Modeling of heat and mass transfer in unsaturated wet porous media with consideration of capillary hysteresis

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Abstract—The capillary hysteresis is an important behavior of liquid-unsaturated porous media. The hysteresis effects on the heat and mass transfer are evident in action in many important cases. The present paper introduces the minimum driving gradient concept into the analytical studies on the transport phenomena in unsaturated wet porous media. The individual phase equations and total saturation equation of mass transfer, and the energy equation for temperature profiles are derived. A hysteretic criterion is introduced with discussions. It is believed that the new efforts on the subject will promote the progress in all the relevant respects of theories and applications.

INTRODUCTION

THE HEAT and mass transfer in liquid-unsaturated porous media is rather complicated. Liquid and gas perfusion, capillary liquid movement and phase transition are included. Furthermore, the existence of the capillary hysteresis in the media causes the problem to be much more complicated. Especially, it is more difficult to quantitatively study such a heat and mass transport process with consideration of the capillary hysteresis. Based on the experiments by Shen [1], Leverrett [2] and others [3–5], the reported uncertainty of water saturation of various soils changes from 1 to 20% because of the capillary hysteresis. It is obvious that the capillary hysteresis has important effects on the heat and mass transfer in many cases for the heat and mass transfer in unsaturated wet porous media.

In view of thermodynamics, the capillary potential is a kind of energy the porous media possess, which should therefore be a single-valued function of physical states of the media. But the relation of capillary potential vs degree of saturation, measured based on the classical theories [2, 3], relies on the saturation variation processes—humidifying or dehumidifying (drying). That is, the measured capillary potential is multi-valued. Since the findings of the capillary hysteresis phenomena [6, 7], there had been a doubtful point existing that a part of energy would appear out of nothing or disappear into nowhere in the saturation changing processes for the heat and mass transport in unsaturated porous media. Although many researchers had contributed to the subject and cumulated a large amount of experimental data and related materials since the 1930s [1–9], the knowledge about the capillary hysteresis had been basically qualitative. In quantitative analysis for engineering applications,

the capillary potential values were calibrated from a series of experiments of different specified processes [10–12]. In recent years, we have carefully and currently studied the update achievements about the capillary hysteresis and made precise experiments to observe the phenomena. As a result, we offered a new idea for the formation of capillary hysteresis. We realized that the main reason of macroscopic liquid flow hysteresis is from the joint effects of liquid–solid–gas contact angle variations during fluid moves, and the micro-liquid flow hysteresis in capillary structures [13]. The capillary potential is deposited in the form of the surface energy by surface deformation before the module of total dynamic potential gradient for local liquid flow reaches a critical value. The capillary potential energy could not transform to dynamic energy of macroscopic liquid flowing until the surface deformative energy became larger than the maximum energy of surface contact. On the basis of the analysis described here, we have presented the concept of the minimum gradient for liquid movement in unsaturated wet porous media, and further, established an isothermal infiltration theory of unsaturated porous media [14], which explains the capillary hysteresis phenomena reasonably (qualitatively and quantitatively). We have also proposed and arranged an experimental method for determination of capillary hysteretic behaviors [15].

Practically, the porous media are often located in non-isothermal surroundings, and the heat transfer is normally strongly relevant to mass migration, such that the capillary hysteresis should give rise to the changes of the heat and mass transfer processes. Based on our previous studies, the present paper will introduce the effects of capillary hysteresis into the analysis of heat transfer phenomena, and establish a new for-

NOMENCLATURE

		Greek symbols	
c	specific heat	α	mass–thermal conductivity
D	diffusivity	β	corrective coefficient for diffusive area of
g	gravitational acceleration		gas phase
$\vec{g}, \vec{G}$	driving gradient	δ	correction for moisture migration in
g_0, G_0	the module of the minimum gradient		equation (50)
h	enthalpy	η	defined in equations (12) and (26)
H	hysteretic criterion	λ	thermal conductivity
$\vec{j}$	vector in direction to $\vec{G}$	μ	dynamic viscosity
$\vec{J}$	flow flux vector	ξ	nonlinear thermal conductivity
k	specific permeability	ρ	density
K	hydraulic conductivity	τ	time
K_t	thermo–hydraulic conductivity	ϕ_i	volume percentage for phase i.
$\vec{l}$	unit vector in upward vertical		
	direction	Subscripts	
n	porosity	a	air
p_c	capillary pressure	at	thermo–mass effect on air flow
r	latent heat of phase change	l	liquid
s	moisture content (percentage to	lt	thermo–mass effect on liquid flow
	saturated)	m	solid matrix
S	mass source per unit volume	s	in saturation state
T	temperature	v	vapor
w_s	mass fraction of vapor in humid air	vt	thermo–mass effect on vapor
w	defined in equation (21)	w	humid air.
z	coordinate in up vertical direction.		

mulation for simulating the heat transfer and moisture migration in unsaturated wet porous media with a consideration of capillary hysteresis.

