}_s}\phi}{Dt} = \alpha\frac{D_{\mathbf{v}_s}p}{Dt}. \tag{19}$$

By inserting (17) and (19) into (18), and rearranging terms, we obtain the fluid's mass balance equation in the MEL-form

$$\frac{D_{\tilde{\mathbf{v}}}p}{Dt} = -\frac{1}{\alpha+\phi\beta_p^\rho}\nabla\cdot\phi\mathbf{V}_r, \tag{20}$$

in which

$$\tilde{\mathbf{V}} \equiv \frac{1}{\alpha+\phi\beta_p^\rho}(\phi\beta_p^\rho\mathbf{V} + \alpha\mathbf{V}_s), \tag{21}$$

or,

$$\frac{D_{\tilde{\mathbf{v}}}p}{Dt} = \frac{1}{\alpha+\phi\beta_p^\rho}\frac{1}{\mu}(\mathbf{k}:\nabla\nabla p + \rho g\nabla\mathbf{k}\cdot\nabla z), \tag{22}$$

in which

$$\tilde{\mathbf{V}} \equiv \mathbf{V} - \frac{1}{\alpha+\phi\beta_p^\rho}\left[\alpha(\mathbf{V}-\mathbf{V}_s) + \frac{1}{\mu}\nabla\mathbf{k} + \rho g\beta_p^\rho\mathbf{k}:\nabla z\right]. \tag{23}$$

We note the effects of (a) the solid's velocity, (b) the heterogeneity in permeability, and (c) gravity, in the fluid's reduced velocity.

Example 2: Transport of a single component in unsaturated flow.
We consider the case of a single γ-component in an ℓ-phase liquid that occupies part of the void space, at saturation S. The same component can also be adsorbed on the solid matrix (s). To eliminate the rate of transfer due to adsorption of the γ-component between the fluid and the solid phases, in the mass balance equation for γ, we write the mass balance equation for the considered component in the porous medium as a whole. With c_ℓ and c_s denoting the concentrations *in the liquid* and on the solid matrix, respectively, and assuming the absence of external sources and sinks, we write this balance equation in the form:

$$\frac{\partial}{\partial t}[\phi S c_\ell + (1-\phi)c_s] = -\nabla\cdot\phi S(c_\ell\mathbf{V} - \mathbf{D}_h\cdot\nabla c_\ell). \tag{24}$$

Assuming that adsorption is governed by a linear equilibrium isotherm,

$$\frac{c_s}{\rho_s} = \mathcal{K}_d c_\ell,$$

in which $\mathcal{K}_d$ is the *partitioning coefficient* (= volume of fluid per unit mass of solid), we rewrite (24) in the form

$$\frac{\partial}{\partial t}[\phi S + (1-\phi)\rho_s\mathcal{K}_d]c_\ell = -\nabla\cdot\phi S(c_\ell\mathbf{V} - \mathbf{D}_h\cdot\nabla c_\ell), \tag{25}$$

or

$$\frac{\partial}{\partial t}(\phi S R_d c_\ell) = -\nabla \cdot \phi S(c_\ell \mathbf{V} - \mathbf{D}_h \cdot \nabla c_\ell), \tag{26}$$

where

$$R_d = 1 + (1-\phi)\rho_s \mathcal{K}_d / \phi S$$

is known as the *retardation factor*.

Noting that $R_d = R_d(\phi, S)$, we have

$$\begin{aligned}\frac{\partial}{\partial t}(\phi S R_d c_\ell) &= \phi S R_d \frac{\partial c_\ell}{\partial t} + S R_d c_\ell \frac{\partial \phi}{\partial t} + \phi R_d c_\ell \frac{\partial S}{\partial t} + \phi S c_\ell \frac{\partial R_d}{\partial t} \\ &= \phi S R_d \frac{\partial c_\ell}{\partial t} + S R_d c_\ell \frac{\partial \phi}{\partial t} + \phi R_d c_\ell \frac{\partial S}{\partial t} \\ &\quad - \rho_s \mathcal{K}_d \phi S c_\ell \left(\frac{1-\phi}{\phi S^2} \frac{\partial S}{\partial t} + \frac{1}{\phi^2 S} \frac{\partial \phi}{\partial t} \right),\end{aligned} \tag{27}$$

and

$$\nabla \cdot [\phi S(\mathbf{D}_h \cdot \nabla c_\ell)] = \nabla(\phi S \mathbf{D}_h) \cdot \nabla c_\ell + \phi S \mathbf{D}_h : (\nabla \nabla c_\ell).$$

We can now rewrite (26) in the Eulerian–Lagrangian formulation, as

$$\frac{1}{c_\ell}\frac{D_{\tilde{\mathbf{v}}} c_\ell}{Dt} + \frac{1}{\phi}\frac{D_{\mathbf{v}}\phi}{Dt} + \frac{1}{S}\frac{D_{\mathbf{v}} S}{Dt} = -\nabla \cdot \mathbf{V} + \frac{\mathbf{D}_h}{c_\ell} : \nabla \nabla c_\ell - \frac{r}{c_\ell}\frac{\partial c_\ell}{\partial t} - \frac{r}{1-\phi}\frac{\partial (1-\phi)}{\partial t}, \tag{28}$$

in which $r = (1-\phi)\rho_b \mathcal{K}_d / \phi S$, and

$$\tilde{\mathbf{V}} \equiv \mathbf{V} - \frac{\nabla(\phi S \mathbf{D}_h)}{\phi S}.$$

We note here the effect of the spatial variations in ϕ, S, and $\mathbf{D}_h$ on the velocity of propagation of the concentration.

A. General Aspects

Although the aforementioned two examples were presented as particular cases, we shall use these examples to address general aspects associated with their specific Eulerian–Lagrangian formulation.

1. Hyperbolic Characteristics

We note that in (14) we differentiate the flux, $\mathbf{k} \cdot \nabla p$, leading to two terms: one associated with $\nabla \mathbf{k}$ and the other with $\nabla \nabla p$. We suggest that the flow equation (Example 1) may be such that $|\nabla \mathbf{k} \cdot \nabla p| \gg |\mathbf{k} : \nabla \nabla p|$ due to a steep gradient in $\mathbf{k}$. Similarly, in the transport equation (Example 2) due to a steep gradient in the hydrodynamic dispersion, we may encounter the case $|\nabla(\phi S \mathbf{D}_h) \cdot \nabla c_\ell| \gg |\phi S \mathbf{D}_h bf : \nabla \nabla c_\ell|$. In both cases the equation becomes *hyperbolic*. The validity of this argument can be demonstrated, for the sake of simplicity and with no affect on the general conclusions, in a 1D case.

Let us consider a problem in which advection dominates. For example, for a 1D case, let the problem be described by a first-order hyperbolic equation in the form

$$\frac{\partial u}{\partial t} + A\frac{\partial u}{\partial x} = f, \tag{29}$$

in which u, A, and f denote a generalized intensive property, a velocity, and a source, respectively.

Consider the case in which transport is due to both advection and diffusion–dispersion. Such a case is described by a parabolic equation in the form

$$\frac{\partial u}{\partial t} + A\frac{\partial u}{\partial x} = B\frac{\partial^2 u}{\partial x^2} + f, \tag{30}$$

in which B denotes a generalized diffusion–dispersion coefficient (e.g., hydrodynamic dispersion).

We note that for a prescribed characteristic length, L_c, the condition $|B| \ll |L_c A|$ will make (30) similar to (29). Furthermore, we may rewrite (30) in the advection–dispersion form

$$\frac{\partial u}{\partial t} + C\frac{\partial u}{\partial x} = \frac{\partial}{\partial x}\left(B\frac{\partial u}{\partial x}\right) + f, \tag{31}$$

where C may be regarded as a kind of velocity that, in view of (30), is related to A and B by

$$C = A + \frac{\partial B}{\partial x}. \tag{32}$$

We note that C is comprised of a velocity component, A (e.g., the phase velocity), and a component resulting from the gradient of the generalized diffusion–dispersion coefficient. The extent to which an advection–dispersion equation is considered hyperbolic (i.e., dominated by advection) is commonly related only to the Peclet number, P_e, which is considered to be a function of the velocity A. However, in view of (31) and (32), we may generalize this definition and write

$$P_e \equiv \frac{L_c C}{B} = \frac{L_c}{B}\left(A + \frac{\partial B}{\partial x}\right). \tag{33}$$

In view of (33), we note that (31) may be dominated by advection also in cases with steep gradients of B, and/or when $A = 0$.

We argue, however, that the hyperbolic characteristic of (31) is not controlled only by P_e. In view of (30), we may construct a valid example for such an argument. Consider the case of $P_e = 0$ (i.e., $C = 0 \Rightarrow A = -\frac{\partial B}{\partial x}$) and $B = B(x)$, such that $|B| \ll |L_c \frac{\partial B}{\partial x}|$. Moreover, the advection–dispersion equation, (33) may be transformed into a pure dispersion equation. To do so, let us multiply (31) by $\lambda(x) \neq 0$, and assume that

$$\lambda\frac{\partial}{\partial x}\left(B\frac{\partial u}{\partial x}\right) - \lambda C\frac{\partial u}{\partial x} = \frac{\partial}{\partial x}\left(B\lambda\frac{\partial u}{\partial x}\right). \tag{34}$$

The equality between both sides of (34) can be ensured if

$$\lambda C = -B\frac{\partial \lambda}{\partial x}, \tag{35}$$

which is solved by

$$\lambda = \lambda_0 \exp\left[-\int_0^x \frac{C(\eta)}{B(\eta)} d\eta\right]. \tag{36}$$

Thus, we may use (36) to rewrite (31) in the form

$$\lambda\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left(B\lambda\frac{\partial u}{\partial x}\right) + \lambda f. \tag{37}$$

We note that (31) and (37) are equivalent. While (31) maybe associated with a high P_e number, (37) with the same characteristics, does not lead to a P_e number, since it does not contain a velocity term. This duality, however, can be resolved by realizing the role of the gradient of B, and using the definition (33) also for equations with $A = 0$.

