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A two-phase mixture model of liquid–gas flow and heat transfer in capillary porous media—I. Formulation

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Abstract—A model for two-phase transport in capillary porous media is presented, in which the two phases are viewed as constituents of a binary mixture. The conservation equations are derived from the classical separate flow model without invoking additional assumptions. The present formulation, owing to its analogy to conventional multicomponent mixture flow theories and to a considerable reduction in the number of the differential equations required for the primary variables, provides an alternative for the theoretical analysis and numerical simulation of two-phase transport phenomena in porous media. Several complicated problems such as boundary layer two-phase flows, conjugate two- and single-phase flows in multiple regions and transient flows are shown to become more tractable within the framework of this new formulation.

1. INTRODUCTION

TWO-PHASE flow through porous media is an important topic which spans a broad spectrum of engineering disciplines. Examples include geothermal systems [1–3], oil reservoir engineering [4, 5], post-accident analysis of nuclear reactors [6, 7], multiphase packed-bed reactors [8], disposal of high-level nuclear wastes [9], porous heat pipes [10, 11], drying [12], condensation enhancement [13, 14], and thermal energy storage.

Traditionally, the problem of two-phase flow in porous media has been approached by the so-called separate flow model (SFM) [4, 5], which is based on a continuum formulation. In this model, the gas and liquid phases are regarded as distinct fluids with individual thermodynamic and transport properties and with different flow velocities. The phenomenon is then mathematically described by the conservation laws for each phase separately and by appropriate interfacial conditions between the two phases. The relative permeabilities of both phases, introduced to account for a decrease in the effective flow cross-section due to the presence of the other fluid, are an important concept in such a formulation.

Due to the inherent nonlinearity of two-phase flow problems, exact solutions are limited to a small class of problems in one dimension, and many simplifying assumptions are employed, e.g. the Buckley–Leverett case [4]. Solving practical problems, which usually involve multi-dimensional effects, gravity and capillarity, requires suitable numerical procedures. The result has been a great number of studies to develop robust numerical algorithms, using both finite element and finite difference methods [15–18].

While the SFM provides a straightforward and rigorous mathematical description of two-phase flow in porous media, its form is generally inconvenient for direct use in numerical simulations due to the fact that a large number of differential equations must be solved (almost twice as many as compared with the single-phase case). This shortcoming becomes even more serious in multi-dimensional situations. Often, in order to reduce the number of equations, various modified formulations are constructed before numerical treatment. For more details the interested reader is referred to reports in oil reservoir engineering [19, 20], as well as in nuclear reactor safety analysis [18, 21, 22].

The main purpose of this work is to develop a new formulation for two-phase flow through capillary porous media that is both physically meaningful and practically useful. In this model, called the two-phase mixture model, the two phases are regarded as constituents of a binary mixture. So as to distinguish this mixture from a conventional multicomponent mixture [23], it is hereafter referred to as a *multiphase* mixture. In this definition, phases are assumed to be distinct and separable components with nonzero interfacial areas, and their mixture represents a single material with a smoothly varying phasic composition. In contrast, a multicomponent mixture is defined as consisting of different chemical components.

In the following, a consistent two-phase mixture model, based on the familiar SFM, is developed, including equations for conservation of mass, momentum and energy, along with boundary/initial conditions. As in a classical multicomponent mixture, all physical properties of a multiphase mixture are consequences of the properties of its constituents; however, their functional forms are not assumed a priori but are rather derived strictly from the SFM. Hence, mathematically, the present formulation is exactly equivalent to the SFM. The differences lie

NOMENCLATURE

c	specific heat
C_k	concentration of component k in a multicomponent mixture
D	capillary diffusion coefficient, equation (25)
$f(s)$	hindrance function, equation (26)
$\mathbf{g}$	gravity vector
h	enthalpy
h_{fg}	latent heat of phase change
$\mathbf{j}$	diffusive mass flux
$J(s)$	capillary pressure function
k	relative permeability
k_{eff}	effective thermal conductivity
K	absolute permeability
$\dot{m}$	mass source
$\mathbf{n}$	unit vector normal to boundaries
p	pressure
q	wall heat flux
$\dot{Q}$	volumetric heat generation rate
s	liquid saturation
S	normalized liquid saturation, equation (52)
S_ϕ	general source term
t	time
T	temperature
u	superficial or Darcian velocity in x-direction
$\mathbf{u}$	superficial or Darcian velocity vector
x	Cartesian coordinate.

Greek symbols

γ_h	two-phase advection correction coefficient, equation (44)
Γ_h	diffusion coefficient in enthalpy equation, equation (45)
$\Delta\rho$	$\rho_l - \rho_v$
ε	porosity
η	similarity variable
λ	relative mobility
μ	viscosity
ν	kinematic viscosity
ρ	density
σ	surface tension
Φ	any field variable
Ω	heat capacitance ratio, equation (43).

Subscripts

c	capillary
k	component
l	liquid
n	normal
r	relative permeability
s	solid matrix
sat	saturated state
v	vapor or gas
α	constituent α in a multiphase mixture
κ	'kinetic' property
ϕ	pertinent to Φ.

Superscript

o	reference.

solely in the form of the governing equations, their physical meanings and amenability to numerical implementation.

After presenting the formulation, the paper points out the analogy between the new model and that describing the transport of a conventional multicomponent mixture in porous media. From this analogy we conclude that the proposed model greatly facilitates the numerical analysis of general transient multi-dimensional two-phase flow through porous media. Moreover, when applied to some specific cases, the proposed model lends new insights into physical phenomena. In a companion paper [24], the capabilities of the two-phase mixture model are demonstrated through application to pressure-driven boiling flow adjacent to a vertical heated plate inside a porous medium, namely the two-phase flow problem of the boundary-layer type.

2. FORMULATION OF THE MODEL

The present formulation for two-phase flow through porous media begins with the definition of a *multiphase* mixture with two flowing phases as constituents. Similar to a classical multicomponent mixture, a multiphase mixture can be thought of as consisting of diffusing constituents (phases). However, in the latter case it should be kept in mind that the interfacial area between constituent elements (phases) is no longer negligibly small but rather of finite scale. As a consequence, two basic physical assumptions underlie such a multiphase mixture formulation. One is that a system of two separable phases can be viewed as a continuum in which any location $\mathbf{r}$ can be simultaneously occupied by both phases (Fig. 1). The other requires that the control volume, on which the model of differential form is based, should be larger than the maximum dimension of any phase element, but much smaller than the characteristic scale of the system.

