

Derivation of Conditions Describing Transport Across Zones of Reduced Dynamics Within Multiphase Systems

S. MAJID HASSANIZADEH

National Institute of Public Health and Environmental Protection, Bilthoven, The Netherlands

WILLIAM G. GRAY

Department of Civil Engineering, University of Notre Dame, Notre Dame, Indiana

Equations for describing flow and transport in multiphase systems can be derived within the context of averaging theory. In some subsurface systems, the balance equations must be three dimensional in one portion of a domain of interest but need be only one or two dimensional in other regions (e.g., across clay lenses or within fractures). Conditions linking the dynamic processes among the different regions are typically obtained heuristically. Here a general framework is presented within which the needed conditions may be derived systematically. Particular conditions for mass, momentum, chemical species, and heat transfer are illustrated between main porous media domains and both a permeable fracture and a semipermeable layer.

INTRODUCTION

In the past two decades considerable progress has occurred in the construction of a sound theoretical basis for description of transport phenomena in general multiphase systems and particularly in porous media. Investigators from different disciplines have employed various methods to expose physical principles as well as assumptions underlying these theories. As a result, equations such as Darcy's law and Fick's law have been shown to be constitutive relations valid under certain restrictive conditions rather than heuristic empirical assumptions. Variables such as pressure, velocity, temperature, energy, stress, etc. appear as thermodynamic variables intimately related to each other through derived thermodynamic relationships.

Despite these advances in the proper description of differential equations for transport in multiphase systems, additional study is required to produce a careful and systematic formulation of conditions at discontinuities and across regions of reduced dynamics (i.e., regions where simplified equations may be applied). These conditions, referred to collectively as interface conditions, are necessary to complete the mathematical description of a well-posed problem. In fact, at discontinuities the interface conditions replace the differential equations.

In the derivation of interface conditions for mass, momentum, and energy conservation in multiphase systems, the interface is often assumed to be a narrow region devoid of thermodynamic properties. Under this assumption, the following jump or interface condition for a general macroscopic thermodynamic property $\bar{\psi}^\alpha$ is typically obtained [e.g., Raats, 1972a; Bowen and Doria, 1973; Bachmat and Bear, 1972; Hassanizadeh and Gray, 1979a, b; Bear, 1979, Appendix A]:

$$[\langle \rho \rangle_\alpha \bar{\psi}^\alpha (\bar{v}^\alpha - \mathbf{W}) - \mathbf{i}^\alpha] \cdot \mathbf{N} = 0 \quad (1a)$$

where

$$[\mathbf{f}] \cdot \mathbf{N} = (\mathbf{f}_1 - \mathbf{f}_2) \cdot \mathbf{N}_1 = (\mathbf{f}_2 - \mathbf{f}_1) \cdot \mathbf{N}_2 \quad (1b)$$

$\langle \rho \rangle_\alpha$ is the phase average density for phase α , \bar{v}^α is the mass-averaged velocity of phase α , \mathbf{W} is the velocity of the surface of discontinuity, \mathbf{i}^α is the macroscopic nonadvective flux of the α phase, and \mathbf{N}_1 and \mathbf{N}_2 are the unit normals to the interface of the main domains 1 and 2 pointing outwards from the main domains, respectively ($\mathbf{N}_1 = -\mathbf{N}_2$). Although (1a) has wide applicability for some multiphase flow situations, the assumption that the interface possesses no thermodynamic properties lacks generality. Even for the simple case of two porous media with different porosities, the interface condition above for momentum will give incorrect results. In general situations, the right-hand side of (1a) must be nonzero. That is, one must obtain

$$[\langle \rho \rangle_\alpha \bar{\psi}^\alpha (\bar{v}^\alpha - \mathbf{W}) - \mathbf{i}^\alpha] \cdot \mathbf{N} = f_b^\alpha \quad (2)$$

where f_b^α accounts for the contribution of the interface to thermodynamic properties of the α phase. Equations similar to (2) have been suggested by Raats [1972b], Bedford [1973], and Bear and Verruijt [1987].

In some cases, the zone between two media may actually be a volume as opposed to an idealized surface. This region will naturally be able to store and transport mass and other thermodynamic properties. For such cases, even (2) may be inadequate and a more general formulation of conservation laws is required. For example, when a permeable fracture separates two porous media, the transport of thermodynamic properties within the fracture may play an essential role in the overall behavior of the system. Alternatively, a clay lens separating two aquifers will dramatically affect the flow and transport in the ground water system, although the lens itself may be treated simply as an interface or intermedia zone.

In the current presentation, the intermedia zone between two multiphase media is considered to have a finite thickness attaining mass as well as all other usual thermodynamic properties. This zone need not be narrow. However, it will be modeled as a two-dimensional domain separating the main three-dimensional domains. This type of zone is referred to here as a general interface. Transport and storage of mass and other thermodynamic properties within and across the interface (i.e., in the tangential as well as the normal direction to

Copyright 1989 by the American Geophysical Union.

Paper number 88WR03973.
0043-1397/89/88WR0-3973\$05.00

the interface) is accounted for. Such types of interfaces will be called nonsimple interfaces. The nonsimple interface condition is shown to be a generalized form of (2). It is a differential equation relating transport and storage of the interfacial thermodynamic properties to normal fluxes into and out of the two neighboring main domains. The special case of an intermedia zone of negligible thickness but of thermodynamic importance will be called a simple interface.

The derivation of jump conditions for a general interface does not completely characterize the flow and transport. Constitutive postulates, similar to those needed to completely define a multiphase body, are needed to fully describe interface behavior. The postulates supplement the jump conditions. Although the general jump conditions are universal, the constitutive postulates vary depending on the system under study.

In this paper, the above-mentioned general interface condition is derived and its application to some cases of practical interest involving nonsimple interfaces will be illustrated. In these applications, the rationale for obtaining supplementary constitutive postulates will also be provided. Interface conditions for simple interfaces will be presented in a subsequent work where a number of commonly encountered situations are considered.

THE NATURE OF MACROSCOPIC DISCONTINUITIES IN MULTIPHASE SYSTEMS

At the microscopic scale, a multiphase system is composed of two or more phases separated by surfaces or interfaces at which the material properties and thermodynamic quantities may undergo discontinuities. Use of volume-averaging techniques allows a macroscopic description of a multiphase system to be constructed where the aforementioned discontinuities are incorporated into the governing equations. This averaging process is a transformation from the microscale to the macroscale. At the macroscopic scale, a multiphase system is composed of two or more continua superimposed on each other. Therefore initially, the consideration of surfaces of discontinuity at the macroscopic scale may seem to be unnecessary. The averaging process might be expected to remove all discontinuities, even those between two distinctly different neighboring media. For example, consider the hypothetical situation depicted in Figure 1. In Figure 1a, the phase average mass density of the fluid is plotted as a function of space. It appears that as the averaging volume is moved from the single-phase fluid region I to the single-phase solid region III, a continuous variation in the average mass density is obtained. In other words, when considered at the macroscopic scale, no definite surface of discontinuity which marks the boundary of two different media seems to exist. This observation, however, is not valid. In fact, the averaging procedure may not be carried out in regions R_1 and R_2 . When applying the averaging technique to a particular domain, the center of the averaging volume may not get closer than D to the boundary of that domain, where D is the characteristic size of the averaging volume [Hassanizadeh and Gray, 1979a, Appendix A]. Moreover, a major restriction in the macroscopicization process is that the characteristic size of the averaging volume must be much smaller than the length over which gross inhomogeneities in macroscopic properties are encountered [Hassanizadeh and Gray, 1979a]. Clearly, this restriction is not satisfied in regions R_1 and R_2 where the macroscopic characteristic length of the region is of the same order of magnitude as the characteristic size of the averaging volume.

In light of these considerations, a proper application of the averaging procedure to the hypothetical situation discussed here should give the plot depicted in Figure 1b instead of that in Figure 1a. From this figure, it is evident that at the macroscopic scale, narrow regions (such as R_1 and R_2) where rapid changes in material properties occur are not discernable and must be treated as singular surfaces. Additionally, interface conditions must be provided which establish relationships between material properties at the bounding sides of regions R_1 and R_2 . Thermodynamic processes in regions I to III are described by localized macroscopic differential equations of balance. The situation depicted in Figure 1b shows a "simple interface" where the discontinuity persists despite the macroscopicization process.

In addition to the simple interface discussed above, situations may exist where the intermedia zone has a considerable thickness; but, for practical reasons, a three-dimensional modeling of macroscopic processes within the zone may not be of interest. Examples of such zones include a permeable fracture within a porous medium, or a thick layer with low horizontal permeability separating two aquifers. These zones may be described mathematically as two-dimensional domains separating the two main media. They are accounted for as interfaces and will be referred to here as nonsimple interfaces. Additional constitutive conditions must be provided which relate material properties of the main domains to those of the interface.

In the idealized situation depicted in Figure 1, the interfaces are stationary. However, other situations exist where the discontinuity surface or zone may be moving. An example is the formation of filter cake in filtration problems. Also, an important class of moving discontinuity surfaces involves rapid variations in properties of fluids flowing through a porous medium. Examples are interfaces between two miscible fluids with different densities such as a salt water-freshwater interface, interfaces between immiscible fluids (such as the interface between saturated and unsaturated regions or an interface between water and organic phases), a reaction front in a reacting porous medium, a wave front, etc. A final special type of a discontinuity surface is the external boundary of a domain of interest.