2. Discontinuity

In what follows, we still address the differentiation of the divergence of, say, the flux $\mathbf{k} \cdot \nabla p$ [or $\frac{\partial}{\partial x}(B\frac{\partial u}{\partial x})$ as in (31)]. In view of a possible discontinuity in $\mathbf{k}$ (or B), such operation may be questionable.

Let us first draw attention to the fact that a discontinuity in B will also condition $\frac{\partial u}{\partial x}$ to be discontinuous. In such a case, u is not differentiable in the classical sense and, instead, we have to use generalized functions, e.g., the Heaviside step function. This conclusion applies also to $\frac{\partial B}{\partial x}$. This is discussed, for example, in Rudin [14], Antosik et al. [15], and Zemanian [16].

A gradient of a discontinuous B will lead to the appearance of a δ-function. We note that in (31), $\frac{\partial B}{\partial x}$ does not appear on the r.h.s. as a coefficient multiplying $\frac{\partial u}{\partial x}$. Instead, it was moved to the l.h.s. of (31), to be associated with a pathline, characteristic, equation. In view of (32) this yields a mathematically well-posed ordinary differential equation (with the δ-function on its r.h.s.), in the form,

$$\frac{dx}{dt} = \frac{\partial B}{\partial x}. \tag{38}$$

Hence, in terms of generalized functions, the conditions of being mathematically well-posed and physically meaningful remain intact, even when $\mathbf{k}$ is discontinuous.

3. Relevance

Differentiating the product $B\frac{\partial u}{\partial x}$ will result in a nondivergence form of the accompanying balance equation, which, in view of the possible physically irrelevance between these factors, may seem questionable.

Nondivergence procedures can be found (e.g., Oran and Boris, [17]; Gyarmati, [18]) in reference to simulating shock waves propagation. In such problems, the fluid mass density, ρ, and its velocity, $\mathbf{V}$, are discontinuous across the shock front. Nevertheless, the divergence (Eulerian formulation) form of its mass balance equation,

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \rho \mathbf{V} = 0,$$

is written in the nondivergence form (Eulerian–Lagrangian formulation):

$$\frac{D_v \rho}{Dt} + \rho \nabla \cdot \mathbf{V} = 0.$$

We further note that transonic flows are often simulated (Miles [19]; Nixon [20]) on the basis of associating the velocity with a potential function, Φ, such that

$$\mathbf{V} = \nabla \Phi.$$

Thus, the analogy, $A = \frac{\partial B}{\partial x}$, with the proposed methodology becomes obvious.

Altogether, both approachs, the divergence and the nondivergence one, are valid for various balance equations. The decision as to which one to use in a particular case depends, for example, on the simulation procedure (Samarsky, [21]; Forsythe and Wasow, [22]).

4. Simulation

The fact that ∇p may be discontinuous does not imply that $\nabla\nabla p$ [or $\frac{\partial^2 u}{\partial x^2}$ as in (30)] cannot be approximated for simulation purposes. As an example, in transonic aerodynamics we simulate the 2D motion equation in terms of a potential, Φ, function, in the form

$$\left[a^2 - \left(\frac{\partial \Phi}{\partial x}\right)^2\right]\frac{\partial^2 \Phi}{\partial x^2} - 2\frac{\partial \Phi}{\partial x}\frac{\partial \Phi}{\partial y}\frac{\partial^2 \Phi}{\partial x \partial y} + \left[a^2 - \left(\frac{\partial \Phi}{\partial y}\right)^2\right]\frac{\partial^2 \Phi}{\partial y^2} = 0,$$

in which a denotes the sound speed, and the terms $\nabla\nabla\Phi$ are approximated, although the velocity, $\mathbf{V}(= \nabla\Phi)$, is discontinuous at the shock front.

Furthermore, following Atkinson [23], both the divergence and the nondivergence formulations may yield the same discretized forms. In view of (31), consider the divergence operator, $\mathcal{L}$, in the form

$$\mathcal{L}u \equiv \frac{\partial}{\partial x}\left(B\frac{\partial u}{\partial x}\right) = 0. \tag{39}$$

The discretization of $\mathcal{L}u$ is known to be robust. An equivalent discrete form to the above divergence operator, $\mathcal{L}$, is

$$\mathcal{D}U \equiv \frac{\partial}{\partial x}(bU_{\bar{x}}) = 0, \tag{40}$$

in which U and b denote the approximate values of u and B, respectively, assigned at an i node of a prescribed grid, and $U_{\bar{x}}$ denotes the approximation for $\frac{\partial u}{\partial x}$. Two valid forms are obtained by differentiating (39) and (40), respectively. These are

$$\mathcal{L}u \equiv \frac{\partial B}{\partial x}\frac{\partial u}{\partial x} + B\frac{\partial^2 u}{\partial x^2} = 0 \tag{41}$$

and

$$\mathcal{D}U \equiv \frac{\partial b}{\partial x}U_{\bar{x}} + b_i\frac{\partial U_{\bar{x}}}{\partial x} = 0. \tag{42}$$

If we choose the b_i terms to be equal to the *central differences* approximation for $B(\equiv B_{i+0.5})$, namely

$$b_i = B_{i+0.5} \equiv (B_i + B_{i+1})/2, \tag{43}$$

then, in view of (43), expressions (41) and (42) become equivalent for a *central differences* approximation. Moreover, it is demonstrated by Samarsky [21] that the *central differences* approximation of (39), for a discontinuous B coefficient, will yield only first-order accuracy. Such may not be the case when approximating (42) by the MEL-formalism.

V. PRIMARY VARIABLES

When we consider a transport problem in a porous medium domain containing multiple multicomponent fluid phases, in a deformable porous medium, we usually have a rather large number of independent variables that together describe the behavior of the system. For example, we need one mass concentration for every component of every phase (including the solid in the case of adsorption), one pressure for every fluid phase, one saturation value for every fluid phase, one

fluid velocity (= density of momentum) for every fluid phase, the velocity of the solid matrix, and a temperature for each phase. To solve for these variables, we have a number of mass (of phases and components), momentum and energy balance equations (in the form of second-order partial differential equations).

However, due to various relationships among the variables, including definitions, constitutive relations and thermodynamic ones, especially, when the system is assumed to be under equilibrium conditions, only a relatively small number of variables are *primary* ones (or *base variables*) for which a solution is required. For every primary variable, a balance equation with appropriate initial and boundary conditions has to be solved. Often, these equations are coupled to each other due to exchange terms and to thermodynamic relations between adjacent phases in equilibrium. All other variables may be derived from the primary ones, by making use of the thermodynamic relationships, the constitutive relations, the definitions, and the remaining balance equations, which now serve as definitions.

In the theory of thermodynamics, *Gibbs phase rule* states that under the assumption of equilibrium among all phases and components, and thermal equilibrium, the number of primary variables (= number of degrees of freedom), NF, for a system of NP phases and NC components, is given by

$$NF = NC - NP + 2.$$

Bear and Nitao [24], following the development of Gibbs phase rule, proposed a *rule for the number of degrees of freedom*, NF (abbreviated NF-rule, or NFR) for a system composed of multiple multicomponent phases in a deformable porous medium, under nonisothermal conditions. They assumed that the system is (1) in thermal equilibrium, i.e., all phases and components have the same temperature) at all times; (2) in chemical equilibrium, i.e., that the chemical potential of a component is the same in all phases; and (3) in mechanical equilibrium, i.e., that the statically derived capillary pressure relations is applicable, or that the system undergoes only slow and small changes, so that it can be assumed to undergo a succession of equilibrium states such that it is always close to equilibrium. Under such conditions, they found that

$$NF = NC + NP + 4.$$

If Darcy's law is used to determine the velocities of the NP fluid phases, NF is reduced by NP.

When the solid matrix is nondeformable, the NF is reduced by 3.

When isothermal conditions prevail, the NF is reduced by 1.

In what follows, we shall make use of this rule under the assumption that equilibrium conditions prevail.

VI. EULER–LAGRANGE FORMULATION IN TERMS OF PRIMARY VARIABLES

We can now combine the discussions presented in the previous sections. Let $a_k, k = 1, 2, \ldots, NF$, denote the NF primary variables of a problem. This means that all the variables of the problem can be expressed in terms of these ones. Actually, it should be noted that primary variables may be introduced into the sets of balance equations and the *holonomic constraints*, but not into *nonholonomic constraints* (i.e., ones that cannot be integrated). We then need to solve NF balance equations.

Thus, if e denotes a typical variable, then $e = e(a_k)$, with a_k as a symbol meaning *all* a_k's. For example, we may have $S = S(a_k)$. However, we may select S itself as a primary variable. In general, model coefficients may also be functions of the a_k's, e.g., $\phi = \phi(a_k), \mathbf{k} = \mathbf{k}(a_k)$.

Let us introduce coefficients defined by

$$\chi_k^e = \frac{1}{e}\frac{\partial e}{\partial a_k} \equiv \frac{\partial \ln e}{\partial a_k}, \text{ e.g., } \chi_k^\phi = \frac{1}{\phi}\frac{\partial \phi}{\partial a_k}, \text{ etc.,} \tag{44}$$

for all model variables and coefficients. We may then write

$$\frac{\partial e}{\partial t} = e\chi_k^e \frac{\partial a_k}{\partial t}, \nabla e = e\chi_k^e \nabla a_k,$$

in which the *summation convention* should be invoked. This means that

$$\chi_k^e \nabla a_k \equiv \sum_{k=1}^{k=NF} \chi_k^e \nabla a_k.$$

We note that the χ's need not be constant; they may depend on the a_k's.