In addition to the above conceptual definition of the multiphase mixture, several mean mixture properties need to be defined before proceeding to construct the conservation equations.

The mixture density and mixture velocity are defined, respectively, as

$$\rho = \rho_l s + \rho_v (1-s) \tag{1}$$

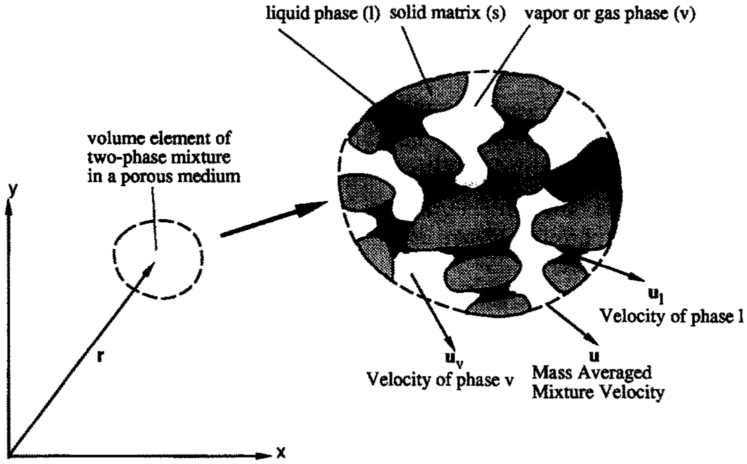

FIG. 1. Schematic illustration of a control volume containing a multiphase mixture.

$$\rho\mathbf{u} = \rho_l\mathbf{u}_l + \rho_v\mathbf{u}_v \tag{2}$$

where s is the liquid saturation denoting the volumetric fraction of the void space occupied by liquid and $\mathbf{u}$ is the superficial (or Darcian) velocity vector based on the total cross-sectional area of both the fluid and the porous medium. Since the superficial velocity of a phase is related to its intrinsic velocity by the phase volume fraction, equation (2) implies that the mixture velocity is a mass-weighted average of the intrinsic phase velocities multiplied by the porosity. The specification of the mixture pressure is more involved because of the difference between liquid and gas pressures due to capillary forces. Here this difficulty is circumvented by using a modified Chavent's pressure variable [19]. Let

$$\nu(s) = \frac{1}{\dfrac{k_{rl}(s)}{\nu_l} + \dfrac{k_{rv}(s)}{\nu_v}} \tag{3}$$

represent a *mean* kinematic viscosity of the two-phase mixture, and define relative mobilities by

$$\lambda_l(s) \equiv \lambda(s) = \nu(s)k_{rl}(s)/\nu_l \tag{4}$$

and

$$\lambda_v(s) \equiv 1 - \lambda(s) = \nu(s)k_{rv}(s)/\nu_v. \tag{5}$$

The *pseudo* mixture pressure is then defined as [19]

$$p = \frac{p_l + p_v}{2} + \frac{1}{2}\int_0^{p_c} [\lambda_v(\xi) - \lambda_l(\xi)]\,\mathrm{d}\xi. \tag{6}$$

Subscripts l and v refer to the liquid and vapor (or any kind of gas) phases, respectively. The term ν represents the kinematic viscosity, k_r is the relative permeability of a phase as usually introduced in the classical SFM, and p_c, the capillary pressure, denotes the difference between the pressures of the two phases due to interfacial surface tension.

Obviously, when the capillary force is negligibly small, $p = p_l = p_v$. Moreover, as the liquid saturation, s, approaches unity (pure liquid) or zero (pure vapor), the mixture pressure defined in equation (6) reduces to the appropriate single-phase pressures. These observations show that the definition in equation (6) is consistent with a mixture theory. Later, we show that this definition can greatly simplify the momentum conservation equation for a bulk mixture.

Having defined the basic mean properties of a two-phase mixture, we now formulate conservation equations for such a mixture by starting from the governing equations for each individual phase, which are available from the SFM. In the following, the SFM is first summarized.

2.1. *Separate flow model (SFM)*

As discussed by Scheidegger [4] or Bear [5], the conventional form of the equations governing two-phase, immiscible, incompressible flow through a porous medium are:

(1) The differential equations expressing the principle of mass conservation for two phases:

$$\rho_l\left[\varepsilon\frac{\partial s}{\partial t} + \nabla\cdot\mathbf{u}_l\right] = \dot{m}_l \tag{7}$$

$$\rho_v\left[\varepsilon\frac{\partial(1-s)}{\partial t} + \nabla\cdot\mathbf{u}_v\right] = \dot{m}_v \tag{8}$$

where ε is the porosity of the porous medium, and $\dot{m}_l$ and $\dot{m}_v$ are mass sources of liquid and vapor, respectively, which may arise due to internal phase change or chemical reactions. In the absence of any external mass source or sink,

$$\dot{m}_l + \dot{m}_v = 0. \tag{9}$$

Equations (7) and (8) assume that the porous medium is not deformable and the fluids are incompressible.

(2) The Darcy flow model, reflecting relationships of flow velocities with phase pressures:

$$\mathbf{u}_1 = -K\frac{k_{r1}}{\mu_1}(\nabla p_1 - \rho_1 \mathbf{g}) \tag{10}$$

$$\mathbf{u}_v = -K\frac{k_{rv}}{\mu_v}(\nabla p_v - \rho_v \mathbf{g}) \tag{11}$$

where the presence of body acceleration has been taken into account. In equations (10) and (11), K is the absolute permeability of the porous medium, and k_r the relative permeability of a phase.

(3) The definition of capillary pressure, p_c, between two phases:

$$p_c = p_v - p_1. \tag{12}$$

The capillary pressure, p_c, is further assumed to be adequately represented by Leverett's well-known J function [4]:

$$p_c = \left(\frac{\varepsilon}{K}\right)^{1/2} \sigma J(s) \tag{13}$$

in which σ is the vapor–liquid interfacial tension.