DERIVATION OF GENERAL INTERFACE CONDITIONS

Consider a domain between two different multiphase media as depicted in Figure 2 which is not to be fully modeled in three dimensions. This domain exists either by virtue of its own thermodynamic properties (e.g., a thin clay lens between two sandy media) and/or as a consequence of applying a macroscopicization procedure to the two neighboring domains. From a microscopic point of view, the interface region may be considered as a domain in its own right. That is to say, it is a medium composed of two or more phases separated from each other by singular surfaces at which the material properties undergo jump discontinuities.

The actual boundaries of the interface zone with main domains I and II are denoted by B_1 and B_2 in Figure 2. Macroscopic properties for these main domains are defined no closer to the transition zone than A_1 and A_2 , respectively. Thus for example, the centroids of the last row of averaging volumes which lie totally within domain I will fall on the mathematical surface A_1 . The shaded region between A_1 and A_2 forms the interface zone, V . Denote the thickness of the interface by b . This thickness is assumed to be much smaller than the lateral

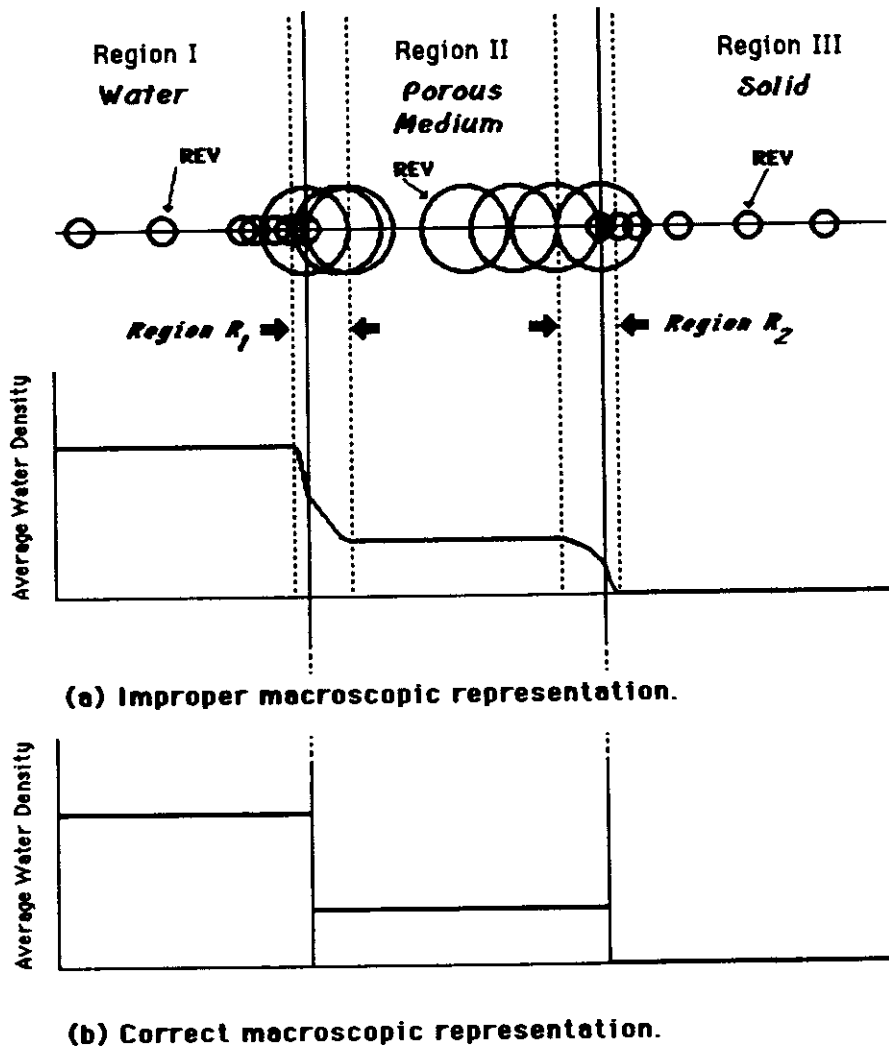


Fig. 1. Variation of average water density with position in the domain.

extent of the domain. Also, based on the discussion presented in the previous section, the restriction

$$b \geq D_1 + D_2 \quad (3)$$

must be satisfied. For a simple interface the equality sign holds; that is, boundaries B_1 and B_2 coincide.

In this development it is assumed that the interface curva-

ture is very small so that the averaging volume remains independent of space as well as time. However, spatial and temporal variations of b are admissible as long as the above assumption (3) is not compromised.

With these considerations in mind, macroscopic conservation laws are sought which relate macroscopic properties of the interface zone to those of the main domains. A mac-

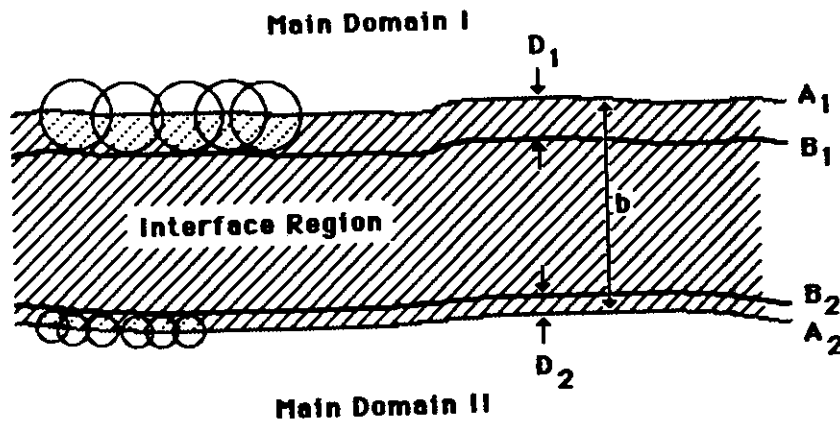


Fig. 2. Nonsimple interface between two main domains.

roscopecization or averaging process is conveniently advanced within the framework of the approach adopted by Gray [1982] for transforming three-dimensional point equations to two-dimensional averaged equations.

For microscopic processes in a multiphase system, the governing equations in each phase are the classical balance laws of continuum mechanics. They may be represented by the general form

$$\frac{\partial(\rho\psi)}{\partial t} + \nabla \cdot (\rho\mathbf{v}\psi) - \nabla \cdot \mathbf{i} - \rho f = \rho G \quad (4)$$

where

- ρ mass density;
- ψ thermodynamic property;
- \mathbf{i} nonadvective flux vector;
- \mathbf{v} velocity vector;
- f external supply;
- G net rate of production.

Individual balance laws are obtained by substituting appropriate quantities from Table 1 into (4). Variables of Table 1 are defined in the notation.

For averaging this equation, a representative elementary volume (REV) is defined which is essentially constant in time and space. This REV is depicted in Figure 3. Note that in the direction (approximately) normal to the interface, the length scale of the REV is greater than b while in the lateral directions, the length scale is smaller than or the same as b . The volume of the REV is denoted as δV_b and its cross section by δS . The area of intersections of A_1 and A_2 in δV_b are denoted as δA_1 and δA_2 , respectively. Additionally, the portion of the boundary surface of δV_b which is in the intermedia zone, not including δA_1 and δA_2 , is indicated as δA . The interfacial area of the α phase with another phase β within the REV and within the intermedia zone is $\delta A_{\alpha\beta}$. Finally, a distribution function $\gamma_{\alpha}^b(\mathbf{x}, t)$ is defined such that

$$\gamma_{\alpha}^b(\mathbf{x}, t) = 1 \quad \text{for } \mathbf{x} \text{ in the } \alpha \text{ phase within the interface zone}$$

$$\gamma_{\alpha}^b(\mathbf{x}, t) = 0 \quad \text{otherwise}$$

Throughout this work, superscript b is employed to label variables associated with the interface. Application of the averaging procedure of Gray [1982] to (4) yields

$$\begin{aligned} & \frac{\partial}{\partial t} (b\langle\rho\rangle_{\alpha}^b \bar{\psi}^{ba}) + \nabla' \cdot (b\langle\rho\rangle_{\alpha}^b \bar{\mathbf{v}}^{ba} \bar{\psi}^{ba}) - \nabla' \cdot (b\bar{\mathbf{i}}^{ba}) - b\langle\rho\rangle_{\alpha}^b \bar{f}^{ba} \\ & - b\langle\rho\rangle_{\alpha}^b \bar{G}^{ba} - \sum_{\beta \neq \alpha} \frac{1}{\delta S} \int_{\delta A_{\alpha\beta}} [\rho\psi(\mathbf{w} - \mathbf{v}) + \mathbf{i}] \cdot \mathbf{n}^{\alpha\beta} da \\ & = \frac{1}{\delta S} \int_{\delta A_1} \gamma_{\alpha}^b [\rho\psi(\mathbf{v} - \mathbf{w}) - \mathbf{i}] \cdot \mathbf{n} da \\ & + \frac{1}{\delta S} \int_{\delta A_2} \gamma_{\alpha}^b [\rho\psi(\mathbf{v} - \mathbf{w}) - \mathbf{i}] \cdot \mathbf{n} da \end{aligned} \quad (5)$$

TABLE 1. Corresponding Variables for Specific Balance Laws Based on General Equation (4)

Property	ψ	\mathbf{i}	f	G
Mass	1	0	0	0
Species	ω	\mathbf{i}	0	r
Momentum	\mathbf{v}	\mathbf{t}	\mathbf{g}	0
Energy	$E + 1/2 \mathbf{v} \cdot \mathbf{v}$	$\mathbf{t} \cdot \mathbf{v} + \mathbf{g}$	$\mathbf{g} \cdot \mathbf{v} + h$	0
Entropy	η	Φ	b	Γ

where \mathbf{w} is the velocity of the area of integration, the prime denotes a two-dimensional spatial vector, and \mathbf{n} on δA_1 and δA_2 points out of domains I and II, respectively. Furthermore,

$$\langle\rho\rangle_{\alpha}^b = \frac{1}{b\delta S} \int_{\delta V_b} \rho \gamma_{\alpha}^b dv \quad (6a)$$

$$\bar{\psi}^{ba} = \frac{1}{b\langle\rho\rangle_{\alpha}^b \delta S} \int_{\delta V_b} \rho \psi \gamma_{\alpha}^b dv \quad (6b)$$

$$\bar{\mathbf{i}}^{ba} = \frac{1}{b\delta S} \int_{\delta V_b} (\mathbf{i} - \rho \bar{\mathbf{v}}^{ba} \bar{\psi}^{ba}) \gamma_{\alpha}^b dv \quad (6c)$$

$$\bar{\psi}^{ba} = \psi - \bar{\psi}^{ba} \quad (6d)$$

Also, $\bar{\mathbf{v}}^{ba}$, \bar{f}^{ba} , and G^{ba} are defined analogously to $\bar{\psi}^{ba}$. All microscopic quantities are functions of time and three spatial dimensions, whereas the averaged quantities depend on time and only the two spatial dimensions tangent to the interface. Note that in these definitions the integral is divided by $b\delta S$ because $b\delta S$ is the actual volume of the transition zone within the REV.