BASIC ASSUMPTIONS AND THE CONSERVATIVE LAWS

The present paper is limited to studying porous media with the assumptions below :

(1) The medium is macroscopically continuous in space (an imaginative continuous medium) and isotropic for physical properties.

(2) Liquid moves due to both the capillary potential and gravitational potential, and is ruled by the minimum gradient assumption [14] described below.

(3) The humid air in medium pores are assumed locally saturated thermodynamically, and the phase change between liquid and its vapor occurs when the local temperature varies. The humid air moves only by thermal diffusion.

(4) The gas pressure is assumed constant everywhere so that there is no sweeping flow of fluids in the medium.

(5) The local thermodynamic equilibrium is maintained anyhow.

(6) The temperature is higher than the freezing point of the liquid so that the phase transition between liquid and its solid states is not considered.

(7) The matrix of the porous medium is assumed rigid.

The minimum gradient for liquid movement in capillary porous media is assumed such that the liquid flow would happen only if the magnitude of the total driving potential gradient, $|\vec{G}|$, exceeds the module of a minimum gradient, G_0, which should be a single-valued function of liquid saturation. Liquid movement would be impossible when the magnitude of total gradient, $|\vec{G}|$, is less than G_0. This assumption reflects the hysteretic behavior of capillary porous media, and we could assure it that a 'friction' should be overcome by the external force.

Arbitrarily take a control volume within the porous medium with the characteristics mentioned above, and apply the mass conservative law to its solid matrix (m), air (a), vapor (v) and liquid water (l) as

$$\frac{\partial(\rho_i\phi_i)}{\partial\tau} = -\nabla\cdot\vec{J}_i + S_i \quad (i = \text{m,a,v,l}) \qquad (1)$$

where ρ_i is the substantial density of phase i, ϕ_i is the volume percentage of phase i, ϕ_i is the volume percentage of phase i, $\vec{J}_i$ is the mass flux, S_i is the mass source of unit volume, and τ denotes the time.

Applying the energy conservative law to the control volume unit gives rise to

change rate of energy in the unit = apparent heat flux + conducted heat + heat generated

that is

$$\frac{\partial}{\partial\tau}\left(\sum_i\rho_i\phi_ih_i\right) = -\nabla\cdot\left(\sum_i h_i\vec{J}_i\right) + \nabla\cdot(\lambda^*\nabla T) + q_v \quad (2)$$

where h_i is the specific enthalpy of phase i, q_v is the generated heat rate in the unit, T denotes temperature, and λ^* is the nominal thermal conductivity of moist porous medium which should include the effects of heat conduction of matrix, gas and liquid phases, and the effects of micro convective and radiative heat transfer in medium pores. Normally, the nominal thermal conductivity λ^* is also briefly called the thermal conductivity of the moist porous medium because the pure heat conduction is not meaningful macroscopically in such a case.

DETERMINATION OF MASS SOURCES AND FLOW VECTORS

Solid matrix

The mass flux of solid matrix should be null if there is no solid grain dissolved and/or deposited into the fluid, that is

$$S_m = 0. \qquad (3)$$

When the volume of the solid matrix changes due to temperature variation, and/or due to humidifying or dehumidifying, the mass flux of the solid matrix should be dependent upon the variations of local temperature and moisture content. We do not consider the situation temporarily in this paper. Hence, from assumption (7), we have

$$\vec{J}_m = \vec{0}. \qquad (4)$$

Humid air in medium pores

The air and water vapor in pores exist in the form of humid air. Because air does not change its phase form in the temperature range considered, the mass source of air should be null, i.e.

$$S_a = 0. \qquad (5)$$

There is a phase change between local liquid and its vapor, which produces mass sources in liquid and vapor, respectively [16]. Changes in local temperatures would give rise to shift the thermodynamic saturation state of local humid air, so that

$$S_v = \rho_w \phi_w \frac{\partial w_s}{\partial \tau}$$

where subscript w denotes humid air, w_s is the mass fraction of vapor in saturated humid air. w_s is only the function of temperature if the total pressure remains constant, so that

$$S_v = \rho_w \phi_w \frac{dw_s}{dT} \frac{\partial T}{\partial \tau}. \qquad (6)$$