Equations (7)–(13) constitute a full system of governing equations for the unknown vector velocities $\mathbf{u}_1$ and $\mathbf{u}_v$, scalar pressures p_1 and p_v, and scalar liquid saturation, s.

2.2. *Conservation of mass*

The mass conservation equation for a two-phase mixture can readily be obtained by addition of the phase conservation equations (7) and (8). Note that the production of the vapor phase, $\dot{m}_v$, must come at the expense of the liquid phase (equation (9)). Hence,

$$\varepsilon\frac{\partial \rho}{\partial t} + \nabla\cdot(\rho\mathbf{u}) = 0. \tag{14}$$

It is clear that the continuity equation is just a duplicate of the corresponding equation for single-phase mixture flow. Since the mixture density is strongly variable, the multiphase mixture flow should be categorized as compressible.

2.3. *Conservation of momentum*

The development of the equation governing the conservation of momentum for a two-phase mixture needs a few algebraic manipulations. First, the momentum equations, equations (10) and (11), for the two phases are multiplied by their respective phase densities, and the resultant identities are then added together. This yields

$$\rho\mathbf{u} = -\frac{K}{v(s)}[(\lambda_1\nabla p_1 + \lambda_v\nabla p_v) - (\lambda_1\rho_1 + \lambda_v\rho_v)\mathbf{g}]. \tag{15}$$

From the definition of the mixture pressure in equation (6), it is easy to show that

$$\lambda_1\nabla p_1 + \lambda_v\nabla p_v = \nabla p. \tag{16}$$

Thus, the momentum equation for the two-phase mixture can be recast as

$$\mathbf{u} = -\frac{K}{\mu(s)}[\nabla p - \rho_k(s)\mathbf{g}] \tag{17}$$

where the mixture viscosity is defined as

$$\mu(s) = \rho(s)\cdot v(s). \tag{18}$$

It should be noted that, in equation (17), we have introduced a new mixture density, $\rho_k(s)$, appearing before the body acceleration. This density is defined as

$$\rho_k(s) = \rho_1\lambda_1(s) + \rho_v\lambda_v(s). \tag{19}$$

We shall refer to this quantity from now on as the *kinetic* mixture density, in order to distinguish it from the conventional *static* density, $\rho(s)$, defined by equation (1). The kinetic density acquires its name because of its dependence on the relative mobilities of the phases. The two kinds of densities are generally different from each other.

2.4. *Conservation of liquid mass*

Now we have developed one vectorial and one scalar governing equation for the unknowns, $\mathbf{u}$ and p. However, all mean physical properties of the two-phase mixture, as defined in equations (1), (3), (18) and (19), are strongly dependent on the constituent concentration, namely the liquid saturation, s. Therefore, in order to complete the mathematical system, one also needs a governing equation for the liquid saturation, which is given by the statement for conservation of liquid mass. This statement can be mathematically derived using the difference of the two mass conservation equations for the phases, equations (7) and (8). This results in

$$\varepsilon(\rho_1+\rho_v)\frac{\partial s}{\partial t} - \nabla\cdot\left[\frac{K}{v(s)}(\lambda_1\nabla p_1 - \lambda_v\nabla p_v) - (\rho_1\lambda_1 - \rho_v\lambda_v)\mathbf{g}\right] = \dot{m}_1 - \dot{m}_v. \tag{20}$$

Since $\lambda_1 + \lambda_v = 1$, it can be seen that

$$\begin{aligned}\lambda_1\nabla p_1 - \lambda_v\nabla p_v &= -2\lambda_1\lambda_v\nabla p_c \\ &\quad + (\lambda_1-\lambda_v)(\lambda_1\nabla p_1 + \lambda_v\nabla p_v) \\ &= -2\lambda_1\lambda_v\nabla p_c + (\lambda_1-\lambda_v)\nabla p.\end{aligned} \tag{21}$$

Thus, equation (20) can be rewritten as

$$\begin{aligned}\varepsilon(\rho_1+\rho_v)\frac{\partial s}{\partial t} &+ 2\nabla\cdot\left[\frac{K}{v}\lambda(1-\lambda)p_c'\nabla s\right] \\ &+ \nabla\cdot\left[\frac{K}{v}(\rho_1\lambda - \rho_v(1-\lambda))\mathbf{g}\right] \\ &- \nabla\cdot\left[\frac{K}{v}(2\lambda-1)\nabla p\right] = \dot{m}_1 - \dot{m}_v\end{aligned} \tag{22}$$

where p_c' is the derivative of the capillary pressure function with respect to the liquid saturation. Next, substituting the momentum equation, equation (17), and using the continuity equation, equation (14), and after several algebraic manipulations, we obtain

$$\varepsilon\frac{\partial(\rho_l s)}{\partial t}+\nabla\cdot[\rho\mathbf{u}\lambda(s)] = \nabla\cdot\left(-\frac{K}{\nu}\lambda(1-\lambda)p_c'\nabla s\right)$$

$$-\nabla\cdot\left(\frac{K}{\nu}\lambda(1-\lambda)(\rho_l-\rho_v)\mathbf{g}\right)+\dot{m}_l. \quad (23)$$

Now we introduce a total mass flux $\mathbf{j}$ defined as

$$\mathbf{j} = -D(s)\nabla s+f(s)\frac{K\Delta\rho}{\nu_v}\mathbf{g} \quad (24)$$

where $D(s)$ is the so-called capillary diffusion coefficient, i.e.

$$D(s) = \frac{K}{\nu(s)}\lambda(1-\lambda)\cdot[-p_c'(s)] \quad (25)$$

and $f(s)$, expressed as

$$f(s) = k_{rv}(s)\lambda(s) \quad (26)$$

is here termed the hindrance function for phase migration and eventual separation. The physical meaning of the function $f(s)$ is similar to the well-known hindrance function in sedimentation theories and the reader is referred to ref. [25] for further details on its properties.