When developed in the work by Gray [1982], (5) was used as a two-dimensional balance law for a region of primary interest with thickness b . The terms on the right side were sources for that region. Here the application is different. Equation (5) serves as a link between two domains where dynamic processes are occurring. The subsequent derivation is designed to illustrate how this linkage can be properly accounted for when the dynamics of the regions neighboring the intermedia zone is of paramount interest. Therefore the source terms must be formulated in terms of the properties of domains I and II at the boundaries of the interface zone. Equation (A4) of Appendix A relates the integral over an area to volume-averaged quantities and may be invoked to express the right-hand side of (5) in terms of volume-averaged quantities. Thus (5) becomes

$$\begin{aligned} & \frac{\partial}{\partial t} (b\langle\rho\rangle_{\alpha}^b \bar{\psi}^{ba}) + \nabla' \cdot (b\langle\rho\rangle_{\alpha}^b \bar{\mathbf{v}}^{ba} \bar{\psi}^{ba}) - \nabla' \cdot (b\bar{\mathbf{i}}^{ba}) - b\langle\rho\rangle_{\alpha}^b \bar{f}^{ba} \\ & - b\langle\rho\rangle_{\alpha}^b \bar{G}^{ba} - \sum_{\beta \neq \alpha} \frac{1}{\delta S} \int_{\delta A_{\alpha\beta}} [\rho\psi(\mathbf{w} - \mathbf{v}) + \mathbf{i}] \cdot \mathbf{n}^{\alpha\beta} da \\ & = [\langle\rho\rangle_{\alpha} \bar{\psi}^{\alpha} (\bar{\mathbf{v}}^{\alpha} - \mathbf{W}) - \bar{\mathbf{i}}^{\alpha}] \cdot \mathbf{N} \end{aligned} \quad (7)$$

where the notation of (1) is employed. In this equation, $\langle\rho\rangle_{\alpha}$, $\bar{\psi}^{\alpha}$, $\bar{\mathbf{v}}^{\alpha}$, and $\bar{\mathbf{i}}^{\alpha}$ are macroscopic properties of phase α obtained by averaging over REV's associated with domains I and II. Equation (7) is the general form of the jump condition for a macroscopic interface. It relates the properties of the two main domains to each other through the properties of the intermedia zone. The last term in the left side of (7) accounts for the exchange of thermodynamic properties between the α phase and all other phases present within the intermedia zone. This exchange may be brought about by chemical and mechanical interactions. The exchange term is subject to the following restriction:

$$\sum_{\beta \neq \alpha} \frac{1}{\delta S} \int_{\delta A_{\alpha\beta}} [\rho\psi(\mathbf{w} - \mathbf{v}) + \mathbf{i}] \cdot \mathbf{n}^{\alpha\beta} da = 0 \quad (7')$$

and plays an essential role in the development of correct interface conditions for multiphase systems.

Any additional information on $\bar{\mathbf{i}}^{ba}$ and the exchange term must be based on the constitution of the intermedia zone and obtained using a constitutive theory. Such an approach is in line with the macroscopic description of multiphase systems in

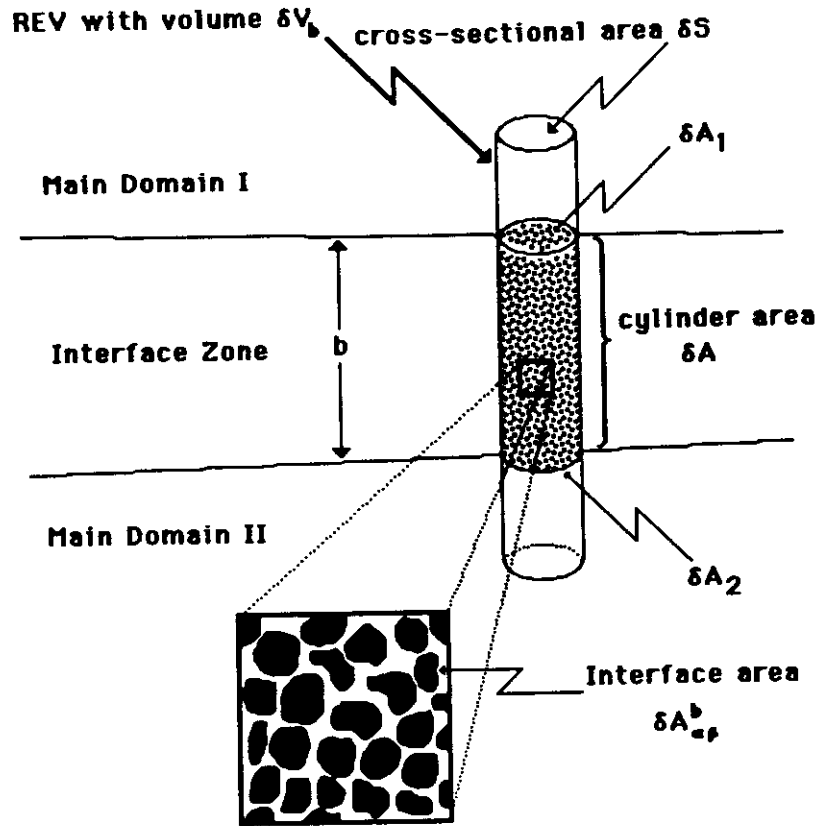


Fig. 3. Averaging volume for a nonsimple interface.

three dimensions. An example of application of constitutive theory to equations of balance similar to (7) is the work by Gray [1983] on derivation of constitutive relations for vertically averaged equations of steam water flow in porous media. The coefficients and functional forms obtained through constitutive analysis must be subjected to experimental verification.

Fully general macroscopic equations of balance of mass, momentum, energy, and entropy are obtained from (7) by selecting appropriate quantities from Table 1. In order to demonstrate the significance of transport terms in the left side of (7) for multiphase systems as well as some simplifications that can be obtained, two special cases of practical importance in porous media flow modeling are considered here. These cases involve nonsimple interfaces separating two main domains.

CONDITIONS FOR A PERMEABLE FRACTURE WITHIN A POROUS MEDIUM

Consider a fracture which is filled with crushed materials within a porous medium such that the fracture has a higher permeability than the surrounding media. Flow is saturated but the fluid is multicomponent. Essentially, the flow within the fracture is two dimensional. However, there is exchange of mass and other thermodynamic properties with the neighboring porous media. It is, of course, possible to model the whole domain as an inhomogeneous system, but then the fracture flow must be considered as three dimensional. However, in situations where the fracture is essentially homogeneous, this approach will result in excessive computational effort. Instead, the porous medium can be conveniently modeled as two three-dimensional systems separated by a two-dimensional fracture interface. Equation (7) then serves as the appropriate differential equation for the fracture zone.

As a special case, the following assumptions will be applied.

1. The deformation of the solid phase in the fracture is such that at the interface between the main domains and the fracture (i.e., at the boundaries of the fracture):

$$\bar{v}^S \cdot N = W \cdot N$$

2. Phase change within the fracture between solid and fluid is negligible such that

$$\rho\psi(w - v) \cdot n^{\alpha\beta} = 0 \quad \text{for all } \psi$$

3. The dependence of fluid mass density on composition is negligible such that it depends only on pressure and temperature.

The saturation of the α phase within the fracture is denoted by $s^{\beta\alpha}$ such that $\langle \rho \rangle_a^b = \epsilon^b s^{\beta\alpha} \langle \rho \rangle^{b\alpha}$, where $\langle \rho \rangle^{b\alpha}$ is the intrinsic average mass density of the α phase within the fracture and ϵ^b is the porosity of the fracture. If notation is now simplified by omitting averaging overbars and brackets, (7) becomes

$$\begin{aligned} & \frac{\partial (b\epsilon^b s^{\beta\alpha} \rho^{b\alpha} \psi^{b\alpha})}{\partial t} + \nabla' \cdot (b\epsilon^b s^{\beta\alpha} \rho^{b\alpha} v^{b\alpha} \psi^{b\alpha}) - \nabla' \cdot (b i^{b\alpha}) \\ & - b\epsilon^b s^{\beta\alpha} \rho^{b\alpha} f^{b\alpha} - b\epsilon^b s^{\beta\alpha} \rho^{b\alpha} G^{b\alpha} - \sum_{\beta \neq \alpha} \frac{1}{\delta S} \int_{\delta A_{\alpha\beta}} i \cdot n^{\alpha\beta} da \\ & = [\rho^{\alpha} \psi^{\alpha} u^{\alpha} - i^{\alpha}] \cdot N \end{aligned} \tag{8}$$

subject to

$$\sum_{\beta \neq \alpha} \frac{1}{\delta S} \int_{\delta A_{\alpha\beta}} i \cdot n^{\alpha\beta} da = 0 \tag{8'}$$

where u^{α} is the Darcian velocity defined by

$$u^{\alpha} = \epsilon s^{\alpha} (v^{\alpha} - v^s) \tag{8''}$$

The definitions of Table 1 will be used along with (8) to obtain the particular balance equations.