With these relations, we may rewrite (7), which is a typical balance equation in a transport model, in the form

$$\begin{aligned}(\chi_k^\phi + \chi_k^S)\frac{D_{\mathbf{v}} a_k}{Dt} + \chi_k^e \frac{D_{\tilde{\mathbf{v}}_{(k)}} a_k}{Dt} \\ = -\nabla \cdot \mathbf{V} + \mathbf{D}_h^E : [\chi_k^e(\nabla + \chi_m^e \nabla a_m) + \nabla \chi_k^e] \cdot \nabla a_k - \frac{1}{\phi S e} f_{\alpha\to\beta}^E + \frac{\rho}{e}\Gamma^E,\end{aligned} \tag{45}$$

[no summation on subscript (k)], where

$$\tilde{\mathbf{V}}_{(k)} \equiv \mathbf{V} - \nabla \mathbf{D}_h^E - \mathbf{D}_h^E : (\chi_m^S + \chi_m^\phi)\nabla a_m$$

is the reduced velocity, associated with the propagation of the primary variable a_k, along a characteristic pathline. We recall that the summation convention is invoked, so that on the l.h.s. of (45) we sum $2NF$ terms.

We note here, and as a rule, that whenever we have a diffusive flux of an extensive quantity (here E), expressed by a Fickian-type flux law, the velocity of propagation of that extensive quantity is reduced. Part of the reduction stems from the heterogeneity in the coefficient of the diffusive–dispersive flux, D_h^E.

A second form of (45) is

$$(\chi_k^\phi + \chi_k^S + \chi_k^e)\frac{D_{\tilde{\mathbf{v}}_{(k)}} a_k}{Dt} = -\nabla \cdot \mathbf{V} + \chi_k^e \mathbf{D}_h^E : \nabla\nabla a_k - \frac{1}{\phi S e} f_{\alpha\to\beta}^E + \frac{\rho}{e}\Gamma^E, \tag{46}$$

where

$$\tilde{\mathbf{V}}_{(k)} \equiv \mathbf{V} - \mathcal{B}_{(k)}[\nabla \mathbf{D}_h^E + \mathbf{D}_h^E : (\chi_m^S + \chi_m^\phi + \chi_m^e)\nabla a_m] - \mathcal{A}_{(k)} \mathbf{D}_h^E : \nabla \chi_k^e,$$

in which

$$\mathcal{B}_{(k)} = \frac{\chi_k^e}{\chi_k^\phi + \chi_k^S + \chi_k^e}, \mathcal{A}_{(k)} = \frac{1}{\chi_k^\phi + \chi_k^S + \chi_k^e}, \text{ no summation on } k.$$

Let us focus attention on one of the primary variables. As an example, let S be selected as one of the primary variables, with k referring to all NF primary variables, and r referring to the remaining $(NF-1)$ ones, i.e., $e = e(S, a_r), \phi = \phi(S, a_r)$, and

$$\frac{\partial e}{\partial t} = e\chi_S^e \frac{\partial S}{\partial t} + e\chi_r^e \frac{\partial a_r}{\partial t}, \nabla e = e\chi_S^e \nabla S + e\chi_r^e \nabla a_r.$$

We note that

$$\chi_k^e \frac{\partial a_k}{\partial t} = \chi_S^e \frac{\partial S}{\partial t} + \lambda_r^e \frac{\partial a_r}{\partial t}, \chi_k^e \nabla a_k = \chi_S^e \nabla S + \chi_r^e \nabla a_r, \text{ etc.,}$$

and that

$$\chi_r^S = 0, \chi_S^S = \frac{1}{S}.$$

Then, from (46), we obtain the balance equation

$$(\chi_S^\phi + \chi_S^S + \chi_S^e)\frac{D_{\mathbf{V}_{(s)}} S}{Dt} + (\chi_r^\phi + \chi_r^e)\frac{D_{\mathbf{V}_{(r)}} a_r}{Dt}$$
$$= -\nabla \cdot \mathbf{V} + \chi_S^e \mathbf{D}_h^E : \nabla\nabla S + \chi_r^e \mathbf{D}_h^E : \nabla\nabla a_r - \frac{1}{\phi Se} f_{\alpha\to\beta}^E + \frac{\rho}{e}\Gamma^E, \quad (47)$$

where

$$\tilde{\mathbf{V}}_{(S)} \equiv \mathbf{V} - \mathcal{B}_{(S)}[\nabla \mathbf{D}_h^E + \mathbf{D}_h^E : (\chi_S^S + \chi_S^\phi + \chi_S^e)\nabla S] - \mathcal{A}_{(S)} \mathbf{D}_h^E : \nabla \chi_S^e,$$

$$\tilde{\mathbf{V}}_{(r)} \equiv \mathbf{V} - \mathcal{B}_{(r)}[\nabla \mathbf{D}_h^E + \mathbf{D}_h^E : (\chi_r^\phi + \chi_r^e)\nabla a_r$$
$$+ \mathbf{D}_h^E : (\chi_S^S + \chi_S^\phi + 3\chi_S^e)\nabla S] - \mathcal{A}_{(r)} \mathbf{D}_h^E : \nabla \chi_r^e, \quad (48)$$

in which

$$\mathcal{B}_{(S)} = \frac{\chi_S^e}{\chi_S^\phi + \chi_S^S + \chi_S^e}, \mathcal{A}_{(S)} = \frac{1}{\chi_S^\phi + \chi_S^S + \chi_S^e}, \text{ no summation on } S,$$

$$\mathcal{B}_{(r)} = \frac{\chi_r^e}{\chi_r^\phi + \chi_r^e}, \mathcal{A}_{(r)} = \frac{1}{\chi_r^\phi + \chi_r^e}, \text{ no summation on } r.$$

The same equation can be obtained from (7).

Equation (46) constitutes a single equation (= balance equation for E) in the NF primary variables, a_k, of the problem. On the l.h.s. of each such equation we have NF terms, each involving a material derivative of one of the primary variables. Each material derivative is associated with a reduced velocity, $\tilde{\mathbf{V}}_{(k)}$. We have NF such equations, so that we have a complete set, and, in principle, a solution for all a_k's can be obtained. All other variables can be calculated from the primary ones, making use of definitions, thermodynamic relations, the remaining balance equations (which now serve as *definitions*), and constitutive relations.

Finally, we may rewrite (46) in the general form

$$(\chi_k^\phi + \chi_k^S + \chi_k^e)\mathcal{L}_k = RHS^E, k = 1, 2, \ldots, NF, \quad (49)$$

where

$$\mathcal{L}_k \equiv \frac{D_{\tilde{\mathbf{v}}_k} a_k}{Dt}, \quad (50)$$

and RHS^E denotes the r.h.s. of (46).

Each of the NF primary variables is being translated along its own characteristic path defined by

$$\frac{D_{\tilde{\mathbf{v}}_{(k)}}}{Dt}\mathbf{x}^{(k)} = \tilde{\mathbf{V}}_{(k)}, \quad (51)$$

where $\mathbf{x}^{(k)}$ is the spatial location of the particle of the kth primary variable.

Let us assume that the RHS^E's of all NF equations are known. For example, in a numerical model, we may freeze the value of the r.h.s. at the previous time interval. Or, we may assume some initial value, and then update in an iteration process. Then we have a set of NF equations for the NF unknown values, $\mathcal{L}_k$. We assume that all the χ_k^e's are known (although this is not always the case, as the χ_k^e's may depend on the a_k's; iterations may then be required). These equations may then be solved by some simple direct method. Then the value of each a_k can be determined in the considered domain by the method of characteristics, with the reduced velocity, $\tilde{\mathbf{V}}_{(k)}$, along the characteristic path defined by (51), and

$$\frac{D_{\tilde{\mathbf{v}}_{(k)}} a_k}{Dt} = \mathcal{L}_k, k = 1, 2, \ldots, NF. \tag{52}$$

Consider the following example. Let saturation, S, phase pressure, p, and temperature, T, represent three (of the NF) primary variables of a problem. The remaining $NF - 3$ primary variables will be denoted by $a_r, r = 1, 2, \ldots, NF - 3$.