Because the humid air is postulated as saturated, the mass transport occurs only by the thermal-driven mass diffusion because concentration diffusion is not considered here, so [17]

$$\vec{J}_a = \beta D_a \rho_w \nabla (1 - w_s) = \beta D_a \rho_w \frac{dw_s}{dT} \nabla T \qquad (7)$$

$$\vec{J}_v = -\beta D_v \rho_w \nabla w_s = -\beta D_v \rho_w \frac{dw_s}{dT} \nabla T \qquad (8)$$

where D_a and D_v are the thermo-mass diffusion coefficients for air and vapor, respectively, and β is the corrective coefficient for diffusive areas of gas phase in the porous medium.

Liquid water

The mass source of liquid water is resulted from the local vapor condensation, $S_l = -S_v$, and so

$$S_l = -\rho_w \phi_w \frac{dw_s}{dT} \frac{\partial T}{\partial \tau}. \qquad (9)$$

The liquid water moves under the action of capillarity and gravitation. If $\vec{g}$ is the total driving potential gradient for local liquid movement, then,

$$\vec{g} = \nabla (p_c - \rho_l g z) = \nabla p_c - \rho_l g \vec{l}_z \qquad (10)$$

where p_c is the capillary pressure, g is the gravitational acceleration, z is the upward coordinate in vertical direction, and $\vec{l}_z$ is the unit vector in the z-direction. We have [18]

$$\vec{J}_l = \frac{\rho_l k}{\mu_l} \vec{g} \frac{|\vec{g}| - \eta g_0}{|\vec{g}|}. \qquad (11)$$

Here, k is the specific permeability of the medium, μ_l is the dynamic viscosity of water, g_0 is the module of minimum gradient, and the scalar quantity, η, is defined as

$$\eta = \begin{cases} \dfrac{|\vec{g}|}{g_0}, & |\vec{g}| < g_0 \\ 1, & |\vec{g}| \geqslant g_0 \end{cases}$$

or

$$\eta = \frac{\min(|\vec{g}|, g_0)}{g_0}. \qquad (12)$$

It should be mentioned that the capillary pressure here is the static pressure when $\vec{g} = \vec{0}$, which should be the only function of moisture saturation and be different from that ordinarily measured. Generally, p_c is a function of liquid moisture content and temperature, or $p_c = p_c(\rho_l, T)$. From equation (10), we get

$$\vec{g} = \frac{\partial p_c}{\partial \phi_l} \nabla \phi_l + \frac{\partial p_c}{\partial T} \nabla T - \rho_l g \vec{l}_z. \qquad (13)$$

Substituting equation (13) into (11) produces

$$\vec{J}_l = \frac{\rho_l k}{\mu_l} (\vec{g} - \eta g_0 \vec{j})$$

or

$$\vec{J}_l = \frac{\rho_l k}{\mu_l} \left(\frac{\partial p_c}{\partial \phi_l} \nabla \phi_l + \frac{\partial p_c}{\partial T} \nabla T - \rho_l g \vec{l}_z - g_0 \vec{j} \right). \qquad (14)$$

Here

$$\vec{\jmath} = \frac{\vec{g}}{|\vec{g}|} \qquad (15)$$

is the unit vector in the direction of $\vec{g}$.

GOVERNING EQUATIONS FOR HEAT TRANSFER AND MOISTURE MIGRATION

Mass transfer equations of individual phases

The mass transfer equations of air, vapor and liquid are conducted below. The solid matrix is not included here because the rigid matrix is assumed. Substituting equations (5)–(9) and (14) into (1), we obtain the equations of mass conservation for air, vapor and liquid, respectively, as

$$\frac{\partial(\rho_a \phi_a)}{\partial \tau} = -\nabla \cdot (n\rho_a D_{at} \nabla T) \qquad (16)$$

$$\frac{\partial(\rho_v \phi_v)}{\partial \tau} = \nabla \cdot (n\rho_v D_{vt} \nabla T) + W \frac{\partial T}{\partial \tau} \qquad (17)$$

$$\frac{\partial(\rho_l \phi_l)}{\partial \tau} = \nabla \cdot [n\rho_l (D_l \nabla \phi_l + D_{lt} \nabla T + K \vec{1}_z - \eta G_0 \vec{\jmath})]$$
$$- W \frac{\partial T}{\partial \tau} \qquad (18)$$