Mass

$$\frac{\partial(b\epsilon^b s^{ba} \rho^{ba})}{\partial t} + \nabla' \cdot (b\epsilon^b s^{ba} \rho^{ba} \mathbf{v}^{ba}) = [\rho^a \mathbf{u}^a] \cdot \mathbf{N} \quad (9)$$

This equation relates the storage and flux of mass of the fluid in the plane of the fracture to the mass entering (leaving) the fracture from (into) the main domains. Additional relations for ρ^{ba} , s^{ba} , and \mathbf{v}^{ba} must be provided by constitutive equations of state and by the momentum balance. The fracture orientation, thickness, and porosity are assumed to be known functions of position and time or known functions of the thermodynamic variables of the flow system.

Momentum

$$\frac{\partial(b\epsilon^b s^{ba} \rho^{ba} \mathbf{v}^{ba})}{\partial t} + \nabla' \cdot (b\epsilon^b s^{ba} \rho^{ba} \mathbf{v}^{ba} \mathbf{v}^{ba}) - \nabla' \cdot (b\mathbf{t}^{ba}) - b\epsilon^b s^{ba} \rho^{ba} \mathbf{g} - \sum_{\beta \neq \alpha} \frac{1}{\delta S} \int_{\delta A_{\alpha\beta}} \mathbf{t} \cdot \mathbf{n}^{\alpha\beta} da = [\rho^a \mathbf{v}^a \mathbf{u}^a - \mathbf{t}^a] \cdot \mathbf{N} \quad (10)$$

Multiply (9) by \mathbf{v}^{ba} and subtract from (10) to obtain

$$b\epsilon^b s^{ba} \rho^{ba} \frac{\partial \mathbf{v}^{ba}}{\partial t} + b\epsilon^b s^{ba} \rho^{ba} \mathbf{v}^{ba} \cdot \nabla' \mathbf{v}^{ba} - \nabla' \cdot (b\mathbf{t}^{ba}) - b\epsilon^b s^{ba} \rho^{ba} \mathbf{g} - \sum_{\beta \neq \alpha} \frac{1}{\delta S} \int_{\delta A_{\alpha\beta}} \mathbf{t} \cdot \mathbf{n}^{\alpha\beta} da = [\rho^a (\mathbf{v}^a - \mathbf{v}^{ba}) \mathbf{u}^a - \mathbf{t}^a] \cdot \mathbf{N} \quad (11)$$

This equation requires constitutive assumptions in order to be easily applied. First, based on the work of Hassanizadeh and Gray [1980] and of Gray [1983], the fluid phase stress may be approximated as

$$\mathbf{t}^{ba} = -\epsilon^b s^{ba} p^{ba} \mathbf{1}'' \quad (12)$$

$$\mathbf{t}^a = -\epsilon^a s^a p^a \mathbf{1} \quad (13)$$

Appendix B motivates the relation

$$\sum_{\beta \neq \alpha} \frac{1}{\delta S} \int_{\delta A_{\alpha\beta}} \mathbf{t} \cdot \mathbf{n}^{\alpha\beta} da = p^{ba} \nabla' (b\epsilon^b s^{ba}) - [p^a \epsilon^a \mathbf{N}] + \epsilon^b s^{ba} [p^a] \mathbf{N} - bR''^a \cdot \mathbf{u}^{ba} - bR_N''^a [\chi^a \mathbf{u}^a \cdot \mathbf{N}] \mathbf{N} \quad (14)$$

where p is the thermodynamic pressure, R''^a is the medium resistance to the flow within the fracture, $R_N''^a$ accounts for resistance to the flow from domain I and II across the fracture, \mathbf{u}^{ba} is the two-dimensional Darcy velocity vector tangent to the fracture, and χ_1^a and χ_2^a apportion the resistance to the flow entering the fracture from domains I and II, respectively. Equations (12) through (14) make use of the fact that porous media flow is macroscopically inviscid. Additionally, equations of state for the α phase relate the mass density to pressure and temperature:

$$\rho^a = \rho^a(p^a, T^a) \quad (15a)$$

$$\rho^{ba} = \rho^{ba}(p^{ba}, T^{ba}) \quad (15b)$$

Substitution of (12) through (14) into (11) results in

$$b\epsilon^b s^{ba} \rho^{ba} \frac{\partial \mathbf{v}^{ba}}{\partial t} + b\epsilon^b s^{ba} \rho^{ba} \mathbf{v}^{ba} \cdot \nabla' \mathbf{v}^{ba} + \nabla' (b\epsilon^b s^{ba} p^{ba}) - b\epsilon^b s^{ba} \rho^{ba} \mathbf{g} - p^{ba} \nabla' (b\epsilon^b s^{ba}) + [\epsilon^a p^a] \mathbf{N} - \epsilon^b s^{ba} [p^a] \mathbf{N} + bR''^a \cdot \mathbf{u}^{ba} + bR_N''^a [\chi^a \mathbf{u}^a \cdot \mathbf{N}] \mathbf{N} = [\rho^a (\mathbf{v}^a - \mathbf{v}^{ba}) \mathbf{u}^a + \epsilon^a p^a \mathbf{1}] \cdot \mathbf{N} \quad (16)$$

The term involving pressure on the right side of (16) cancels with the same term on the left side. When the flow in the porous medium is slow such that inertial terms are negligible, (16) reduces further to

$$b\epsilon^b s^{ba} (\nabla' p^{ba} - \rho^{ba} \mathbf{g}) - \epsilon^b s^{ba} [p^a] \mathbf{N} + bR''^a \cdot \mathbf{u}^{ba} + bR_N''^a [\chi^a \mathbf{u}^a \cdot \mathbf{N}] \mathbf{N} = 0 \quad (17)$$

This equation has components in directions normal and tangential to the interface zone. The tangential components of this equation, after rearrangement, yield an equivalent form of Darcy's law within the fracture:

$$\mathbf{u}^{ba} = -\epsilon^b s^{ba} (R''^a)^{-1} \cdot (\nabla' p^{ba} - \rho^{ba} \mathbf{g}) \quad (18)$$

Equations (9), (15), and (18) provide four equations in terms of five unknowns ρ^{ba} , s^{ba} , p^{ba} , and \mathbf{u}^{ba} when the flow is isothermal. An additional needed equation for multiphase flow is normally provided by a relationship between s^{ba} and the capillary pressure.

The mass and momentum equations for the fractures can be solved only in conjunction with the equations of mass and momentum of the two main domains. Additional equations which link the interface zone process to $\mathbf{u}_1^a \cdot \mathbf{N}_1$, and $\mathbf{u}_2^a \cdot \mathbf{N}_2$ can be obtained from the normal component of (17):

$$-b\epsilon^b s^{ba} \rho^{ba} \mathbf{g} \cdot \mathbf{N}_1 - \epsilon^b s^{ba} (p_1^a - p_2^a) + bR_N''^a (\chi_1^a \mathbf{u}_1^a \cdot \mathbf{N}_1 - \chi_2^a \mathbf{u}_2^a \cdot \mathbf{N}_2) = 0 \quad (19)$$

Equation (19) may be rearranged to the form

$$\{bR_N''^a \chi_1^a \mathbf{u}_1^a \cdot \mathbf{N}_1 + \epsilon^b s^{ba} [(p^{ba} - p_1^a) - \chi_1^a b\rho^{ba} \mathbf{g} \cdot \mathbf{N}_1] - \{bR_N''^a \chi_2^a \mathbf{u}_2^a \cdot \mathbf{N}_2 + \epsilon^b s^{ba} [(p^{ba} - p_2^a) - \chi_2^a b\rho^{ba} \mathbf{g} \cdot \mathbf{N}_2]\} = 0 \quad (20)$$

because $0 \leq \chi_1^a \leq 1$ and $\chi_1^a + \chi_2^a = 1$.

Equation (20) describes the transfer of momentum in the normal direction between the main domains and the fracture. This equation may be split into two parts by selecting χ_1^a (and thereby χ_2^a) such that each of the bracketed quantities is individually zero. This allows two equations to be written, one accounting for momentum transfer between domain I and the fracture and another accounting for transfer between domain II and the fracture. Thus from (20) it follows that

$$\mathbf{u}_1^a \cdot \mathbf{N}_1 = \frac{-\epsilon^b s^{ba}}{R_N''^a} \left[\frac{p^{ba} - p_1^a}{b\chi_1^a} - \rho^{ba} \mathbf{g} \cdot \mathbf{N}_1 \right] \quad (21a)$$

$$\mathbf{u}_2^a \cdot \mathbf{N}_2 = \frac{-\epsilon^b s^{ba}}{R_N''^a} \left[\frac{p^{ba} - p_2^a}{b\chi_2^a} - \rho^{ba} \mathbf{g} \cdot \mathbf{N}_2 \right] \quad (21b)$$

The constitutive parameter $\chi_1^a (= 1 - \chi_2^a)$ may be specified based on the system under consideration. The following selected cases are examples: (1) when the interface zone is permeable but the flow normal to the zone is negligible such that the pressure is hydrostatic, $\chi_1^a = 0.5$; (2) when the main domain I is impermeable to the α phase, $\chi_1^a = 0.0$ and $p_1^a = p^{ba}$; (3) when $R_N''^a$ is infinite such that the interface zone is impermeable, (21) reduce to $\mathbf{u}_1^a \cdot \mathbf{N}_1 = \mathbf{u}_2^a \cdot \mathbf{N}_2 = 0$; and (4) when main domains I and II have the same properties (porosity, permeability, temperature, density), $\chi_1^a = \chi_2^a = 0.5$. Other cases which may exist may be modeled by appropriate selection of a value of χ_1^a between 0.0 and 1.0.