Since we have explicitly introduced here pressure and temperature as primary variables, we may express $\nabla \cdot \mathbf{V}$, appearing on the r.h.s. of (47), in terms of S, p, T, noting that $\rho = \rho(p, T)$. We obtain

$$-\nabla \cdot \mathbf{V} = \frac{1}{\phi\mu}[\rho g \nabla \mathbf{k} : \nabla z + \mathbf{k} : \nabla\nabla p + (\nabla \mathbf{k} + \rho g \beta_p^\rho \mathbf{k} : \nabla z) \cdot \nabla p + \rho g \mathbf{k} \chi_T^\rho \nabla T \cdot \nabla z]. \tag{53}$$

Then, from (46) we obtain

$$\begin{aligned}
&(\chi_p^\phi + \chi_p^e)\frac{D_{\mathbf{v}_{(p)}} p}{Dt} + (\chi_T^\phi + \chi_T^e)\frac{D_{\mathbf{v}_{(T)}} T}{Dt} + (\chi_S^\phi + \chi_S^S + \chi_S^e)\frac{D_{\mathbf{v}_{(S)}} S}{Dt} + (\chi_r^\phi + \chi_r^e)\frac{D_{v_{(r)}} a_r}{Dt} \\
&= \left(\chi_p^e \mathbf{D}_h^E + \frac{\mathbf{k}}{\phi\mu}\right) : \nabla\nabla_p + \chi_p^e \chi_p^\phi \mathbf{D}_h^E : \nabla p \nabla p + \chi_T^e \mathbf{D}_h^E : (\nabla\nabla T + \chi_T^\phi \nabla T \nabla T) \\
&\quad + \chi_S^e \mathbf{D}_h^E : [\nabla\nabla S + (\chi_S^\phi + 1)\nabla S \nabla S] + \chi_r^e \mathbf{D}_h^E : (\nabla\nabla a_r + \chi_r^\phi \nabla\phi\nabla\phi) \\
&\quad + \frac{\rho g}{\phi\mu}\nabla \mathbf{k} : \nabla z - \frac{1}{\phi S e} f_{\alpha\to\beta}^E + \frac{\rho}{e}\Gamma^E,
\end{aligned} \tag{54}$$

where summation is invoked only for r. The various reduced velocities are

$$\begin{aligned}
\tilde{\mathbf{V}}_p = \mathbf{V} - \frac{1}{\chi_p^\phi + \chi_p^e}\mathbf{D}_h^E : [&(\chi_T^\phi \chi_p^e + \chi_p^\phi \chi_T^e)\nabla T + (\chi_S^\phi \chi_p^e + \chi_p^\phi \chi_S^e + \chi_p^e)\nabla S \\
&+ (\chi_r^\phi \chi_p^e + \chi_p^\phi \chi_r^e)\nabla a_r] - \frac{1}{\chi_p^\phi + \chi_p^e}\left[\nabla(\chi_p^e \mathbf{D}_h^E) + \frac{1}{\phi\mu}(\nabla \mathbf{k} + \beta_p^\rho \rho g \mathbf{k} : \nabla z)\right],
\end{aligned}$$

$$\begin{aligned}
\tilde{\mathbf{V}}_T = \mathbf{V} - \frac{1}{\chi_T^\phi + \chi_T^e}\mathbf{D}_h^E : [&(\chi_S^\phi \chi_T^e + \chi_T^\phi \chi_S^e + \chi_T^e)\nabla S + (\chi_r^\phi \chi_r^e + \chi_T^\phi \chi_r^e)\nabla a_r] \\
&- \frac{1}{\chi_T^\phi + \chi_T^e}\left[\nabla(\chi_T^e \mathbf{D}_h^E) + \frac{1}{\phi\mu}(\chi_T^\rho \rho g \mathbf{k} : \nabla z)\right],
\end{aligned}$$

$$\tilde{\mathbf{V}}_S = \mathbf{V} - \frac{1}{\chi_S^S + \chi_S^\phi + \chi_S^e}\mathbf{D}_h^E : (\chi_S^\phi \chi_r^e + \chi_r^\phi \chi_S^e + \chi_r^e)\nabla a_r - \frac{1}{\chi_S^S + \chi_S^e + \chi_S^\phi}\nabla(\chi_S^e \mathbf{D}_h^E),$$

$$\tilde{\mathbf{V}}_{a_r} = \mathbf{V} - \frac{1}{\chi_e^r + \chi_r^\phi} \nabla(\chi_r^e \mathbf{D}_h^E).$$

We note the material derivatives of S, p, and T on the l.h.s. of (54), as well as of all other primary variables. We have included gradients of the primary variables S, T, and a_r in the modified velocity, $\tilde{\mathbf{V}}_p$. Similarly, we have included gradients of S and a_r in $\tilde{\mathbf{V}}_T$, and gradients of a_r in $\tilde{\mathbf{V}}_S$. Equation (54) is but one form of rewriting (46); other forms, with different definitions for the reduced velocities, are also possible. The selection of the expressions for the modified velocity presented above is based on the assumption that pressure changes are evolving more rapidly than those of temperature, which, in turn, are assumed to evolve more rapidly than those of saturation. In a numerical scheme of solution (to be discussed in a sequel article), this will allow us to solve for pressure by taking values of the remaining primary variables at an early iteration, and then proceed to update the values of these variables.

VII. EXAMPLE

We have established a methodology for expressing the balance equation for any extensive quantity in a MEL formulation in terms of selected primary variables. Let us demonstrate the methodology through an example.

We consider the flow of a single liquid phase (essentially water) in the unsaturated zone under isothermal conditions. The porous medium is deformable, i.e., $\partial\phi/\partial t \neq 0$. However, for the purpose of this example, we'll greatly simplify the deformation model.

A. Conceptual Model

The following assumptions constitute the conceptual model:

- **[A.1]** The unsaturated zone contains a liquid (essentially water) and a gas. We assume that the gas is at approximately atmospheric pressure. The movement of only the water is being considered.
- **[A.2]** The system is under isothermal conditions.
- **[A.3]** The water carries a nonvolatile contaminant that can adsorb on the solid. We assume that the contaminant in the liquid and on the solid are in equilibrium.
- **[A.4]** The dispersive and diffusive fluxes of the liquid's mass are much smaller than the advective one and can be neglected. There are no liquid sources within the domain (e.g., no evaporation or condensation).
- **[A.5]** In the averaged momentum balance equations for the two phases, we neglect the exchange of momentum across their common microscopic interface.
- **[A.6]** In the averaged momentum balance equations for the liquid and for the porous medium as a whole, we neglect inertial effects and fluid–fluid momentum transfer. This reduces the averaged momentum balance equation to Darcy's law, with an effective permeability that is a function of the saturation.
- **[A.7]** The effect of fluid shear stress, τ, is much smaller than that of pressure in the expression for total stress.
- **[A.8]** The solid matrix is deformable.
- **[A.9]** The solid's density remains constant.
- **[A.10]** External loads are not changed, so that the total stress within the considered domain remains unchanged with time.

B. Mathematical Model

The above conceptual model leads to the following mathematical one.

Mass balance equation for the liquid phase (ℓ):

$$\frac{\partial(\phi S_\ell \rho_\ell)}{\partial t} = -\nabla \cdot (\phi S_\ell \rho_\ell V_\ell), \tag{55}$$

where S_ℓ is the liquid's saturation. The same equation can be written in a form that emphasizes the relative velocity ($\mathbf{V}_r = \mathbf{V}_\ell - \mathbf{V}_s$), defined by Darcy's law, viz., in the form

$$\frac{\partial(\phi S_\ell \rho_\ell)}{\partial t} = -\rho_\ell \nabla \cdot (\phi S_\ell \mathbf{V}_r) - \rho_\ell \mathbf{V}_s \cdot \nabla(\phi S_\ell) - \phi S_\ell \rho_\ell \nabla \cdot \mathbf{V}_s - \phi S_\ell \mathbf{V}_\ell \cdot \nabla \rho_\ell. \tag{56}$$

Mass balance equation for the solid matrix (s):

With assumption [A.9], and neglecting the mass of the adsorbate on the solid, we have

$$\frac{\partial}{\partial t}(1-\phi) = -\nabla \cdot [(1-\phi)\mathbf{V}_s], \tag{57}$$

or

$$\nabla \cdot \mathbf{V}_s = \frac{1}{1-\phi}\left(\frac{\partial \phi}{\partial t} + \mathbf{V}_s \cdot \nabla \phi\right) \equiv \frac{1}{1-\phi}\frac{D_{\mathbf{v}_s}\phi}{Dt}. \tag{58}$$

Mass balance equation for a contaminant in a porous medium:

This equation has already been presented above, in the form of (26). For convenience, we shall rewrite it here:

$$\frac{\partial(\phi S_\ell R_d c_\ell)}{\partial t} = -\nabla \cdot \phi S_\ell (c_\ell \mathbf{V}_\ell - \mathbf{D}_h \cdot \nabla c_\ell), \tag{59}$$

where the retardation factor is defined by

$$R_d = R_d(\phi, S_\ell) = 1 + (1-\phi)\rho_s \mathcal{K}_d / \phi S_\ell.$$

Momentum balance equation for the liquid phase:

Making use of assumptions [A.6] and [A.7], this equation takes the form of Darcy's law

$$\mathbf{q}_{r\ell} = \phi S_\ell (\mathbf{V}_\ell - \mathbf{V}_s) = -\frac{\mathbf{k}_\ell(S_\ell, \gamma_{\ell_g})}{\mu_\ell} \cdot (\nabla p_\ell + \rho_\ell g \nabla z), \tag{60}$$

in which p_ℓ is the pressure in the liquid, $\mu = \mu(c_\ell)$ is the liquid's dynamic viscosity, assumed to be a function of the contaminant's concentration, c_ℓ, and $\mathbf{k}_\ell$ is the liquid's effective permeability. The latter depends on the saturation, S_ℓ, and on the surface tension, γ_{ℓ_g}, which, in turn is a function of c_ℓ (as we have assumed here, isothermal conditions).

Momentum balance equation for the porous medium:

Since we consider here a deformable solid matrix, a balance of momentum for the porous medium, as a whole, is required. It is obtained by summing up the three macroscopic momentum balance equations for the individual phases, in order to eliminate the terms that express interphase momentum transfer between the fluids and the solid across common (microscopic) boundaries. For the case in which inertial effects, friction *within* the fluid phases, and the capillary force arising from the surface tension between the two fluids at their common curved boundary can be neglected, Bear and Bachmat [25] develop the averaged momentum balance equation for the porous medium as a whole (= *equilibrium equation*, in the form

$$\nabla \cdot \sigma_t + \rho_b g \nabla z = 0, \tag{61}$$

where $\rho_b(= \phi S_\ell \rho_\ell(p_\ell, c_\ell) + \phi(1 - S_\ell)\rho_g(p_g) + (1 - phi)\rho_s)$ is the bulk density of the porous medium, and $\boldsymbol{\sigma}_t$ denotes the *total stress* (a symmetric tensor). Usually, we assume $\rho_s = \text{const}$. Thus, ρ_b can be taken as known, once we know p_ℓ and c. For an unsaturated zone, assuming $p_g = 0$, they express the total stress in terms of the *effective stress* (a symmetric tensor), $\boldsymbol{\sigma}'_s$, and the pressure in the fluid, p_ℓ, in the form

$$\boldsymbol{\sigma}_t = \boldsymbol{\sigma}'_s - \zeta(S_\ell) p_\ell \boldsymbol{\delta}, \tag{62}$$

where $\zeta(S_\ell)$ is a coefficient that takes into account the presence of gas in the void space.