With the above definition, equation (22) eventually reduces to

$$\varepsilon\frac{\partial(\rho_l s)}{\partial t}+\nabla\cdot[\rho\mathbf{u}\lambda(s)] = -\nabla\cdot\mathbf{j}+\dot{m}_l. \quad (27)$$

This equation is a direct manifestation of the liquid-phase mass balance. The total mass flux $\mathbf{j}$ is a combination of the capillarity-induced diffusive flux and the gravity-induced migrating flux, as seen from its definition, equation (24). For a two-phase system, one composition conservation equation such as equation (27) is sufficient since overall constituent conservation calls for $s_l+s_v = 1$.

In equations (14), (17) and (27) the basic variables pertinent to each constituent (phase) have been ignored. Fortunately, however, within the frame of this formulation, definite algebraic relations exist between relative motions of the bulk mixture and each phase. These relations can be derived as follows.

From the definition of the mixture pressure, equation (6), it is evident that

$$\nabla p = \lambda\nabla p_l+(1-\lambda)\nabla p_v \quad (28)$$

and operating a vectorial gradient over the capillary pressure equation (12), one obtains

$$\nabla p_c = \nabla p_v-\nabla p_l. \quad (29)$$

Solving equations (28) and (29) simultaneously for ∇p_l and ∇p_v in terms of ∇p and ∇p_c, we get

$$\nabla p_v = \nabla p+\lambda\nabla p_c \quad (30)$$

$$\nabla p_l = \nabla p+(1-\lambda)\nabla p_c. \quad (31)$$

Further, substituting these results into the SFM, and recognizing the relationship between ∇p and $\rho\mathbf{u}$ on a mixture level, yields

$$\rho_l\mathbf{u}_l = \lambda\rho\mathbf{u}+\mathbf{j} \quad (32)$$

$$\rho_v\mathbf{u}_v = (1-\lambda)\rho\mathbf{u}-\mathbf{j} \quad (33)$$

where $\mathbf{j}$ is the diffusive mass flux as defined in equation (24). Note that $\rho_\alpha\mathbf{u}_\alpha$ in equations (32) and (33) represents the true mass flowrate of the αth constituent, while $\lambda_\alpha\rho\mathbf{u}$ is the virtual mass flowrate of the same constituent in the bulk stream of the whole mixture, which has a mixture mean velocity. Thus, we conclude that the quantity $\mathbf{j}$ has a clear physical meaning as a diffusive mass flux, though initially it is defined only for mathematical convenience.

Furthermore, with the aid of equations (32) and (33), the flow characteristics of individual phases can readily be obtained, once one has solved the flow problem of the bulk mixture. Thus, the detailed flow aspects of each phase are not smeared out in the present model; they are still accessible wherever they are needed. This is why the model is called the *two-phase mixture model*, rather than simply a mixture model, implying that, in the latter, the intrinsic two-phase characteristics are usually lost.

2.5. *Conservation of energy*

For nonisothermal two-phase flows, one more governing equation is required to determine the temperature field. This can be obtained from the total energy conservation equation for a combined solid matrix-multiphase mixture system and by invoking the assumption that local thermodynamic equilibrium prevails among the solid matrix, vapor and liquid phases (i.e. $T = T_s = T_l = T_v$); thus [2]

$$\frac{\partial}{\partial t}[(1-\varepsilon)\rho_s h_s+\varepsilon s\rho_l h_l+\varepsilon(1-s)\rho_v h_v]$$

$$+\nabla\cdot(\rho_l\mathbf{u}_l h_l+\rho_v\mathbf{u}_v h_v) = \nabla\cdot(k_{\mathrm{eff}}\nabla T)+\dot{Q} \quad (34)$$

where k_{eff} is the effective thermal conductivity of the combined three-phase system and $\dot{Q}$ is a volumetric heat source. The enthalpies in equation (34) are related to the temperature by

$$h_s = c_s T+h_s^\circ \quad (35a)$$

$$h_l = c_l T \quad (35b)$$

$$h_v = c_v T+[(c_l-c_v)T_{\mathrm{sat}}+h_{fg}] \quad (35c)$$

where it is assumed that $h_l|_{T=0} = 0$ and $(h_v-h_l)|_{T=T_{\mathrm{sat}}} = h_{fg}$.

The advective term in the energy equation, equation (34), can be further decomposed into contributions due to the bulk mixture motion and intrinsic relative phase motion; that is,

$$\sum_\alpha \rho_\alpha\mathbf{u}_\alpha h_\alpha = \rho\mathbf{u}h_\kappa+\sum_\alpha(h_\alpha-h_\kappa)(\rho_\alpha\mathbf{u}_\alpha-\lambda_\alpha\rho\mathbf{u}),$$

$$\alpha = \mathrm{l}, \mathrm{v} \tag{36}$$

where the mixture enthalpy h_κ is defined as

$$h_\kappa = h_\mathrm{l}\lambda + h_\mathrm{v}(1-\lambda). \tag{37}$$

Again, such a definition gives kinetic characteristics to the mixture enthalpy; this is why we add the subscript κ and refer to it as the *kinetic* mixture enthalpy, h_κ. On the other hand, a *static* mixture enthalpy is ordinarily defined as

$$\rho h = \rho_\mathrm{l} s h_\mathrm{l} + \rho_\mathrm{v}(1-s)h_\mathrm{v}. \tag{38}$$

From the definitions of these two mixture enthalpies, the corresponding mixture specific heats can be obtained as

$$c_\kappa = c_\mathrm{l}\lambda + c_\mathrm{v}(1-\lambda) \tag{39}$$

$$\rho c = \rho_\mathrm{l} s c_\mathrm{l} + \rho_\mathrm{v}(1-s)c_\mathrm{v}. \tag{40}$$

Now, using the above decomposition and with the help of equations (37) and (38), the energy equation can be simplified to the following form, in which only mixture variables are involved:

$$\frac{\partial}{\partial t}[(1-\varepsilon)\rho_\mathrm{s} h_\mathrm{s} + \varepsilon\rho h] + \nabla\cdot(\rho\mathbf{u}h_\kappa) = \nabla\cdot(k_\mathrm{eff}\nabla T) + \nabla\cdot[(h_\mathrm{v}-h_\mathrm{l})\mathbf{j}] + \dot{Q}. \tag{41}$$

The physical meanings of all the terms appearing in equation (41) are quite clear, since the equation strongly resembles the classical formulation describing heat transfer of a single-phase multicomponent mixture inside porous media. Nevertheless, several particular and salient points are worth outlining. First, equation (41) is a variable-property equation, in which all physical properties are strongly dependent on the liquid saturation. Also, we include a source term to describe possible volumetric heating. Secondly, the second term on the RHS accounts for the energy flux due to relative phase motion, including both sensible and latent heat transport. Lastly, equation (41) is valid throughout a whole problem domain, which may simultaneously involve single- and two-phase subregions.