Mass Balance for Species

The balance of mass for a species existing in the α phase reads

$$\begin{aligned} \frac{\partial (b\epsilon^b s^{ba} \rho^{ba} \omega^{ba})}{\partial t} + \nabla' \cdot (b\epsilon^b s^{ba} \rho^{ba} \omega^{ba} \mathbf{v}^{ba}) - \nabla' \cdot \mathbf{j}^{ba} \\ = b\epsilon^b s^{ba} \rho^{ba} r^{ba} + \sum_{\beta \neq \alpha} \frac{1}{\delta S} \int_{\delta A_{\alpha\beta}} \mathbf{j} \cdot \mathbf{n}^{\alpha\beta} da \\ + [\rho^\alpha \omega^\alpha \mathbf{u}^\alpha - \mathbf{j}^\alpha] \cdot \mathbf{N} \end{aligned} \quad (22)$$

The first term on the right side accounts for homogeneous reactions and/or decay, and the second term denotes the heterogeneous mass exchange of the species between the α phase and all other phases as a result of adsorption and interphase diffusion process.

Constitutive equations have to be provided for \mathbf{j}^{ba} and $\sum_{\beta \neq \alpha} (1/\delta S) \int_{\delta A_{\alpha\beta}} \mathbf{j} \cdot \mathbf{n}^{\alpha\beta} da$. In particular, a Fickian type relation may be employed for \mathbf{j}^{ba} :

$$\mathbf{j}^{ba} = \rho^{ba} \mathbf{D}^{ba} \cdot \nabla' \omega^{ba} \quad (23)$$

where \mathbf{D}^{ba} is the dispersion tensor for the fracture zone.

To complete the description of the mass transfer problem, constitutive relations for $\mathbf{j}_1^\alpha \cdot \mathbf{N}_1$ and $\mathbf{j}_2^\alpha \cdot \mathbf{N}_2$ must be proposed in terms of $(\omega_1^\alpha, \omega^{ba})$ and $(\omega_2^\alpha, \omega^{ba})$ respectively. A reasonable proposition may be obtained by analogy with (21) using a mass transfer resistance coefficient $R_N^{\omega\alpha}$ and weighting parameter $\chi_1^{\omega\alpha}$ and $\chi_2^{\omega\alpha}$ such that

$$\mathbf{j}_1^\alpha \cdot \mathbf{N}_1 = (\omega^{ba} - \omega_1^\alpha) / (\chi_1^{\omega\alpha} R_N^{\omega\alpha}) \quad (24a)$$

$$\mathbf{j}_2^\alpha \cdot \mathbf{N}_2 = (\omega^{ba} - \omega_2^\alpha) / (\chi_2^{\omega\alpha} R_N^{\omega\alpha}) \quad (24b)$$

The resistance coefficients must be obtained empirically depending on the system under study. Note that $\chi_1^{\omega\alpha}$ and $\chi_2^{\omega\alpha}$ sum to 1.0 and are related to the resistance to the nonadvective fluxes. For example, when there is no resistance to a dispersive flux from domain I into the fracture zone, $\chi_1^{\omega\alpha} = 0.0$ and therefore for a finite flux, $\omega^{ba} = \omega_1^\alpha$. When the resistance to dispersive flux into the fracture is the same for both bounding domains, $\chi_1^{\omega\alpha} = \chi_2^{\omega\alpha} = 0.5$. Other cases may also be considered in the context of the relations given in (24). Equations (22) through (24) together with the transport equation for domains I and II comprise a set of equations to be solved for ω^{ba} and the mass fraction in I and II.

Energy Balance

$$\begin{aligned} \frac{\partial}{\partial t} \{ b\epsilon^b s^{ba} \rho^{ba} (E^{ba} + \frac{1}{2} \mathbf{v}^{ba} \cdot \mathbf{v}^{ba}) \} \\ + \nabla' \cdot \{ b\epsilon^b s^{ba} \rho^{ba} (E^{ba} + \frac{1}{2} \mathbf{v}^{ba} \cdot \mathbf{v}^{ba}) \mathbf{v}^{ba} \} \\ - \nabla' \cdot (b\mathbf{t}^{ba} \cdot \mathbf{v}^{ba} + b\mathbf{q}^{ba}) - b\epsilon^b s^{ba} \rho^{ba} (h^\alpha + \mathbf{g} \cdot \mathbf{v}^{ba}) \\ = \sum_{\beta \neq \alpha} \frac{1}{\delta S} \int_{\delta A_{\alpha\beta}} (\mathbf{t} \cdot \mathbf{v} + \mathbf{q}) \cdot \mathbf{n}^{\alpha\beta} da \\ + [\rho^\alpha (E^\alpha + \frac{1}{2} \mathbf{v}^\alpha \cdot \mathbf{v}^\alpha) \mathbf{u}^\alpha - \mathbf{t}^\alpha \cdot \mathbf{v}^\alpha - \mathbf{q}^\alpha] \cdot \mathbf{N} \end{aligned} \quad (25)$$

Multiply (9) with $(E^{ba} + \frac{1}{2} \mathbf{v}^{ba} \cdot \mathbf{v}^{ba})$, take the inner product of (10) with \mathbf{v}^{ba} , and subtract the results from (25) to obtain the internal energy equation

$$\begin{aligned} b\epsilon^b s^{ba} \rho^{ba} \left(\frac{\partial E^{ba}}{\partial t} + \mathbf{v}^{ba} \cdot \nabla' E^{ba} \right) \\ - b\mathbf{t}^{ba} : \nabla' \mathbf{v}^{ba} - \nabla' \cdot (b\mathbf{q}^{ba}) - b\epsilon^b s^{ba} \rho^{ba} h^{ba} \\ = \sum_{\beta \neq \alpha} \frac{1}{\delta S} \int_{\delta A_{\alpha\beta}} [\mathbf{t} \cdot (\mathbf{v} - \mathbf{v}^{ba}) + \mathbf{q}] \cdot \mathbf{n}^{\alpha\beta} da \\ + [\rho^\alpha \{ (E^\alpha + \frac{1}{2} \mathbf{v}^\alpha \cdot \mathbf{v}^\alpha) - (E^{ba} + \frac{1}{2} \mathbf{v}^{ba} \cdot \mathbf{v}^{ba}) \} \mathbf{u}^\alpha \\ - \mathbf{t}^\alpha \cdot (\mathbf{v}^\alpha - \mathbf{v}^{ba}) - \mathbf{q}^\alpha] \cdot \mathbf{N} \end{aligned} \quad (26)$$

Some of the quantities in this equation, such as s^{ba} , ρ^{ba} , \mathbf{v}^{ba} , and \mathbf{t}^{ba} , have been introduced in the equations of mass and momentum balance discussed earlier. Here, additional constitutive equations are needed for E^{ba} and \mathbf{q}^{ba} in terms of temperature and temperature gradient. The following linear relations are employed (where the dependence of E^{ba} on pressure has been neglected for simplicity):

$$dE^{ba} = C_v^{ba} dT^{ba} \quad (27)$$

$$\mathbf{q}^{ba} = \kappa^{ba} \cdot \nabla' T^{ba} \quad (28)$$

$$\begin{aligned} \sum_{\beta \neq \alpha} \frac{1}{\delta S} \int_{\delta A_{\alpha\beta}} [\mathbf{t} \cdot (\mathbf{v} - \mathbf{v}^{ba}) + \mathbf{q}] \cdot \mathbf{n}^{\alpha\beta} da \\ = - \sum_{\beta} \lambda^{\alpha\beta} (T^{ba} - T^{b\beta}) \end{aligned} \quad (29a)$$

subject to

$$\sum_{\alpha} \sum_{\beta} \lambda^{\alpha\beta} (T^{ba} - T^{b\beta}) = 0 \quad (29b)$$

where T^{ba} is the temperature of the α phase within the fracture. Substitution of (12)–(16) and (27)–(29) into (26) yields

$$\begin{aligned} b\epsilon^b s^{ba} \rho^{ba} C_v^{ba} \left(\frac{\partial T^{ba}}{\partial t} + \mathbf{v}^{ba} \cdot \nabla' T^{ba} \right) \\ + b\epsilon^b s^{ba} \rho^{ba} \nabla' \cdot \mathbf{v}^{ba} - \nabla' \cdot (b\kappa^{ba} \cdot \nabla' T^{ba}) \\ - b\epsilon^b s^{ba} \rho^{ba} h^{ba} = - \sum_{\beta} \lambda^{\alpha\beta} (T^{ba} - T^{b\beta}) \\ + [\rho^\alpha \{ (E^\alpha + \frac{1}{2} \mathbf{v}^\alpha \cdot \mathbf{v}^\alpha) - (E^{ba} + \frac{1}{2} \mathbf{v}^{ba} \cdot \mathbf{v}^{ba}) \} \mathbf{u}^\alpha \\ + \epsilon^\alpha p^\alpha (\mathbf{v}^\alpha - \mathbf{v}^{ba}) - \mathbf{q}^\alpha] \cdot \mathbf{N} \end{aligned} \quad (30)$$