¿From assumption [A.10], it follows that

$$\frac{\partial}{\partial t}\boldsymbol{\sigma}_t \equiv 0, \frac{\partial}{\partial t}\boldsymbol{\sigma}'_s = \frac{\partial}{\partial t}[\zeta(S_\ell)p_\ell \boldsymbol{\delta}], \frac{\partial \sigma'_s}{\partial t} = \frac{\partial \zeta(S_\ell)p_\ell}{\partial t}, \tag{63}$$

in which $\sigma'_s = \frac{1}{3}\sigma'_{sii}$ is the first invariant of the effective stress tensor.

Modeling porous medium deformation:

Introducing the momentum balance Eq. (61) is the first step in modeling porous medium deformation. Let us supplement this equation by introducing other elements of the deformation model, until a complete model is derived. Already from (62), we may note the coupling between the flow and deformation models, through p_ℓ.

Assuming, as an example, that the solid matrix is isotropic and elastic, the constitutive relationship is [25]

$$\boldsymbol{\sigma}'_s = \mu'_s(\nabla \cdot \mathbf{w})\boldsymbol{\delta} + \lambda'_s[\nabla \mathbf{w} + (\nabla \mathbf{w})^T] = \mu'_s \epsilon_{sk}\boldsymbol{\delta} + 2\lambda'_s \epsilon, \tag{64}$$

with

$$\epsilon_{sk} = \epsilon_{ii} = \nabla \cdot \mathbf{w}, \epsilon = \frac{1}{2}[\nabla \mathbf{w} + (\nabla \mathbf{w})^T], \mathbf{V}_s = \frac{D_{\mathbf{v}_s}\mathbf{w}}{Dt}, \tag{65}$$

where ϵ and ϵ_{sk} denote the strain and the dilatation of the solid skeleton, respectively, $\mathbf{w}$ denotes the skeleton's displacement, and λ'_s, μ'_s are the two Lamè constants of the skeleton.

We also need the mass balance equation for the solid matrix (57), or (58). We may rewrite the last equation in the form

$$\nabla \cdot \mathbf{V}_s \equiv \frac{D_{\mathbf{v}_s}\epsilon_{sk}}{Dt} = \frac{1}{1-\phi}\frac{D_{\mathbf{v}_s}\phi}{Dt}. \tag{66}$$

Let us regard the issue of porous medium deformation in the given domain as a separate problem, with variables:

$$\boldsymbol{\sigma}_t, \boldsymbol{\sigma}'_s, \sigma'_s, \mathbf{w}, \mathbf{V}_s, \boldsymbol{\epsilon}, \epsilon_{sk}, \text{ and } \phi,$$

i.e., 27 *scalar variables*. Given p and c from the remaining flow and contaminant transport problem, we have the following 27 equations: (61)—3 equations, (62)—6 equations, (64)—6 equations, (65)—0 equations, (66)—2 equations, i.e., 27 scalar equations. Thus, given p and c, the deformation problem can be fully described by a closed set of equations, which is decoupled from the flow and transport problem.

The large number of variables can be reduced to 3 primary ones, for which we have to solve the three scalar partial differential equations (61). Making use of the constitutive equation in terms of $\mathbf{w}$, we may easily rewrite (61) in terms of $\mathbf{w}$, and select the components w_i as primary variables:

$$(\mu'_s + \lambda'_s)\nabla(\nabla \cdot \mathbf{w}) - \nabla[\zeta(S)p] + \lambda'_s \nabla \cdot \nabla \mathbf{w} + \rho_b g \nabla z = 0.$$

We note that in view of the relationships between ϕ, ϵ_{sk}, and σ'_s, we may write the (experimentally derived) constitutive relationship symbolically as

$$\phi = \phi(\sigma'_s), \tag{67}$$

or, in view of the relationship

$$\sigma'_s = (3\lambda'_s + 2\mu'_s)\epsilon_{sk}.$$

¿From the solid's mass balance equation, (66), it follows that $\phi = \phi(\epsilon_{sk})$, or, explicitly

$$\frac{1-\phi}{1-\phi_0} = \exp(\epsilon_{sk}), \tag{68}$$

with $\phi = \phi_0$ for $\epsilon_{sk} = 0$.

Once $\mathbf{w}$ has been determined, we can determine all other nonprimary variables from the equations and definitions listed above.

Having, thus, established the complete deformation model (except for initial and boundary conditions), we can now return to the flow and transport model.

The complete flow and contaminant transport model:

In addition to the variables that describe the deformation of the solid matrix [including ϕ, obeying (67)], we have the 7 scalar variables:

$$S_\ell, \rho_\ell, p_\ell, c_\ell, V_{\ell i}.$$

To solve for these variables, we have 7 balance equations: (56), (59), (60)—3 equations, and the two constitutive relations:

$$\rho_\ell = \rho_\ell(p_\ell, c_\ell), \tag{69}$$

$$p_c = p_c(S_\ell, \gamma_{\ell g}(c_\ell)) = -p_\ell. \tag{70}$$

We also need information on

$$R_d = R_d(S_\ell, \phi), \mu = \mu(c_\ell), \mathbf{k} = \mathbf{k}(S_\ell, \gamma_{\ell g}),$$

$$\gamma_{g\ell} = \gamma_{g\ell}(c_\ell), \zeta = \zeta(S_\ell), S_\ell = S_\ell(p_c, \gamma_{\ell g}),$$

neglecting the effects of changes in ϕ on $\mathbf{k}$, which we have not counted as variables.

In what follows, we shall assume that the deformation model can be decoupled, thus focussing on the flow and transport model. In principle, the methodology presented above is also valid for an anisotropic porous medium, with appropriate constitutive relationships. We shall, therefore, extend the discussion below to such a model, making use of (67) as a constitutive relationship, assuming that σ'_s has been determined from the deformation model. We also note that $\mathbf{V}_s$ can be determined from that model.

C. Primary Variables

At this point, we note that for the model considered here: two phases, three components, isothermal flow, and a deformable porous medium, the number of primary variables is given by $NF = NC$. However, since we have assumed gas pressure to be always atmospheric, NF is reduced to 2.

We select pressure, p_ℓ, and contaminant concentration, c_ℓ. Henceforth, they will be denoted as p and c, respectively. Similarly, ρ, μ, and S will be used to denote ρ_ℓ, μ_ℓ, and S_ℓ, respectively.

We note that the functional relations (67) and (69) are not given in terms of primary variables.

To obtain a solution, we have to solve two balance equations. We select to solve the liquid mass balance equation, (56), and the contaminant mass balance equation, (59).

Once we have solved these equations, and, obviously, we have to provide appropriate initial and boundary conditions for them, all other variables can be determined.

The mathematical model, or more specifically, the balance equations, have been presented in their Eulerian form. Let us now employ the methodology presented above to rewrite the model in its MEL formulation.

D. MEL Formulation

1. *Mass Balance Equation for the Liquid*

In order to rewrite (56) in the MEL form, we note:

a. From (69), we have

$$\frac{\partial \rho}{\partial t} = \rho\left(\chi_p^\rho \frac{\partial p}{\partial t} + \chi_c^\rho \frac{\partial c}{\partial t}\right), \nabla\rho = \rho(\chi_p^\rho \nabla p + \chi_c^\rho \nabla c), \tag{71}$$

in which the χ's, defined in (44), are known (here and everywhere else).

b. From (70), we have

$$\frac{\partial S}{\partial t} = S\left(\chi_p^S \frac{\partial p}{\partial t} + \chi_c^S \frac{\partial c}{\partial t}\right), \nabla S = S(\chi_p^S \nabla p + \chi_c^S \nabla c), \tag{72}$$

where, because p_c and $\gamma_{\ell g}$ are not primary variables, we have introduced

$$\chi_p^S = \frac{\partial p_c}{\partial tp}\chi_{p_c}^S = -\chi_{p_c}^S, \chi_c^S = \frac{d\gamma_{\ell g}}{dc}\chi_{\gamma_{\ell g}}^S.$$

We note the slightly different structure of the χ's whenever the dependence is not directly on primary variables, but through some intermediate functional relationship. These modif ied χ's are also known. Alternatively, we could modify the original definition of $\chi_{a_k}^e$ by replacing a_k by any variable, not necessarily a primary one, as long as the relationship between e and that variable is known.