The general representation of energy conservation, equation (41), may further be recast into forms which are more suitable in various applications. The following two subsections are designed for this purpose.

2.5.1. *Isothermal two-phase flows.* A two-phase region can often be assumed to be isothermal without much loss of accuracy. This is especially true for single-component two-phase flow with phase change, because the thermodynamic relationships require a nearly isothermal condition in the two-phase region [11, 26]. For a uniform temperature field, the energy equation, equation (41), reduces identically to the liquid mass conservation equation, equation (27), in the two-phase region. This outcome is physically intuitive since if the system has no temperature gradient, the energy transport will be caused solely by phase change controlled by mass transfer. In recognition of the fact that equation (41) is a unified formulation representing both the temperature equation in the single-phase regions and the liquid saturation equation in the two-phase region, an efficient single-domain methodology, using equation (41), can be proposed for solving complicated problems involving multiple regions [27]. More details are presented below.

After a few manipulations, equation (41) can be transformed into the following more useful form, which contains only one variable, the mixture enthalpy, h, defined in equation (38):

$$\Omega\frac{\partial(\rho h)}{\partial t} + \nabla\cdot(\gamma_\mathrm{h}\rho\mathbf{u}h) = \nabla\cdot(\Gamma_\mathrm{h}\nabla h) + \nabla\cdot[\Gamma_\mathrm{h}(h-h_\mathrm{vsat})\nabla\ln\rho] + \nabla\cdot\left(f(s)\frac{K\Delta\rho h_\mathrm{fg}}{\nu_\mathrm{v}}\mathbf{g}\right) + \dot{Q}. \tag{42}$$

The coefficients newly introduced in equation (42), namely the heat capacitance ratio Ω, the advection correction coefficient γ_h and the diffusion coefficient Γ_h are defined, respectively, as

$$\Omega = \varepsilon + \frac{\rho_\mathrm{s}c_\mathrm{s}(1-\varepsilon)}{\rho}\frac{\mathrm{d}T}{\mathrm{d}h} \tag{43}$$

$$\gamma_\mathrm{h} = \frac{\dfrac{\rho_\mathrm{l}h_\mathrm{lsat}}{\mu_\mathrm{l}}k_\mathrm{rl}(s) + \dfrac{\rho_\mathrm{v}h_\mathrm{vsat}}{\mu_\mathrm{v}}k_\mathrm{rv}(s)}{\dfrac{\rho_\mathrm{l}h_\mathrm{lsat}}{\mu(s)}(s) + \dfrac{\rho_\mathrm{v}h_\mathrm{vsat}}{\mu(s)}(1-s)} \tag{44}$$

and

$$\Gamma_\mathrm{h} = \frac{\rho(s)D(s)}{\rho_\mathrm{l}} + k_\mathrm{eff}\frac{\mathrm{d}T}{\mathrm{d}h} \tag{45}$$

where the term $\mathrm{d}T/\mathrm{d}h$ denotes the derivative of the temperature with respect to the mixture enthalpy. It should be stressed that equation (42) represents the temperature equation in a single-phase region, whereas it reduces to the liquid saturation equation in the isothermal two-phase region. The relationships of the mixture enthalpy with either the temperature or the liquid saturation can be explicitly written as

$$T = \begin{cases} \dfrac{h}{c_\mathrm{l}} & h \leqslant h_\mathrm{lsat} \\ T_\mathrm{sat} & h_\mathrm{lsat} < h \leqslant h_\mathrm{vsat} \\ T_\mathrm{sat} + \dfrac{h-h_\mathrm{vsat}}{c_\mathrm{v}} & h_\mathrm{vsat} < h \end{cases} \tag{46}$$

$$s = \begin{cases} 1 & h \leqslant h_\mathrm{lsat} \\ \dfrac{\rho}{\rho_\mathrm{l}}\left(\dfrac{h_\mathrm{vsat}-h}{h_\mathrm{fg}}\right) & h_\mathrm{lsat} < h \leqslant h_\mathrm{vsat}. \\ 0 & h_\mathrm{vsat} < h \end{cases} \tag{47}$$

From the definition (46), it follows that

$$\frac{dT}{dh}=\begin{cases}\frac{1}{c_l} & h \leqslant h_{lsat}\\ 0 & h_{lsat} < h \leqslant h_{vsat}\cdot\\ \frac{1}{c_v} & h_{vsat} < h\end{cases} \quad (48)$$

Four observations can be made regarding equations (42)–(48). First, by means of equations (46) and (47), the temperature and liquid saturation can be uniquely determined from the mixture enthalpy. Secondly, the solid matrix does not contribute to two-phase transport in the isothermal two-phase region. Thirdly, within single-phase regions no correction ($\gamma_h = 1$ in this case) needs to be made for the convective term in equation (42). Lastly, both the second and third terms on the RHS vanish within single-phase regions.

Equations (14), (17) and (42) establish a one-domain formulation for flow problems in multiple regions, if the two-phase region can be assumed to be isothermal. The formulation is attractive, since there is no need to track the moving interfaces between different regions, complex interfacial boundary conditions are not required to match, and it is amenable to solution with existing numerical algorithms [28].