where

$$D_{at} = \frac{\beta D_a \rho_w}{n\rho_a} \frac{dw_s}{dT} \qquad (19)$$

$$D_{vt} = \frac{\beta D_v \rho_w}{n\rho_v} \frac{dw_s}{dT} \qquad (20)$$

$$W = \rho_w \phi_w \frac{dw_s}{dT} \qquad (21)$$

$$D_l = \frac{k}{n\mu_l} \frac{\partial p_c}{\partial \phi_l} \qquad (22)$$

$$D_{lt} = -\frac{k}{n\mu_l} \frac{\partial p_c}{\partial T} \qquad (23)$$

$$K = \frac{k\rho_l g}{n\mu_l} \qquad (24)$$

$$G_0 = \frac{k}{n\mu_l} g_0 \qquad (25)$$

where n is the porosity of the medium, and η and $\vec{\jmath}$ are defined as follows:

$$\eta = \frac{\min(|\vec{G}|, G_0)}{G_0} \qquad (26)$$

$$\vec{\jmath} = \frac{\vec{G}}{|\vec{G}|} \qquad (27)$$

with

$$\vec{G} = \frac{k}{n\mu_l} \vec{g}. \qquad (28)$$

Moisture transport equation

Define the moisture saturation s as the ratio of total moisture content (liquid and vapor) to its liquid-saturated moisture content as

$$\rho_l n s = \rho_l \phi_l + \rho_v \phi_v. \qquad (29)$$

Adding equation (17) and equation (18), and mentioning $\rho_l \approx ns$, we can arrange the moisture transport equation as follows

$$\frac{\partial s}{\partial \tau} = \nabla \cdot (D_m \nabla s + D_t \nabla T + K \vec{1}_z + \eta G_0 \vec{\jmath}) \qquad (30)$$

where D_m, D_t and K are the mass diffusivity, the thermo–mass diffusivity and the hydraulic conductivity, respectively, which are defined as

$$D_m = -\frac{k}{n\mu_l} \frac{\partial p_c}{\partial s} \qquad (31)$$

$$D_t = D_{vt} + D_{lt} = \frac{\beta D_v \rho_w}{n\rho_v} \frac{dw_s}{dT} - \frac{k}{n\mu_l} \frac{\partial p_c}{\partial T} \qquad (32)$$

and $\vec{G}$ can be also expressed as

$$\vec{G} = -D_m \nabla s - D_{lt} \nabla T - K \vec{1}_z. \qquad (33)$$

Energy equation

Equation (2) can be transformed to the following form, with the definition of specific heat of phase i, $c_i = dh_i/dT$. We have

$$\sum_i h_i \frac{\partial(\rho_i \phi_i)}{\partial T} + \sum_i \rho_i c_i \phi_i \frac{\partial T}{\partial \tau} = -\sum_i \nabla h_i \cdot \vec{J}_i$$
$$- h_i \nabla \cdot \vec{J}_i + \nabla \cdot (\lambda^* \nabla T) + q_v. \qquad (34)$$

Substituting equation (1) and the relation for S_i and $\vec{J}_i$ into equation (34), with $\nabla h_i = dh_i/dT \, \nabla T$, we can simplify the energy equation as

$$\rho^* c^* \frac{\partial T}{\partial \tau} = (\xi \nabla T + \alpha \nabla s + K_t K \vec{1}_z + K_t \eta G_0 \vec{\jmath})$$
$$\cdot \nabla T + \nabla \cdot (\lambda^* \nabla T) + q_v \qquad (35)$$

where ξ and α are called the nonlinear thermal conductivity and the mass–thermal conductivity, respectively, which are defined as

$$\xi = (c_v D_v - c_a D_a)\beta \rho_w \frac{dw_s}{dT} - \frac{c_l \rho_l k}{\mu_l} \frac{\partial p_c}{\partial T} \qquad (36)$$

$$\alpha = -\frac{c_l \rho_l k}{\mu_l} \frac{\partial p_c}{\partial s} \qquad (37)$$

and K_t is called the thermo–hydraulic conductivity

$$K_t = c_l n \rho_l. \qquad (38)$$

In equation (35), the nominal density, ρ^* of the control volume denotes the ratio of the total mass to the volume, while the nominal specific heat c^* is defined as

$$c^* = \frac{1}{\rho^*}\left(\sum_i \rho_i c_i \phi_i + r\rho_w \phi_w \frac{dw_s}{dT}\right) \quad (39)$$

where $r = (h_v - h_l)$ is the latent heat of phase transition.