Often, in heat transport problems in porous media, the effects of potential forces and kinetic energy and radiation are neglected. For that case (30) reduces to

$$\begin{aligned} b\epsilon^b s^{ba} \rho^{ba} C_v^{ba} \left(\frac{\partial T^{ba}}{\partial t} + \mathbf{v}^{ba} \cdot \nabla' T^{ba} \right) - \nabla' \cdot (b\kappa^{ba} \cdot \nabla' T^{ba}) \\ = - \sum_{\beta} \lambda^{\alpha\beta} (T^{ba} - T^{b\beta}) + [\rho^\alpha (E^\alpha - E^{ba}) \mathbf{u}^\alpha - \mathbf{q}^\alpha] \cdot \mathbf{N} \end{aligned} \quad (31)$$

The first term on the right-hand side of this equation accounts for the exchange of heat between the α phase and all other phases within the transition zone as the fluid phase passes through this zone. This equation can be employed to solve for the temperature of the α phase in the fracture zone. However, this equation must be solved in conjunction with equations of balance for the two main domains as well as the balance equations for the other phases in the system. Constitutive functions are also needed which describe the nonadvective heat transfer between the main domains and the fracture. These can be expressed, for example, by analogy with mass transfer hypotheses (24) as

$$\mathbf{q}_1^\alpha \cdot \mathbf{N}_1 = (T^{ba} - T_1^\alpha) / (\chi_1^{T\alpha} R_N^{T\alpha}) \quad (32a)$$

$$\mathbf{q}_2^\alpha \cdot \mathbf{N}_2 = (T^{ba} - T_2^\alpha) / (\chi_2^{T\alpha} R_N^{T\alpha}) \quad (32b)$$

The heat transfer resistance coefficients, $R_N^{T\alpha}$ and $\chi_1^{T\alpha} (= 1 - \chi_2^{T\alpha})$, must be obtained empirically depending on the characteristics of the system under study.

The solution of the energy balance simplifies significantly when all phases at a point may be considered to be at local thermal equilibrium, i.e., at the same temperature. In this case, (31) may be summed over all α phases and the resultant equation may be solved in conjunction with the balance equation for the main domain to obtain the temperature distribution T^b

within the fracture and the temperature distribution in domains I and II.

CONDITIONS FOR A SEMIPERMEABLE LAYER WITHIN A POROUS MEDIUM

Consider a thin layer within a porous medium which has a much lower permeability than the surrounding domains. In this case the transport of matter within the layer in the tangential direction will not be significant and storage within the layer is also considered unimportant. However, the role of the layer in the exchange of thermodynamic properties between the porous media on the two sides of the layer is important. In developing balance equations for this case, assumptions 1-4 described in the previous section are adopted. Furthermore, because storage and transport of thermodynamic properties in the plane of the layer are negligible, the time and spatial derivatives in the equations of balance for the layer may be neglected. The following equations are obtained as simplifications of balances derived in the preceding section.

Mass Balance (from Equation (9))

Neglect the left hand side of (9) to obtain

$$[\rho^a \mathbf{u}^a] \cdot \mathbf{N} = 0 \quad (33)$$

which is simply a statement of continuity of normal flux. Note that if storage, but not transport, were important, the time derivative term could be retained. However, that case is not being considered here.

Momentum Balance (from Equation (17))

With the tangential flow in the layer assumed to be negligible, the tangential components of (17) reduce to the statement of hydrostatic equilibrium. However, the normal components, equations (21), will remain as they account for flow across the layer. When storage is negligible, p^{ba} may be eliminated from consideration and (33) indicates that the flow entering one side of the layer is equal to the flow leaving the other side.

Elimination of p^{ba} between (21a) and (21b) yields

$$\begin{aligned} \rho_1^a \mathbf{u}_1^a \cdot \mathbf{N}_1 &= \rho_2^a \mathbf{u}_2^a \cdot \mathbf{N}_1 \\ &= - \frac{\rho_1^a \rho_2^a \varepsilon^b s^{ba}}{R_N^a (\chi_1^a \rho_1^a + \chi_2^a \rho_2^a)} \left[\frac{p_2^a - p_1^a}{b} - \rho^{ba} \mathbf{g} \cdot \mathbf{N}_1 \right] \end{aligned} \quad (34)$$

where use has been made of the fact that $\chi_1^a + \chi_2^a = 1$ and $\mathbf{N}_2 = -\mathbf{N}_1$. This equation is of the same form as is commonly used in describing flow across a semipermeable layer, where R_N^a is the resistance of the medium to the flow. Note that when $\rho_1^a = \rho_2^a$, the constitutive parameters χ_1^a and χ_2^a disappear from (34). When $\rho_1^a \neq \rho_2^a$, selection of $\chi_1^a = \chi_2^a = 0.5$ is appropriate.

Mass Balance for Species (from Equation (23))

When the rate of accumulation of a chemical species within the α phase of a layer as well as the lateral transport are negligible, the species mass balance equation (22) becomes

$$\begin{aligned} b \varepsilon^b s^{ba} \rho^{ba} r^{ba} + \sum_{\beta \neq a} \frac{1}{\delta S} \int_{\delta A_{a\beta}} \mathbf{j} \cdot \mathbf{m}^{\beta} da \\ + [\rho^a \omega^a \mathbf{u}^a - \mathbf{j}^a] \cdot \mathbf{N} = 0 \end{aligned} \quad (35)$$

If the homogeneous reaction within the α phase in the layer is negligible, the first term in (35) drops out. If adsorption/desorption processes are negligible, the second term in (35) may also be eliminated. Finally, (33) may be applied such that

(35) reduces to

$$\rho_1^a \mathbf{u}_1^a \cdot \mathbf{N}_1 (\omega_1^a - \omega_2^a) - [\mathbf{j}^a] \cdot \mathbf{N} = 0 \quad (36)$$

The interface zone equation must be solved in conjunction with two constitutive equations such as (24a) and (24b). However, under conditions where the reactions and storage are unimportant such that ω^{ba} is not needed and (36) applies, ω^{ba} may be eliminated between (24a) and (24b). Combination of this result with (36) yields

$$\begin{aligned} \mathbf{j}_1^a \cdot \mathbf{N}_1 &= [\rho_1^a \mathbf{u}_1^a \cdot \mathbf{N}_1 \chi_2^{aa} - (R_N^{aa})^{-1} (\omega_1^a - \omega_2^a)] \\ \mathbf{j}_2^a \cdot \mathbf{N}_2 &= [\rho_2^a \mathbf{u}_2^a \cdot \mathbf{N}_2 \chi_1^{aa} - (R_N^{aa})^{-1} (\omega_2^a - \omega_1^a)] \end{aligned} \quad (37)$$

Equation (37) in conjunction with the equations for the main domains are sufficient conditions for obtaining solutions for mass fractions in the main domain.

Energy Balance (from Equation (31))

When time and space variation in the layer can be neglected, the energy balance in (31) reduces to the form

$$[\varepsilon^a \rho^a (E^a - E^{ba}) \mathbf{u}^a - \mathbf{q}^a] \cdot \mathbf{N} = \sum_{\beta} \lambda^{\alpha\beta} (T^{ba} - T^{b\beta}) \quad (38)$$

This equation must be solved in conjunction with constitutive equation (32a) and (32b) along with balance equation for the main domains. When local thermal equilibrium is achieved, the right-hand side of (38) is zero. If storage is negligible such that (33) also applies then

$$\rho_1^a \mathbf{u}_1^a \cdot \mathbf{N}_1 (E_1^a - E_2^a) - [\mathbf{q}^a] \cdot \mathbf{N} = 0 \quad (39)$$

For this case, T^{ba} is not needed and the conditions (32) can be combined with (39) by a procedure analogous to that used to obtain (37) for species transport. In the current case the result is

$$\mathbf{q}_1^a \cdot \mathbf{N}_1 = \rho_1^a \mathbf{u}_1^a \cdot \mathbf{N}_1 \chi_2^{Ta} (E_1^a - E_2^a) - (R_N^{Ta})^{-1} (T_1^a - T_2^a) \quad (40a)$$

$$\mathbf{q}_2^a \cdot \mathbf{N}_2 = \rho_2^a \mathbf{u}_2^a \cdot \mathbf{N}_2 \chi_1^{Ta} (E_2^a - E_1^a) - (R_N^{Ta})^{-1} (T_2^a - T_1^a) \quad (40b)$$

Because local thermal equilibrium has been assumed, (40) may be summed over all α phases to obtain expressions for the total nonadvective energy transport across the layer. Solution of these equations in conjunction with the energy balances for domains I and II yields the complete temperature profile for the systems of interest.

CONCLUSION

The framework presented here allows for conditions at large-scale interfaces between porous media zones to be derived from fundamental principles. An interface may be either a surface of discontinuity at the microscale or a zone in which transport normal to the boundary surfaces may be accounted for on a global average. The general interface condition, (7), relates the properties at the boundaries of the media to the transport occurring within the interface. The interface condition for a general property has been applied to the specific cases of mass, momentum, chemical species, and energy transport into a fracture of high permeability and across a clay lens of limited permeability. The general techniques presented allow for a complete and rigorous analysis of multiphase systems which undergo jump changes in properties such as temperature, porosity, saturation, permeability.