c. From (70), (67), and (63), we have

$$\begin{aligned}\frac{\partial \phi}{\partial t} &= \frac{d\phi}{d\sigma_s'}\frac{\partial \sigma_s'}{\partial t} = \frac{d\phi}{d\sigma_s'}\frac{\partial [\zeta(S)p]}{\partial t} = \phi\chi_{\sigma_s'}^\phi\left[\left(\zeta - pS\frac{d\zeta}{dS}\chi_{p_c}^S\right)\frac{\partial p}{\partial t} + pS\frac{d\zeta}{dS}\chi_{\gamma_{\ell g}}^S\frac{d\gamma_{\ell g}}{dc}\frac{\partial c}{\partial t}\right] \\ &= \phi\left(A_p\frac{\partial p}{\partial t} + A_c\frac{\partial c}{\partial t}\right)\nabla\phi = \frac{d\phi}{d\sigma_s'}\nabla\sigma_s' = \frac{d\phi}{d\sigma_s'}\nabla[\zeta(S)p] \\ &= \phi(A_p\nabla p + A_c\nabla c),\end{aligned} \tag{73}$$

where

$$A_p = \chi_{\sigma_s'}^\phi\left(\zeta - pS\frac{d\zeta}{dS}\chi_{p_c}^S\right), A_c = \chi_{\sigma_s'}^\phi pS\frac{d\zeta}{dS}\chi_c^S.$$

d. From $\mathbf{k} = \mathbf{k}(S, \gamma_{\ell g})$, and $\mu = \mu(c)$, it follows that

$$\begin{aligned}\nabla\left(\frac{k}{\mu}\right) &= \frac{1}{\mu}\nabla\mathbf{k} + \mathbf{k}\cdot\nabla\left(\frac{1}{\mu}\right) = \frac{1}{\mu}\left(\frac{\partial \mathbf{k}}{\partial S}\cdot\nabla S + \frac{\partial \mathbf{k}}{\partial \gamma_{\ell g}}\cdot\nabla\gamma_{\ell g}\right) - \frac{\mathbf{k}}{\mu^2}\cdot\nabla\mu \\ &= \frac{1}{\mu}\left\{S\frac{\partial \mathbf{k}}{\partial S}\chi_p^S\cdot\nabla p + \left[\frac{\partial \mathbf{k}}{\partial S}S\chi_c^S + \frac{\partial \mathbf{k}}{\partial \gamma_{\ell g}}\frac{d\gamma_{\ell g}}{dc} - \mathbf{k}\chi_c^\mu\right]\cdot\nabla c\right\}.\end{aligned} \tag{74}$$

e. For the l.h.s. of (56), and in view of (69)–(73), we can write

$$\frac{\partial(\phi S\rho)}{\partial t} = \phi S\rho\left[(\chi_p^\rho + \chi_p^S + A_p)\frac{\partial p}{\partial t} + (\chi_c^\rho + \chi_c^S + A_c)\frac{\partial c}{\partial t}\right]. \tag{75}$$

f. Making use of (60) and (74), we write

$$\begin{aligned}\rho\nabla\cdot(\phi S\mathbf{V}_r) &= -\rho\nabla\cdot\left[\frac{\mathbf{k}}{\mu}\cdot(\nabla p+\rho g\nabla z)\right]\\ &= -\rho\nabla\left(\frac{\mathbf{k}}{\mu}\right)\cdot\left[\mu\mathbf{k}^{-1}\frac{\mathbf{k}}{\mu}\cdot(\nabla p+\rho g\nabla z)\right]-\rho\frac{\mathbf{k}}{\mu}\nabla\nabla p-\frac{\rho\mathbf{k}}{\mu}g\nabla\rho\cdot\nabla z\\ &= \rho\left[\phi S^2\chi_{p_c}^S\chi_S^{\mathbf{k}}\cdot\mathbf{V}_r-\chi_p^\rho\frac{\mathbf{k}\rho g}{\mu}\cdot\nabla z\right]\cdot\nabla p-\frac{\mathbf{k}\rho}{\mu}:\nabla\nabla p\\ &\quad+\rho\left[\phi S\left(\chi_{\gamma_{\ell g}}^S S\boldsymbol{\chi}_S^{\mathbf{k}}+\boldsymbol{\chi}_{\gamma_{\ell g}}^{\mathbf{k}}\frac{d\gamma_{\ell g}}{dc}-\chi_c^\mu\mathbf{I}\right)\cdot\mathbf{V}_r-\chi_c^\rho\frac{\mathbf{k}\rho g}{\mu}\cdot\nabla z\right]\cdot\nabla c,\end{aligned} \tag{76}$$

where

$$\boldsymbol{\chi}_S^{\mathbf{k}} = \frac{\partial\mathbf{k}}{\partial S}\mathbf{k}^{-1}, \boldsymbol{\chi}_{\gamma_{\ell g}}^{\mathbf{k}} = \frac{\partial\mathbf{k}}{\partial\gamma_{\ell g}}\mathbf{k}^{-1}.$$

g. From the Solid's mass balance equation, (58), we obtain

$$\nabla\cdot\mathbf{V}_s = \frac{\phi}{1-\phi}\left[A_p\left(\frac{\partial p}{\partial t}+\mathbf{V}_s\cdot\nabla p\right)+A_c\left(\frac{\partial c}{\partial t}+\mathbf{V}_s\cdot\nabla c\right)\right]. \tag{77}$$

h. For the second term on the r.h.s. of (56), and in view of (73) and (72), we write

$$\rho\mathbf{V}_s\cdot\nabla(\phi S) = \rho\phi S\mathbf{V}_s\cdot[(\chi_p^S+A_p)\nabla p+(\chi_c^S+A_c)\nabla c]. \tag{78}$$

i. For the last term on the r.h.s. of (56), and in view of (71), we write

$$\phi S\mathbf{V}\cdot\nabla\rho = \phi S\rho\mathbf{V}\cdot(\chi_p^\rho\nabla p+\chi_c^\rho\nabla c). \tag{79}$$

With the above expressions, (75)–(79), we may now rewrite the liquid mass balance equation, (56), in terms of the primary variables p and c, in the form

$$\begin{aligned}&\phi S\rho\left[\left(\chi_p^\rho+\chi_p^S+\frac{1}{1-\phi}A_p\right)\frac{\partial p}{\partial t}+\left(\chi_c^\rho+\chi_c^S+\frac{1}{1-\phi}A_c\right)\frac{\partial c}{\partial t}\right]\\ &= -\rho\phi S\left[(\chi_p^\rho\mathbf{I}-S\chi_p^S\chi_S^{\mathbf{k}})\cdot\mathbf{V}_r+\left(\chi_p^\rho+\chi_p^S+\frac{1}{1-\phi}A_p\right)\mathbf{V}_s-\chi_p^\rho\frac{\mathbf{k}\rho g}{\phi S\mu}\cdot\nabla z\right]\cdot\nabla p\\ &\quad-\rho\phi S\left\{\left[\chi_{\gamma_{\ell g}}^S S\boldsymbol{\chi}_S^{\mathbf{k}}+\frac{d\gamma_{\ell g}}{dc}\boldsymbol{\chi}_{\gamma_{\ell g}}^{\mathbf{k}}+(\chi_c^\rho-\chi_c^\mu)\mathbf{I}\right]\cdot\mathbf{V}_r\right.\\ &\qquad\left.+\left(\chi_c^\rho+\chi_c^S+\frac{1}{1-\phi}A_c\right)\mathbf{V}_s-\chi_c^\rho\frac{\mathbf{k}\rho g}{\phi S\mu}\cdot\nabla z\right\}\cdot\nabla c+\frac{\mathbf{k}\rho}{\mu}:\nabla\nabla p.\end{aligned} \tag{80}$$

Once we have the Eulerian form of this equation, we can rewrite it in the MEL formulation. We obtain

$$\left(\chi_p^\rho+\chi_p^S+\frac{1}{1-\phi}A_p\right)\frac{D_{\tilde{\mathbf{v}}_p^m}p}{Dt}+\left(\chi_c^\rho+\chi_c^S+\frac{1}{1-\phi}A_c\right)\frac{D_{\tilde{\mathbf{v}}_c^{mc}}}{Dt} = \frac{\mathbf{k}}{\phi S\mu}:\nabla\nabla p, \tag{81}$$

in which

$$\tilde{\mathbf{V}}_p^m = \frac{\chi_p^\rho \mathbf{I} - S\chi_p^S \boldsymbol{\chi}_S^{\mathbf{k}}}{\chi_p^\rho + \chi_p^S + \frac{1}{1-\phi}A_p} \cdot \mathbf{V}_r + \mathbf{V}_s - \frac{k\rho g}{\phi S\mu} \frac{\chi_p^S}{\chi_p^\rho + \chi_p^S + \frac{1}{1-\phi}A_p} \cdot \nabla z,$$

$$\tilde{\mathbf{V}}_c^m = \frac{\chi_{\gamma_{\ell g}}^S S\boldsymbol{\chi}_S^{\mathbf{k}} + \frac{d\gamma_{\ell g}}{dc}\boldsymbol{\chi}_{\gamma_{\ell g}}^{\mathbf{k}} + (\chi_c^\rho - \chi_c^\mu)\mathbf{I}}{\chi_c^\rho + \chi_c^S + \frac{1}{1-\phi}A_c} \cdot \mathbf{V}_r + \mathbf{V}_s$$

$$- \frac{\mathbf{k}\rho g}{\phi S\mu} \frac{\chi_c^\rho}{\chi_c^\rho + \chi_c^S + \frac{1}{1-\phi}A_c} \cdot \nabla z. \quad (82)$$

Following the definition in (51), let us note the interpretation of the *reduced velocities*, $\tilde{\mathbf{V}}_p^m$, and $\tilde{\mathbf{V}}_c^m$, defined above. We are dealing with the movement of a particle in the continuum corresponding to the mass of the phase. Motion in this mass continuum is associated with changes in pressure and concentration. The velocity $\tilde{\mathbf{V}}_p^m$ expresses the instantaneous velocity of propagation of the pressure in the mass continuum. Similarly, $\tilde{\mathbf{V}}_c^m$ expresses the instantaneous velocity of propagation of the concentration of the component in the mass continuum. In each case, the velocity of propagation is tangent to the instantaneous trajectory, or *characteristic curve* along which the considered property (pressure, concentration) would travel, maintaining its instantaneous value.