2.5.2. *Nonisothermal two-phase flows.* Transport in unsaturated porous media constitutes another aspect of two-phase flow and heat transfer in engineering applications [29]. In this case, the two phases are usually of different chemical components; the combination of water and air is a typical example. Now, the temperature distribution in the two-phase zone is no longer uniform but principally of interest. An alternative form of equation (41), in terms of temperature, is thus preferred. This can be achieved by substituting the relationship of enthalpy vs temperature, given by equation (35), into equation (41). After proper arrangement, it follows that

$$[(\rho c)_s\varepsilon+\rho c(1-\varepsilon)]\frac{\partial T}{\partial t}+\rho c_\kappa \mathbf{u}\cdot\nabla T+(c_l-c_v)\mathbf{j}\cdot\nabla T = \nabla\cdot(k_{eff}\nabla T)+\dot{Q} \quad (49)$$

where phase change between the two phases has not been considered.

2.6. *Constitutive relationships*

Closure of the system of conservation equations obtained above for a multiphase mixture requires constitutive equations for the relative permeabilities, k_{rl} and k_{rv}, the capillary pressure function, $J(s)$, and the effective thermal conductivity, k_{eff}. In the petroleum and nuclear reactor safety literature, the simplest correlations used for k_{rl} and k_{rv} are power functions of liquid saturations, s; i.e.

$$k_{rl} = S^n \quad (50)$$

$$k_{rv} = (1-S)^n \quad (51)$$

where S is the normalized liquid saturation (known as holdup in chemical engineering) and is defined as

$$S=\frac{(s-s_{li})}{(1-s_{li})} \quad (52)$$

where s_{li} is the irreducible liquid saturation. This static (or residual) liquid saturation cannot be removed by drainage, but only by evaporation. Then, the range of the variation in the normalized saturation is between 0 and 1.

It is worthwhile pointing out that linear functions ($n = 1$) of the relative permeabilities are usually employed for geothermal systems due to their simplicity and accuracy [1, 30, 31], while cubic forms are widely used in petroleum and nuclear safety engineering [6, 32, 33].

The capillary pressure function, $J(s)$, is generally multivalued. In gas–liquid systems, the experimentally obtained J-values typically lie between two limiting curves, known as the drainage and imbibition curves. The drainage curve is obtained when the liquid saturation, s, is decreased steadily from its maximum value (which is generally equal to unity). On the other hand, the imbibition curve corresponds to measurements conducted when the liquid saturation is steadily increased from its residual value, s_{li}, to unity.

Consequently, one must decide which of these multiple values should be used in a theoretical analysis of a specific two-phase flow system. In the literature, drainage data, imbibition data, or an average curve between these two limits, has been employed. Udell [26] correlated imbibition capillary pressure data obtained by Leverett [34] with

$$J = 1.417(1-S)-2.120(1-S)^2+1.263(1-S)^3 \quad (53)$$

for applications in drying and porous heat pipes.

In contrast, Grosser *et al.* [35] argued that a drainage curve should be used in transient analysis of co-current two-phase flow in a trickle reactor (a type of chemical reactor). Their J-function was correlated as

$$J = 0.48+0.036\ln\left(\frac{1-s}{s}\right) \quad (54)$$

and was further extended to the counter-current case [36], and applied to the analysis of transient two-phase flow in packed beds [37].

In nuclear reactor safety analysis, both drainage and imbibition capillary pressure data are correlated to obtain the following widely used J-function

$$J=\frac{(S^{-1}-1)^{0.175}}{\sqrt{5}}. \quad (55)$$

Although numerous constitutive correlations for the J-function exist, it should be noted that the governing equations obtained here for a multiphase mixture are not limited to a certain correlation. This is because all correlations behave as decreasing J-functions with increasing liquid saturation, and thus produce an always positive capillary diffusion coefficient, D.

The effective thermal conductivity for a composite system consisting of the solid matrix and the flowing mixture, k_{eff}, is also a function of the liquid saturation. The roughest estimation of k_{eff} can be written as

$$k_{\text{eff}} = k_s(1-\varepsilon)+k_l\varepsilon s+k_v\varepsilon(1-s) \tag{56}$$

where k_s is the thermal conductivity of the solid matrix. Alternatively, a more elaborate function can take the form [38]

$$k_{\text{eff}} = k_{sv}+\sqrt{(s)}(k_{sl}-k_{sv}) \tag{57}$$

where k_{sv} is the thermal conductivity when the liquid saturation is zero and k_{sl} corresponds to the case when the porous medium is fully saturated with liquid. Other much more sophisticated correlations for k_{eff} are available in the literature; see for example ref. [39].

2.7. *Initial/boundary conditions*

In order to make problems well-posed, appropriate boundary and initial conditions are needed in the present two-phase mixture formulation. Initial conditions are usually known or taken from a steady-state solution.

Various types of hydrodynamic boundary conditions are possible. The first and most common type is the impermeable condition, which requires no mass exchange through the wall. If the wall is at rest in the chosen frame of reference, this implies that the normal component of the two-phase mixture velocity must vanish; i.e.

$$\mathbf{u}\cdot\mathbf{n} = 0. \tag{58}$$

However, a slip condition is allowed at the impermeable surface, since Darcy's law is used here to formulate the momentum equation for the two-phase mixture.

Other important types of hydrodynamic boundary conditions include constant mass flow rates of the two-phase mixture and constant pressures along permeable surfaces; both can be directly implemented in the present formulation.

The present formulation also requires boundary conditions for the liquid saturation. Either the liquid saturation itself or its gradient should be specified at the boundaries. For example, in condensing or boiling flows, three zones often appear near cooled or heated bodies, namely, two single-phase (pure liquid and vapor) regions sandwiching a two-phase region [11, 14, 40, 41]. The boundary condition for liquid saturation is, therefore, zero at the boundary adjacent to the vapor region, and unity at the other boundary. Another type of boundary condition for the liquid saturation can be obtained for an imposed wall heat flux, q. For an isothermal two-phase region, the energy conservation equation, equation (49), at a heated/cooled surface reduces to

$$\mathbf{j}\cdot\mathbf{n} = \frac{-q}{h_{fg}} \tag{59}$$

or, in another form,

$$-D\frac{\partial s}{\partial n}+f(s)\Delta\rho g_n = \frac{-q}{h_{fg}}. \tag{60}$$

In the absence of body acceleration, this simplifies to

$$-D\frac{\partial s}{\partial n} = \frac{-q}{h_{fg}}. \tag{61}$$

It can be seen that a version similar to the so-called second type of boundary condition in classical mass transfer theories is generated here.