APPENDIX A: EQUIVALENCE OF AREA- AND VOLUME-AVERAGED FLUXES

Consider an arbitrary surface, A , lying within a multiphase domain, and an REV whose cross section intersecting A is ΔA with a normal unit vector \mathbf{n} . If ΔA is a plane, \mathbf{n} is constant within the REV. The characteristic length of ΔA will also be the same as that of the REV. One may define average quantities based on this REV in the usual fashion. Additionally, the volume-averaged flux of a given quantity ψ will be

$$\langle \langle \rho \rangle_v \bar{\psi}^{\alpha} \bar{\mathbf{v}}^{\alpha} - \mathbf{i}^{\alpha} \rangle \cdot \mathbf{N} = \frac{1}{\Delta V} \left(\int_{\Delta V} \gamma^{\alpha} (\rho \psi \mathbf{v} - \mathbf{i}) \, dv \right) \cdot \mathbf{n} \quad (A1)$$

where \mathbf{N} is the unit vector normal to A at the centroid of ΔA . The vector \mathbf{N} is identical to \mathbf{n} . However, to be systematic in notation, here \mathbf{n} is used in the microscopic domain, and \mathbf{N} is employed in the macroscopic domain. The integral on the right side of (A1) may be written as

$$\frac{1}{\Delta V} \int_{-D/2}^{D/2} \left(\int_{\Delta A_{(i)}} \gamma^{\alpha} (\rho \psi \mathbf{v} - \mathbf{i}) \cdot \mathbf{n} \, da \right) dl \quad (A2)$$

where $\Delta A_{(i)}$ are other cross sections of the REV having the same unit normal vector \mathbf{n} . Now using the mean value theorem, one may replace the line integral in (A2) to obtain

$$\frac{D}{\Delta V} \int_{\Delta A} \gamma^{\alpha} (\rho \psi \mathbf{v} - \mathbf{i}) \cdot \mathbf{n} \, da \quad (A3)$$

Finally, with $\Delta A \equiv \Delta V/D$, (A3) may be substituted for the right side of (A1) to obtain

$$\langle \langle \rho \rangle_v \bar{\psi}^{\alpha} \bar{\mathbf{v}}^{\alpha} - \mathbf{i}^{\alpha} \rangle \cdot \mathbf{N} = \frac{1}{\Delta A} \int_{\Delta A} \gamma^{\alpha} (\rho \psi \mathbf{v} - \mathbf{i}) \cdot \mathbf{n} \, da \quad (A4)$$

which is the desired relation of equality of volume- and area-averaged fluxes.

An alternative derivation of this relation follows from using theorem IV of Hassanizadeh and Gray [1979a]:

$$\int_V \nabla \cdot \langle \mathbf{f} \rangle^{\alpha} \, dv = \int_A \frac{1}{\Delta A} \int_{\Delta A} \mathbf{f} \gamma^{\alpha} \cdot \mathbf{n} \, da \, dA \quad (A5)$$

where V is any volume with the boundary A . Applying the divergence theorem to the left-hand side, one obtains

$$\int_A \langle \mathbf{f} \rangle^{\alpha} \cdot \mathbf{N} \, dA = \int_A \frac{1}{\Delta A} \int_{\Delta A} \mathbf{f} \gamma^{\alpha} \cdot \mathbf{n} \, da \, dA \quad (A6)$$

Because A is an arbitrary surface, one may localize this relation to obtain

$$\langle \mathbf{f} \rangle^{\alpha} \cdot \mathbf{N} = \frac{1}{\Delta A} \int_{\Delta A} \mathbf{f} \gamma^{\alpha} \cdot \mathbf{n} \, da \quad (A7)$$

This relation is a more general equivalent of (A4). Equations similar to (A4) have also been obtained by Bear and Bachmat [1983] using a different approach.

APPENDIX B: CONSTITUTIVE EQUATION FOR

$$\sum_{\alpha \neq \alpha} (1/\delta S) \int_{\delta A_{\alpha\beta}} \mathbf{t} \cdot \mathbf{n}^{\alpha\beta} \, da = \hat{\mathbf{T}}^{\alpha\beta}$$

This term actually denotes the forces on the fluid flowing through an interface zone exerted by other phases. These forces are known to consist of an equilibrium part and a nonequilibrium or dissipative part. These two parts arise from the corresponding parts of the microscopic stress tensor \mathbf{t} :

$$\mathbf{t} = -p\mathbf{1} + \boldsymbol{\tau} \quad (B1)$$

where p is the microscopic pressure (equilibrium part of \mathbf{t}) and $\boldsymbol{\tau}$ is the dissipative part of the stress.

As a first step, evaluate $\hat{\mathbf{T}}^{\alpha\beta}$ at equilibrium:

$$\hat{\mathbf{T}}^{\alpha\beta} \Big|_e = - \sum_{\beta \neq \alpha} \frac{1}{\delta S} \int_{\delta A_{\alpha\beta}} p \mathbf{n}^{\alpha\beta} \, da \quad (B2)$$

From (16) of Gray [1982] one obtains (with f set to 1 in that equation):

$$\sum_{\beta \neq \alpha} \frac{1}{\delta S} \int_{\delta A_{\alpha\beta}} \mathbf{n}^{\alpha\beta} \, da = \frac{1}{\delta S} \int_{\delta A_{\alpha\Gamma}} \gamma_{\alpha}^b \mathbf{n}_1 \, da + \frac{1}{\delta S} \int_{\delta A_{\alpha\beta}} \gamma_{\alpha}^b \mathbf{n}_2 \, da - \nabla'(b\epsilon^{\alpha\beta}) \quad (B3)$$

Now, consider (B2). Recall that $\delta S_{\alpha\beta}$ is the union of all $\alpha\beta$ interfaces within the domain lying between A_1 and A_2 in Figure 2. Therefore (B2) may be written as

$$\hat{\mathbf{T}}^{\alpha\beta} \Big|_e = - \frac{1}{\delta S} \int_{\delta A_{\alpha\beta}^{A_1-A_2}} p \mathbf{n}^{\alpha\beta} \, da - \frac{1}{\delta S} \int_{\delta A_{\alpha\beta}^{B_1-B_2}} p \mathbf{n}^{\alpha\beta} \, da - \frac{1}{\delta S} \int_{\delta A_{\alpha\beta}^{B_2-A_2}} p \mathbf{n}^{\alpha\beta} \, da \quad (B4)$$

Assuming that the porous materials in each of regions $A_1 - B_1$, $B_1 - B_2$, and $B_2 - A_2$ are homogeneous and that the pressure p varies linearly in each of these respective regions, one may reduce (B4) to

$$\hat{\mathbf{T}}^{\alpha\beta} \Big|_e = -p_1 \left(\frac{1}{\delta S} \int_{\delta A_{\alpha\beta}^{A_1-B_1}} \mathbf{n}^{\alpha\beta} \, da \right) - p_2 \left(\frac{1}{\delta S} \int_{\delta A_{\alpha\beta}^{B_1-B_2}} \mathbf{n}^{\alpha\beta} \, da \right) - p^{\beta\alpha} \left(\frac{1}{\delta S} \int_{\delta A_{\alpha\beta}^{B_2-A_2}} \mathbf{n}^{\alpha\beta} \, da \right) \quad (B5)$$

Now, use (B3) to obtain

$$\begin{aligned} \hat{\mathbf{T}}^{\alpha\beta} \Big|_e = & -p_1 \left\{ \frac{1}{\delta S} \int_{\delta A_{\alpha\beta}^{A_1}} \gamma_{\alpha}^b \mathbf{n}_1 \, da - \frac{1}{\delta S} \int_{\delta A_{\alpha\beta}^{B_1}} \gamma_{\alpha}^b \mathbf{n}_1 \, da - \nabla'[D_1 \epsilon_1^{\alpha}] \right\} \\ & - p_2 \left\{ \frac{1}{\delta S} \int_{\delta A_{\alpha\beta}^{A_2}} \gamma_{\alpha}^b \mathbf{n}_2 \, da - \frac{1}{\delta S} \int_{\delta A_{\alpha\beta}^{B_2}} \gamma_{\alpha}^b \mathbf{n}_2 \, da - \nabla'[D_2 \epsilon_2^{\alpha}] \right\} \\ & - p^{\beta\alpha} \left\{ \frac{1}{\delta S} \int_{\delta A_{\alpha\beta}^{A_1}} \gamma_{\alpha}^b \mathbf{n}_1 \, da - \frac{1}{\delta S} \int_{\delta A_{\alpha\beta}^{B_2}} \gamma_{\alpha}^b \mathbf{n}_1 \, da - \nabla'[(b - D_1 - D_2)\epsilon^{\alpha\beta}] \right\} \end{aligned} \quad (B6)$$

Terms such as $\int_{\delta A} \gamma_{\alpha}^b \, da$ are equal to the areal fraction of phase α . Assuming that areal and volume fractions are equal, and also assuming that the fracture is filled with a homogeneous material, one has

$$\frac{1}{\delta S} \int_{\delta A_{\alpha\beta}^{A_1}} \gamma_{\alpha}^b \, da = \frac{1}{\delta S} \int_{\delta A_{\alpha\beta}^{B_2}} \gamma_{\alpha}^b \, da = \epsilon^{\beta\alpha} \quad (B7)$$