2. Mass Balance Equation for the Component in the Porous Medium

This equation is the same as (28) presented above in **Example 2**. However, we have now to rewrite it in terms of the primary variables, p and c. Also, in the example considered here, the solid matrix is deformable. This means that $\mathbf{V} = \mathbf{V}_r + \mathbf{V}_s$, where $\mathbf{V}_r$ is obtained from Darcy's law.

We can now rewrite (28), which was obtained from (26), in the Eulerian–Lagrangian formulation:

$$\left(\chi_p^S + \frac{1-\phi r}{1-\phi}A_p\right)\frac{D_{\tilde{\mathbf{v}}_p^\gamma} p}{Dt} + \left(\chi_c^S + \chi_c^c R_d + \frac{1-\phi r}{1-\phi}A_c\right)\frac{D_{\tilde{\mathbf{v}}_c^\gamma} c}{Dt}$$

$$= \frac{\mathbf{D}_h^E}{c} : \nabla\nabla c + \frac{\rho\mathbf{k}}{\phi S\mu} : \nabla\nabla p, \quad (83)$$

in which

$$\tilde{\mathbf{V}}_p^\gamma = \frac{1}{\chi_p^S + \frac{1-\phi r}{1-\phi}A_p}\left[\left(\chi_p^S + \frac{1}{1-\phi}A_p\right)\mathbf{V}_s - S\chi_p^S\boldsymbol{\chi}_S^{\mathbf{k}} \cdot \mathbf{V}_r\right.$$

$$\left. - \chi_p^\rho \frac{\rho g}{\phi S\mu}\mathbf{k} \cdot \nabla z - \chi_c^c(\chi_p^S + A_p)\mathbf{D}_h^E \cdot \nabla_c\right]. \quad (84)$$

$$\tilde{\mathbf{V}}_c^\gamma = \frac{1}{\chi_c^S + \chi_c^c R_d + \frac{1-r\phi}{1-\phi}A_c}\left\{\left[\chi_{\gamma_{\ell g}}^S S\boldsymbol{\chi}_S^{\mathbf{k}} + \frac{d\gamma_{\ell g}}{dc}\boldsymbol{\chi}_{\gamma_{\ell g}}^{\mathbf{k}} + (\chi_c^c - \chi_c^\mu)\mathbf{I}\right] \cdot \mathbf{V}_r\right.$$

$$+ \left(\chi_c^c + \chi_c^S + \frac{1}{1-\phi}A_c\right)\mathbf{V}_s - \chi_c^\rho \frac{\rho g}{\phi S\mu}\mathbf{k} \cdot \nabla z$$

$$\left. - \frac{\chi_c^c}{\phi S}\nabla\mathbf{D}_h^E - \chi_c^c(\chi_c^S + A_c)\mathbf{D}_h^E \cdot \nabla c\right\}, \quad (85)$$

and $\chi_c^c = 1/c$.

The mass balance equations: (81) for the mass of the liquid phase, and (83) for the mass of a component, may be combined in the matrix form

$$\begin{bmatrix} \chi_p^\rho + \chi_p^S + \frac{A_p}{1-\phi} & \chi_c^\rho + \chi_c^S + \frac{A_c}{1-\phi} \\ \chi_p^S + \frac{1-r\phi}{1-gf}A_p & \chi_c^S + \chi_c^c R_d + \frac{1-r\phi}{1-\phi}A_c \end{bmatrix} \begin{bmatrix} \frac{\partial p}{\partial t} \\ \frac{\partial c}{\partial t} \end{bmatrix} + \begin{bmatrix} \left(\chi_p^\rho + \chi_p^S + \frac{A_p}{1-\phi}\right)\tilde{\mathbf{V}}_p^m & \left(\chi_c^\rho + \chi_c^S + \frac{A_c}{1-\phi}\right)\tilde{\mathbf{V}}_c^m \\ \left(\chi_p^S + \frac{1-r\phi}{1-\phi}A_p\right)\tilde{\mathbf{V}}_p^\gamma & \left(\chi_c^S + \chi_c^c R_d + \frac{1-r\phi}{1-\phi}A_c\right)\tilde{\mathbf{V}}_c^\gamma \end{bmatrix} \cdot \begin{bmatrix} \nabla p \\ \nabla c \end{bmatrix} = \begin{bmatrix} \frac{\mathbf{k}}{\phi S\mu} : \nabla\nabla p \\ \frac{\mathbf{D}_h^E}{c} : \nabla\nabla c + \frac{\rho\mathbf{k}}{\phi S\mu} : \nabla\nabla p \end{bmatrix}. \tag{86}$$

The interpretation of the reduced velocities, $\tilde{\mathbf{V}}_p^\gamma$ and $\tilde{\mathbf{V}}_c^\gamma$, is analogous to that given above for $\tilde{\mathbf{V}}_p^m$ and $\tilde{\mathbf{V}}_c^m$, except that here the considered continuum is that of the mass of a component of a phase.

3. Outline of a Solution Scheme

The passage from the Eulerian description to the MEL one was proposed here because of certain advantages that the latter has over the former (in addition to highlighting the idea of reduced velocities of propagation of various properties, as a consequence of resistance and storage mechanisms).

The two MEL equations to be solved are (81) and (83). They are highly nonlinear, as the various reduced velocities and some of the terms depend on the pressure and the concentration (which are the primary variables of our problem). Furthermore, the two equations are *coupled*. Given the constitutive relationships, the various χ's can be determined at every instant. Similarly, the reduced velocities may be determined at every instant of time. We recall that within the Lagrangian framework velocities are of particles and properties of particles and not *at points in space*. The particles move and properties vary along trajectories. The definition of the velocity $\mathbf{V}^E$ of an extensive quantity E was already given by (51).

To facilitate the solution by some numerical technique, let us rewrite (81) and (83) in the special form:

$$\left[\chi_p^\rho + \chi_p^S + \frac{1}{1-\phi}A_p\right]_i \frac{D_{\tilde{\mathbf{v}}_p^m} p}{Dt} = \frac{\mathbf{k}}{\phi S\mu} : \nabla\nabla p - \left[\left(\chi_c^\rho + \chi_c^S + \frac{1}{1-\phi}A_c\right)\frac{D_{\tilde{\mathbf{v}}_c^m} c}{Dt}\right]_i, \tag{87}$$

$$\left[\chi_c^S + \chi_c^c R_d + \frac{1-\phi r}{1-\phi}A_c\right]_i \frac{D_{\tilde{\mathbf{v}}_c^\gamma} c}{Dt} = \frac{\mathbf{D}_h^E}{c} : \nabla\nabla c + \left[\frac{\rho\mathbf{k}}{\phi S\mu} : \nabla\nabla p - \left(\chi_p^S + \frac{1-\phi r}{1-\phi}A_p\right)\frac{D_{\tilde{\mathbf{v}}_p^\gamma} p}{Dt}\right]_i. \tag{88}$$

The solution of the these two equations involves iterations. We recall that, in a numerical scheme for an unsteady problem, we advance from known values at time t to the new values at time $t+\Delta t$. Within each time step, the solution is based on iterations, starting from time t, until we achieve convergence at $t+\Delta t$. In (87) and (88), $[\cdots]_i$ means the *known* value of $[\cdots]$ at the ith iteration. The values to be solved for in (87) and (88) are for the $i+1$ iteration. In each iteration, once the

values of the $[\cdots]_i$-terms are known, one uses one of the known methods of solution developed for the Eulerian–Lagrangian formulation of field equations. In writing the various $[\cdots]_i$-terms as known values, we have eliminated nonlinearities. Furthermore, the two equations become *uncoupled.*

VIII. CONCLUSIONS

A general approach has been developed and presented for the Eulerian–Lagrangian formulation of models that describe the simultaneous transport of any number of extensive quantities in a porous medium domain that contains multiple multicomponent phases and a deformable solid matrix, under nonisothermal conditions. In general, a rather large number of state variables is needed in order to fully describe such a system. However, because of interrelationships that exist among the various variables, especially under the assumptions of mechanical, thermal, and chemical equilibria considered here, the number of variables can be significantly reduced. We refer to the smallest number of variables that is needed in order to fully describe a given system, as *number of degrees of freedom*, NF. These state variables are then called *primary variables.*

The proposed mathematical model is written in terms of NF preselected intensive quantities that constitute the set of primary (state) variables of the transport problem. The model contains coefficients that are related to changes in state variables with respect to the primary ones. They are derived from the constitutive and thermodynamic relationships that define the behavior of particular porous media, fluids, and components.

Like in the usual Eulerian model, in the Eulerian–Lagrangian formulation, the model is composed of NF partial differential equations, each describing the balance of one of the NF selected extensive quantities. Each balance equation has the form of a *diffusion equation*: its l.h.s. represents temporal changes, expressed as a linear combination of material derivatives of the NF primary variables of the problem. The r.h.s. expresses the spatial distributions of the same variables. This takes the form of a linear combination of Laplacians [or *div grad* ($\equiv \nabla\nabla\cdot$ operators)] of the same state variables.

Each material derivative involves a velocity of propagation of the particle of the corresponding extensive quantity. These velocities are derived as a modification of the phase (mass weighted) relative velocity, by taking into account heterogeneity in matrix properties (such as permeability and porosity), fluid and matrix compressibilities, spatial changes in surface tension, etc. They also involve a term that represents a (downward) vertical velocity component resulting from the effect of gravity. In some cases, these velocities are affected by gradients in the concentrations of the primary variables themselves. For example, the velocity $\tilde{\mathbf{V}}_p^\gamma$ is affected by ∇c.