For isothermal two-phase flows, if the enthalpy formulation, equation (42), is employed, the boundary conditions become

$$h = h_{\text{const}} \tag{62}$$

at constant temperature or liquid saturation boundaries, and

$$-\Gamma_h\frac{\partial h}{\partial n}-\Gamma_h(h-h_{\text{vsat}})\frac{\partial \ln \rho}{\partial n}-f(s)\frac{K\Delta\rho h_{fg}}{\nu_v}g_n = q \tag{63}$$

at a boundary with a specified heat flux q. An adiabatic boundary condition can be obtained from equation (63) by setting $q = 0$. The 2nd and 3rd terms on the LHS of equation (63) vanish in single-phase regions and equation (63) reduces to the familiar version for single-phase fluids.

3. DISCUSSION

In the preceding section, the present model has been rigorously derived from the classical SFM, without invoking additional approximations. In other words, the new model is an alternative, but equivalent, version of the original SFM. Furthermore, in order to understand the concept of a multiphase mixture and the physical meaning of the conservation equations, two underlying physical assumptions are emphasized: first, all constituents (phases) simultaneously occupy regions of space and, secondly, the control volume employed for constructing the governing differential equations is larger than the dimensions of the phase elements, but much smaller than the characteristic length of the physical system. The same assumptions are also utilized in other models of two-phase flow in porous media.

3.1. *Analogy to multicomponent mixture theory*

Table 1 summarizes the proposed two-phase mixture model and compares it with the familiar model for a multicomponent mixture in porous media. Striking similarities are expected since, from the very outset, the multiphase mixture is conceived to be similar to a

Table 1. Summary of conservation equations in the two-phase mixture model and comparison with a multicomponent mixture model†

	Two-phase mixture	Multicomponent mixture
Mass	$\varepsilon\frac{\partial\rho}{\partial t}+\nabla\cdot(\rho\mathbf{u})=0$	$\varepsilon\frac{\partial\rho}{\partial t}+\nabla\cdot(\rho\mathbf{u})=0$
Momentum	$\mathbf{u}=-\frac{K}{\mu(s)}[\nabla p-\rho_{\kappa}(s)\mathbf{g}]$	$\mathbf{u}=-\frac{K}{\mu(C_k)}[\nabla p-\rho(C_k)\mathbf{g}]$
Liquid mass	$\frac{\partial(\rho_l\cdot s)}{\partial t}+\underline{\nabla\cdot[\rho\mathbf{u}\lambda(s)]}=\nabla\cdot[D(s)\nabla s]$ $\underline{-\nabla\cdot\left[f(s)\frac{K\Delta\rho}{\nu_v}\mathbf{g}\right]}+\dot{m}_l$	$\frac{\partial(\rho_k C_k)}{\partial t}+\nabla\cdot(\rho\mathbf{u}C_k)=\nabla\cdot[D(C_k)\nabla C_k]+\dot{m}_k$
Energy	$[(\rho c)_s\varepsilon+\rho c(1-\varepsilon)]\frac{\partial T}{\partial t}+\rho c_{\kappa}\mathbf{u}\cdot\nabla T$ $+\underline{(c_l-c_v)\mathbf{j}\cdot\nabla T}=\nabla\cdot(k_{\mathrm{eff}}\nabla T)+\dot{Q}$	$[(\rho c)_s\varepsilon+\rho c(1-\varepsilon)]\frac{\partial T}{\partial t}+\rho c\mathbf{u}\cdot\nabla T=\nabla\cdot(k_{\mathrm{eff}}\nabla T)+\dot{Q}$

† Underlined are the differences between the two models.

multicomponent mixture. The two differ only in that the former has a finite interfacial area and strong variations in physical properties between constituent elements (phases).

These differences, however, have several important implications. First, the disparity in the properties of the two constituents (liquid and gas) makes the multiphase mixture flow a much stronger variable-property problem than multicomponent mixture flow. This can be expected to cause considerable difficulties in future analytical and numerical studies of two-phase flow problems via the current formulation.

Secondly, under the action of gravity, the large difference between the two phase densities contributes to diffusion of mass between the constituents. Thus, a term associated with this gravitational effect is included in the total diffusive flux. In contrast to the conventional diffusive flux, this gravity-induced migrating flux does not depend on the concentration gradient. The other cause of mass diffusion between the constituents in the multiphase mixture is the capillary force, which is indeed proportional to the concentration (saturation) gradient; thus, a capillary diffusion coefficient is introduced according to conventional practice. The importance played by the gravitational effect in diffusion of mass can be determined by evaluating the relative magnitude of the two driving forces. In systems with small capillary forces (e.g. in high-permeability media), the gravitational effect dominates and is thus responsible for phenomena such as phase separation and flow maldistribution, which are often observed in multiphase reactors and other systems of technological importance, but are as yet little understood. Addressing and clarifying these complicated multi-dimensional phenomena will constitute a large part of future research using the present formulation.

The last difference between the two models, as noted in the energy equation, equation (49), is that the mass diffusion causes sensible heat transfer of the bulk mixture, if the specific heat values of the two constituents differ from each other.

3.2. *Specific examples*

With the general features of the new formulation stated, we now proceed to consider some specific applications. The first example is concerned with one-dimensional two-phase flow with phase change. Under the isothermal assumption for the two-phase region, the liquid mass conservation equation is employed instead of the energy equation. The continuity and liquid mass conservation equations then reduce to

$$\begin{cases}\varepsilon\frac{\partial\rho}{\partial t}+\frac{\partial(\rho u)}{\partial x}=0\\ \varepsilon\rho_l\frac{\partial s}{\partial t}+\frac{\partial[\rho u\lambda(s)]}{\partial x}=-\frac{\partial j}{\partial x}+\dot{m}_l\end{cases}\tag{64}$$