Because \mathbf{n}_1 and \mathbf{n}_2 are constant and terms containing D_1 and D_2 are small, (B6) becomes

$$\hat{\mathbf{T}}^{\alpha\beta} \Big|_e = -p_1 (\epsilon_1^{\alpha} - \epsilon^{\beta\alpha}) \mathbf{N}_1 - p_2 (\epsilon_2^{\alpha} - \epsilon^{\beta\alpha}) \mathbf{N}_2 + p^{\beta\alpha} \nabla'(b\epsilon^{\alpha\beta}) \quad (B8)$$

with $\epsilon^{\alpha} = \epsilon s^{\alpha}$ and $\epsilon^{\beta\alpha} = \epsilon^{\beta} s^{\beta\alpha}$, and by the convention of (1b), equation (B8) may be written as

$$\hat{\mathbf{T}}^{\alpha\beta} \Big|_e = -[p^{\alpha} \epsilon s^{\alpha}] \mathbf{N} + \epsilon^{\beta} s^{\beta\alpha} [p^{\alpha}] \mathbf{N} + p^{\beta\alpha} \nabla'(b\epsilon^{\beta} s^{\beta\alpha}) \quad (B9)$$

Now, for the dissipative part of $\hat{\mathbf{T}}^{\alpha\beta}$, by analogy with constitutive equations for a multiphase body, a relation proportion-

al to the velocity may be proposed. Because \hat{T}^{ba} has components both in the tangential and normal directions of the interface, the following relation is employed:

$$\hat{T}^{ba} - \hat{T}^{ba}|_e = -bR^{ra} \cdot v^{ba} - bR_N^{ba} \chi_1^a (v_1^a \cdot N_1) N_1 - bR_N^{ba} \chi_2^a (v_2^a \cdot N_2) N_2 \quad (B10)$$

where R^{ra} is the resistance of the material of the interface zone to the flow in the tangential direction, R_N^{ra} is the total resistance of the interface zone to normal flow, and χ_1^a and χ_2^a distribute this resistance between the flows crossing the boundaries at positions 1 and 2 such that $\chi_1^a + \chi_2^a = 1$. Note that R_N^{ra} in general depends on the resistance of the main domains as well as the resistance of the interface to normal flow. Thus the constitutive equation used is

$$\frac{1}{\delta S} \int_{\delta A_{\alpha\beta}} t \cdot n^{\alpha\beta} da = -[p^r \epsilon s^r] N + \epsilon^b s^{ba} [p^r] N + p^{ba} \nabla' (b \epsilon^b s^{ba}) - bR^{ra} \cdot v^{ba} - bR_N^{ra} [\chi^r v^r \cdot N] N \quad (B11)$$

NOTATION

$A_1(A_2)$	macroscopic boundary of domain I (or II).
b	thickness of the interface zone between two media.
b	external supply of entropy introduced in Table 1.
$B_1(B_2)$	Actual boundary of domain I (or II).
C_v^{ba}	specific heat capacity at a constant volume of α phase within the interface.
da	infinitesimal element of area.
dv	infinitesimal element of volume.
D	characteristic size of the representative element of volume.
D^{ba}	dispersion tensor for phase α in the interface.
E	internal energy per unit mass.
f	external supply in the general balance equation (4).
f_b^a	contribution of interface to thermodynamic properties of α phase in (2).
g	gravity vector.
G	net rate of production in the general balance equation (4).
h	external supply of energy per unit mass.
i	nonadvective flux vector.
l	unit tensor in three dimensions.
l'	unit tensor in two dimensions.
j	dispersion flux vector.
n	normal unit vector in the microscopic domain.
$n^{\alpha\beta}$	normal unit vector to a microscopic $\alpha\beta$ interface.
N	normal unit vector in the macroscopic domain.
$N_1(N_2)$	normal unit vector to the interface at side 1 (or 2) pointing into the interface.
p	fluid pressure.
q	heat flux vector.
r	rate of mass production (or decay) as a result of homogeneous reactions.
R_1	transition region between two multiphase media (also R_2) (Figure 1).
R''	two-dimensional resistance tensor for the flux in the "plane" of the interface.
R_N^a	resistance of the interface to the normal flow of phase α .
R_N^{Ta}	transfer resistance coefficient of the interface for heat transport in the normal direction.
R_N^{wa}	transfer resistance coefficient of the interface for species mass transport in the normal direction.
R_{het}^{ba}	rate of species mass exchange as a result of hetero-

geneous reaction between phase α and all other phases in the interfaces.

s^a	saturation of phase α .
s^{ba}	saturation of phase α in the interface.
t	time.
\dagger	stress tensor.
T	temperature.
u^a	Darcy velocity of phase α defined in (8c).
u^{ba}	Darcy velocity of phase α in the interface (two-dimensional vector).
V	region of space occupied by the interface (Figure 2).
v	velocity vector.
w	velocity of microscopic interfaces.
W	velocity of macroscopic interfaces.

Greek Letters

γ_a^b	distribution function defined before (5).
Γ	rate of net production of entropy in Table 1.
δA	surface area of the averaging volume lying totally within the interface.
$\delta A_1(\delta A_2)$	cross section of the averaging volume with boundary A_1 (or A_2) of the interface (Figure 3).
$\delta A_{\alpha\beta}$	union of all $\alpha\beta$ interfaces within the averaging volume.
δS	cross-sectional area of the averaging volume.
δV_b	volume of the averaging volume within the interface $\delta V_b = b \delta S$.
ϵ	porosity of the porous medium.
ϵ^a	volume fraction of phase α .
η	internal entropy per unit mass.
κ	heat conductivity tensor.
$\lambda^{\alpha\beta}$	coefficient of local heat transfer between phases α and β .
ρ	mass density.
χ^a	coefficient related to the interface resistance to flow defined used in (B10).
χ^{Ta}	coefficient related to the interface resistance to heat transfer used in (32).
χ^{wa}	coefficient related to the interface resistance to species mass transfer used in (24).
ψ	typical thermodynamic quantity.
ω	mass fraction of species.

Special Notation

$-\alpha$	mass average of an α phase property of main domains.
$-b\alpha$	mass average of an α phase property of the interface.
$\langle \rangle_a$	volume average of an α phase property of main domains.
$\langle \rangle_b$	volume average of an α phase property of the interface.
$\sim b\alpha$	deviation of a property from its average value defined in (6d).
∇	gradient operator in three dimensions.
∇'	gradient operator in two dimensions (in the directions tangential to the interface).
$[]$	jump of a property defined in (1b).
$\sum_{\beta \neq \alpha}$	summation over all phases except phase α .

Subscripts

1(or 2)	thermodynamic property evaluated at side 1 (or 2) of the interface.
---------	---

Superscripts

- ' denotes the tangential components of a vector in the interface.
- " denotes the tangential components of a tensor in the interface.
- b* properties associated with the interface.
- s* properties associated with the solid phase of a porous medium.
- f* properties associated with the fluid phase of a porous medium.
- α properties associated with the phase α .

Acknowledgments. Cooperation between the authors was facilitated, in part by NATO Collaborative Research grant 0213/87. The authors wish to recognize the encouragement of this effort received from the National Institute of Public Health and Environmental Protection (RIVM).

REFERENCES

- Bachmat, Y., and J. Bear, Mathematical formulation of transport phenomena in porous media, paper presented at Proceedings of the Second Symposium on Fundamentals of Transport Phenomena in Porous Media, IAHR, Guelph, Ont., Canada, 1972.
- Bear, J., *Hydraulics of Groundwater*, McGraw-Hill, New York, 1979.
- Bear, J., and Y. Bachmat, On the equivalence of areal and volumetric averages in transport phenomena in porous media, *Adv. Water Resour.*, 6, 59-62, 1983.
- Bear, J., and A. Verruijt, *Modeling Groundwater Flow and Pollution*, D. Reidel, Hingham, Mass., 1987.
- Bedford, A., Jump conditions and boundary conditions for a multi-component theory of composite elastic materials, *Acta Mech.*, 17, 191-200, 1973.
- Bowen, R. M., and M. L. Doria, On the effect of diffusion on growth and decay of acceleration waves in gases, *J. Acoust. Soc. Am.*, 53, 75-82, 1973.
- Gray, W. G., Derivation of vertically averaged equations describing multiphase flow in porous media, *Water Resour. Res.*, 18, 1705-1712, 1982.
- Gray, W. G., Constitutive theory for vertically averaged equations describing steam-water flow in porous media, *Water Resour. Res.*, 19, 1501-1510, 1983.
- Hassanizadeh, M., and W. G. Gray, General conservation equations for multi-phase systems, I, Averaging procedure, *Adv. Water Resour.* 2(3), 131-144, 1979a.
- Hassanizadeh, M., and W. G. Gray, General conservation equations for multi-phase systems, II, Mass, momenta, energy and entropy equations, *Adv. Water Resour.* 2(4), 191-203, 1979b.
- Hassanizadeh, M., and W. G. Gray, General conservation equations for multi-phase systems, III, Constitutive theory for porous media flow, *Adv. Water Resour.* 3(1), 25-40, 1980.
- Raats, P. A. C., The role of inertia in the hydrodynamics of porous media, *Arch. Rational. Mech. Anal.*, 44, 267-280, 1972a.
- Raats, P. A. C., Jump conditions in the hydrodynamics of porous media, paper presented at the Second International Symposium on Fundamentals of Transport Phenomena in Porous Media, IAHR, Guelph, Ont., Canada, 1972b.
- W. G. Gray, Department of Civil Engineering, University of Notre Dame, Notre Dame, IN 46556.
- S. M. Hassanizadeh, National Institute of Public Health and Environmental Protection, P. O. Box 1, 3720 BA Bilthoven, The Netherlands.

(Received July 20, 1988;
revised October 12, 1988;
accepted October 31, 1988.)