In the Eulerian–Lagrangian formulation, the primary (state) variables are not visualized as ones that vary on a space–time grid, as in a (standard) Eulerian formulation. Instead, we visualize changes in the state variables associated with particles of extensive quantities as they travel along *characteristic curves* (or *pathlines*). Because (in principle) each extensive quantity is associated with *all* primary variables, we have on the l.h.s. of each balance equation, a linear combination of the material derivatives of all NF intensive quantities that constitute the set of primary (state) variables of the problem. Accordingly, each *material* (or *hydrodynamic*) *derivative* expresses the temporal rate of change of one of the primary intensive quantities that is associated with an extensive quantity of a particle. Thus, we may have a material derivative of the pressure, in which the latter is propagating at the velocity associated with a mass of phase particle, and a material derivative of the pressure in which the latter is propagating at the velocity associated with the mass of a component of a phase particle.

In the example given in this article, we had two extensive quantities: mass of a fluid phase (in a two-phase system) and, mass of a component of the phase, both in the porous medium as a whole, and two primary variables, pressure and concentration. A balance equation, in the MEL formulation was written for each of the two extensive quantities. In determining the number of primary variables, NF, we have already taken into account the fact that Darcy's law (which is nothing but a simplified averaged linear momentum balance equation for the fluid) is employed for determining the fluid's (mass weighted) velocity, relative to the solid.

The resulting model is highly nonlinear. The various velocities of propagation of the considered primary variables depend on the (continuously varying) values of these variables.

The advantage of the MEL formulated mathematical model presented here lies in its numerical model and in the method of solution of that model.

The EL method of solution has been proven to yield solutions that are free of numerical dispersion. The latter is inevitable in the MEL extension of the Eulerian–Lagrangian technique to the general case of a number of primary variables that describe transport in porous media. There is no difficulty in extending the development to a larger number of primary variables, e.g., saturations, temperature, and concentrations of a number of interacting chemical components. The actual method of solution for such a case will be presented in a sequel article.

List of Main Symbols

a_k	Primary variable.
c_α	Concentration of a component in an α-phase.
e	Amount of E per unit volume of porous medium.
E	Amount of an Extensive quantity.
$\mathcal{D}_\alpha^E$	Coefficient of diffusion of E in an α-phase.
$\mathcal{D}_\alpha^{*E}$	Coefficient of diffusion of E in porous medium.
$\mathbf{D}_{h\alpha}^\gamma$	Coefficient of hydrodynamic dispersion of a E in an α-phase.
$f_{\alpha\to\beta}^E$	Rate of transfer of E from the α-phase to the β-one, across their common microscopic interface per unit volume of porous medium.
g	Gravity acceleration.
h	Specific enthalpy.
$\mathbf{I}$	Unit tensor.
$\mathbf{J}_\alpha'^E$	Dispersive flux of E in the α-phase, due to variations in $\mathbf{V}_\alpha^E$.
$\mathbf{J}_\alpha^{*E}$	Dispersive flux of E in the α-phase, due to variations in $\mathbf{V}_\alpha$.
$\mathbf{J}_{h\alpha}^E$	Sum of diffusive and dispersive fluxes ($\mathbf{J}_\alpha^{*E}$) of E in an α-phase.
$\mathbf{J}^E$	Macroscopic diffusive flux of E.
$\mathbf{k}_\alpha$	Effective permeability of an α-phase.
$\mathcal{K}^d$	Coefficient for partitioning of a component between the α and the solid in a linear equilibrium isotherm.
NC	Number of components.
NF	Number of degrees of freedom.
NP	Number of phases.
p	Pressure.
p_α	Pressure in an α-phase.
p_c	Capillary pressure.
$\mathbf{q}_\alpha$	Specific discharge of an α-phase.
R_d	Retardation coefficient.

S_α Saturation of an α-phase.
S_0 Specific storativity of a porous medium.
t Time.
T Absolute temperature.
$\mathbf{V}_r$ Velocity of a fluid relative to the solid.
$\mathbf{V}_\alpha$ Mass weighted velocity of an α-phase.
$\mathbf{V}_\alpha^E$ Velocity of E of an α-phase.
z Vertical coordinate (positive upward).

Greek letters

α Coefficient of solid matrix compressibility.
β_p^ρ Coefficient of fluid compressibility.
γ Symbol denoting a γ-component.
$\gamma_{\alpha\beta}$ Interfacial tension between α and β-phases.
Γ^E Rate of production of E per unit mass of phase.
μ_α Dynamic viscosity of an α-phase.
ϕ Porosity.
ρ_α Mass density of α-phase.
$\boldsymbol{\sigma}$ Stress tensor.
$\boldsymbol{\sigma}_t$ Total stress tensor.
$\boldsymbol{\sigma}_s'$ Effective stress tensor.
$\boldsymbol{\tau}$ Shear stress. Deviatoric stress.
θ_α Volumetric fraction of an α-phase.
χ_k^e $= (1/e)\partial e/partial a_k$.

Subscripts

g Gaseous phase.
ℓ Aqueous liquid phase.
s Solid.
α α-phase.
β β-phase. Also, a symbol for all other phases except α.

Superscripts

w Water, as a component.
γ γ-component in a phase.

Special symbols

$\nabla \cdot \mathbf{A}$ Divergence of a vector $\mathbf{A}(\equiv \text{div } \mathbf{A})$.
∇A Gradient of a scalar $A(\equiv \text{grad } A)$.
$\frac{D_{\tilde{\mathbf{V}}}(..)}{Dt}$ Material derivative of (..), as observed by an observer traveling at a velocity $\tilde{\mathbf{V}}$.

References

1. S. P. Neuman and S. Sorek, "Eulerian–Lagrangian methods for advection–dispersion," *Proc. 4th Inter. Confer. F. E. W. R.;* FGR, 1982.

2. S. P. Neuman, "Adaptive Eulerian–Lagrangian finite element method for advection–dispersion," *Int. J. Num. Methods in Eng.* **20,** 321–337 (1984).

3. S. Sorek, "Eulerian–Lagrangian formulation for flow in soils," *Adv. Wat. Resour.* **8,** 118–120 (1985a).

4. S. Sorek, "Adaptive Eulerian–Lagrangian method for transport problems in soils," in *Scientific Basis for Water Resources Management,* IASH Publ., **153,** 393–403 (1985b).
5. S. Sorek, "2-D adaptive Eulerian–Lagrangian method for mass transport with spatial velocity distribution," *Transport in Porous Media,* **3,** 473–489 (1988a).
6. S. Sorek, "Eulerian–Lagrangian method for solving transport in aquifers," *Adv. Wat. Resour.* **11,** 67–73 (1988b).
7. S. Sorek, "Numerical experiments with Euler–Lagrange method for a pair of recharge-pumping wells," *Proc. 7th Confer. on Computational Methods in Water Resources,* MIT, 1988c, pp. 219–226.
8. S. Sorek and C. Braester, "An adaptive Eulerian–Lagrangian approach for the numerical simulation of unsaturated flow," *Proc. 6th Inter. Confer. F. E. W. R.,* Portugal, 1986, pp. 87–100.
9. S. Sorek and C. Braester, "Eulerian–Lagrangian formulation of the equations for groundwater denitrification using bacterial activity," *Adv. Wat. Resour.* **11,** 162–169 (1988).
10. L. F. Konikow and J. D. Bredehoeft, *Computer model of two-dimensional solute transport and dispersion in ground water,* U. S. Geological Survey Techniques of Water Resources Investigations, Book 7, Chap. C2, 1978.
11. A. E. Baptista, "Solution of advection dominated transport by Eulerian–Lagrangian method, using the backwards method of characteristics," Ph. D. Dis., MIT, 1987.
12. A. M. Baptista, E. E. Adams, and K. D. Stolzenbach, "The 2-D unsteady, transport equation solved by the combined use of the finite element method and the method of characteristics," in *Finite Elements in Water Resources,* J. P. Laible et al., Eds., Springer–Verlag, New York, 1984, pp. 353–362.
13. J. Bear, *Hydraulics of Groundwater,* McGraw–Hill, New York, 1979.
14. W. Rudin, *Functional Analysis,* McGraw–Hill, New York, 1979.
15. P. Antosik, Y. Mikusinski, and R. Sikorski, *Theory of Distributions,* Elsevier, Amsterdam, PWN-Polish Scientific, Warszawa, 1973.
16. A. H. Zemanian, *Generalised Integral Transformations,* Interscience, New York, 1968.
17. E. S. Oran and J. P. Boris, *Numerical Simulation of Reactive Flow,* Elsevier, New York, 1987.
18. I. Gyarmati, *Non-Equilibrium Thermodynamics,* Springer–Verlag, New York, 1970.
19. J. Miles, *The Potential Theory of Unsteady Supersonic Flow,* The University Press, Cambridge, 1959.
20. D. Nixon, "Basic equations for unsteady transonic flow," Progress in Astronautics and Aeronautics, Unsteady Transonic Aerodynamics, Ed. D. Nixon, **120,** 57–73, AIAA, Washington, 1989.
21. A. A. Samarsky, *Theory of Difference Schemes,* Nauka, Moscow, 1977 (in Russian).
22. G. E. Forsythe and W. R. Wasow, *Finite Difference Methods for Partial Differential Equations,* John Wiley, New York, 1960.
23. A. F. Atkinson, *Discrete and Continuous Boundary Problems,* Academic Press, New York, 1964.
24. J. Bear and J. Nitao, "On the number of primary variables in modeling transport in porous media," *Transport in Porous Media,* **18,** 151–184 (1995).
25. J. Bear and Y. Bachmat, *Introduction to Modeling of Transport Phenomena in Porous media,* Kluwer Acad., Dordrecht, 1990.