in a 1-D Cartesian coordinate system. It can be seen that the two-phase mixture model requires only two governing equations for the variables u and s, while the phase velocities u_l and u_v are algebraically determined from equations (32) and (33). If desired, the pressure profile can subsequently be calculated from the mixture momentum equation. In contrast, in previous studies [43–45] based on the SFM, four differential equations (two continuity and two momentum equations separately for the two phases) must be simultaneously solved for the unknowns: u_l, u_v, p_l and p_v, and the liquid saturation is iteratively determined from the capillary pressure function given by equations (12) and (13). Therefore, equation set (64) is more convenient for the study of transient effects in two-phase flow through porous media with phase change. Furthermore, the form of the equation set lends additional insight for finding possible analytical solutions. To show this, we further neglect internal phase change and the gravity-induced mass flux, as is done in ref. [44]. The governing equations then become

$$\begin{cases} \varepsilon \dfrac{\partial \rho}{\partial t} + \dfrac{\partial(\rho u)}{\partial x} = 0 \\ \varepsilon \rho_1 \dfrac{\partial s}{\partial t} + \dfrac{[\rho u \lambda(s)]}{\partial x} = \dfrac{\partial}{\partial x}\left(D \dfrac{\partial s}{\partial x}\right) \end{cases} \tag{65}$$

If the boundary condition for the velocity u evolves with time in the manner of $t^{-1/2}$, the above equations admit a similarity variable, $\eta = x/\sqrt{(t)}$, which reduces equation (65) to a set of ordinary differential equations. This change of variables known as the Boltzmann transformation in heat conduction problems and applied by O'Sullivan [45] to study the thermodynamic behavior of geological media, is the tool employed by Doughty and Pruess [43] to obtain an exact solution for two-phase flow in a cylindrical coordinate system.

Another commonly encountered 1-D case deals with steady two-phase flow induced by bottom and/or volumetric heating [6, 9]. Due to the continuity requirement and the boundary condition at an impermeable surface, given by equation (58), the mixture velocity vanishes in this case. Hence, equation (64) simplifies to

$$-\frac{\partial j}{\partial x} + \dot{m}_1 = 0. \tag{66}$$

The mass source rate, $\dot{m}_1$, is equal to $\dot{Q}/h_{\mathrm{fg}}$ in the isothermal two-phase zone. After integration and using the boundary condition given by equation (59), one obtains

$$D(s)\frac{\partial s}{\partial x} + f(s)\frac{K\Delta\rho}{v_{\mathrm{v}}} g = \left[q + \int \dot{Q}\,\mathrm{d}x \right] \Big/ h_{\mathrm{fg}}. \tag{67}$$

Equation (67) represents the so-called Lipinski equation [6].

Further scrutiny of the present formulation reveals that boundary layer flows also exist in the two-phase case. Indeed, this type of flow has been noticed by several authors [13, 14, 41]. Regrettably, due to the cumbersome form of the SFM, these flows are never dealt with as strictly as in the classical boundary layer theory [46]. Instead, unjustified assumptions are introduced, and a systematic two-phase boundary layer theory is far from being developed. The companion paper [24] represents a first step in investigating boundary layer flows based on the present formulation.

3.3. *General methodology for numerical solutions*

The present formulation reduces almost by half the number of governing differential equations for the primary variables involved in two-phase flows through porous media, when compared to the SFM. Therefore, it is more suitable for numerical implementation, especially in applications where multi-dimensional effects are present. Furthermore, each of the conservation equations in the model can be cast into the general form

$$\frac{\partial}{\partial t}(\rho\Phi) + \nabla \cdot (\gamma_\phi \rho \mathbf{u} \Phi) = \nabla \cdot (D_\phi \nabla \Phi) + S_\phi \tag{68}$$

where Φ, D_ϕ, and S_ϕ represent any dependent variable, diffusion coefficient, and source term, respectively. Hence, many existing numerical algorithms for solving coupled single-phase transport equations can theoretically be employed. However, we believe that numerical solutions will be more difficult to obtain than in the single-phase case, because of the highly nonlinear nature of the set of transport equations and the presence of strongly varying transport properties.

Another computational advantage of the present formulation over the classical SFM is apparent for problems involving conjugate two-phase flow with adjacent single-phase regions. When using the SFM, multiple region solutions are required due to the differences in the conservation equations for the two- and single-phase regions [27]. The primary numerical difficulty associated with such a method centers on tracking a moving boundary, which is generally an unknown function of space and time. Therefore, sophisticated numerical procedures, such as moving numerical grids and/or coordinate systems, are usually needed. In contrast, since the present formulation for two-phase flow strongly resembles the one for single-phase transport, a unified formulation is derived that is valid throughout the entire domain, including both two- and single-phase regions. With such a continuum formulation, the interfaces between the regions do not require explicit consideration. The need for moving numerical grids and/or coordinate mapping is thus eliminated, as is the need for prescribing complex interfacial boundary conditions between regions internal to the domain.

4. CONCLUSIONS

In this paper, two-phase flow in porous media is conceived as a multiphase mixture flow. A consistent model for the multiphase mixture is presented that can be reduced to the classical theory for multicomponent mixtures when the interfacial area and property differences between the constituents vanish. The present two-phase model is equivalent to the SFM.

The derived conservation equations contain the effects of the finite dimensions of the phase elements and the large property differences between them. These effects manifest themselves explicitly through the diffusive mass flux due to the density difference between the two phases when under the action of gravity and through the contribution of mass transfer to energy transport due to the difference in the enthalpies of the two phases.

The two-phase mixture model opens new prospects for understanding complicated two-phase flows in porous media. It reduces the differential governing equations almost by half when compared to the SFM, rendering it suitable for numerical simulations with even moderate computer resources. The similarity between this formulation and that describing single-phase multicomponent mixture flow provides new insights into several important problems, such as one-dimensional flows with phase change, boundary layer two-phase flows, and combined single- and two-phase flows in a single domain. Another significant advantage is that the formulation does not smear out intrinsic characteristics of the individual phases, although the differential governing equations deal solely with the bulk behavior of the mixture. This is because the formulation embodies simple algebraic relations between the motions of the multiphase mixture and its separable phases.

Future work will consist not only of applying the two-phase mixture model to a variety of practical problems, but also of extending it to multicomponent two-phase flows (e.g. the liquid–vapor–air system) and to flows which include inertia and other non-Darcian effects.

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