HYSTERETIC CRITERION

We introduce a parameter, H, which is defined as

$$H = \frac{|\check{g}| - \eta g_0}{|\check{g}|} \quad (40)$$

which changes from zero to approach unity, as shown in Fig. 1, i.e. when $|\check{g}| \leqslant g_0$, H maintains zero and no liquid may flow locally due to the hysteretic effect. When $|\check{g}| \geqslant g_0$, local liquid begins to flow. Therefore, it is evident that the parameter, H, can describe the hysteretic behavior of liquid flowing. And so, we call it 'the hysteretic criterion'. Substituting equation (40) into (11), we have

$$\check{J}_l = \frac{\rho_l k}{\mu_l} H \check{g}. \quad (41)$$

With the hysteretic criterion, H, the moisture transport equation and energy equation can be rewritten as follows:

$$\frac{\partial s}{\partial \tau} = \nabla \cdot (\bar{D}_m \nabla s + \bar{D}_t \nabla T + \bar{K}\bar{l}_z) \quad (42)$$

$$\rho^* c^* \frac{\partial T}{\partial \tau} = (\bar{\xi}\nabla T + \bar{\alpha}\nabla S + K_t \bar{K}\bar{l}_z)$$

$$\cdot \nabla T + \nabla \cdot (\lambda^* \nabla T) + q_v \quad (43)$$

where the parameters with the cap line are defined as

$$\bar{D}_m = HD_m \quad (44)$$

$$\bar{D}_t = D_{vt} + HD_{lt} \quad (45)$$

$$\bar{K} = HK \quad (46)$$

$$\bar{\xi} = \xi_v + H\xi_l \quad (47)$$

$$\bar{\alpha} = H\alpha. \quad (48)$$

Equations (42) and (43) are in form the same as those in which the capillary hysteresis is not in consideration [16, 17]. The definitions of the parameters with cap li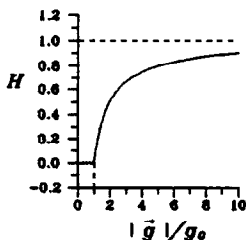ne indicate that the classical transport properties of heat and mass transfer in liquid-unsaturated porous media are relevant to the hysteretic criterion, H. It is obvious that, on the basis of theories not considering hysteresis, the transport properties are the functions of temperature and moisture variations, which lose their own meaning of physical nature. This can explain why the traditionally measured data of these properties are varied with the physical state changing traces.

If the intensity of heat transfer is small enough, the simplified energy equation is normally used for analysis as follows [16]

$$\rho^* c^* \frac{\partial T}{\partial \tau} = \nabla \cdot (\lambda_e \nabla T) \quad (49)$$

where λ_e is the effective thermal conductivity. Using the method of ref. [16], a similar analysis shows that this effective thermal conductivity is also relevant to hysteretic criterion as

$$\lambda_e = \lambda^* + \delta_v + H\delta_l \quad (50)$$

where δ_v and δ_l correct the effect of vapor and liquid migration, respectively. This is in accordance with the experimental results [16, 19]. The hysteretic effect becomes more intense when s is moderate, and hence, the measured data for λ_e would be somewhat disperse for moderate liquid saturation if no corrections applied.

DISCUSSION

(1) The heat and mass transfer processes in liquid-unsaturated porous media are influenced by the initial conditions, such as the initial temperature profile and the initial moisture distribution. From equations (33) and (35), the initial effects can be reflected because the parameter η, defined in equations (12) and (26), is the function of state variations. Even though the boundary conditions are fixed, the final steady state is still dependent upon the initial conditions.

(2) The directions, in which moisture migrates and heat transports, are uncertain without the variation details, and it is difficult to keep the same conditions in the same type of experiments, even if the experiments are arranged carefully.

(3) The thermal and moisture state of the media is normally unstable. The instability is due to the capillary hysteresis, because in some cases the liquid in the media cannot flow when the total driving potential is not high enough to overcome the hysteretic obstacle. This would influence the heat transfer because the liquid can directly carry the energy from here to there when it is in motion.

(4) The introduction of the hysteretic criterion can supply convenience for analysis of stability and transport processes.

CONCLUDING REMARKS

This paper introduces the capillary hysteresis effects into the modeling of heat and mass transfer in unsatu-

FIG. 1. Hysteretic criterion.

rated wet porous media with the minimum driving potential gradient assumption. As a result, the governing equations for individual phases and total moisture migration, and the energy equation for temperature distributions, are derived so as to establish the systematic formulation for heat and mass transfer of unsaturated wet porous media in consideration of capillary hysteretic behaviors. Although the media to be analyzed are restricted by the assumptions taken, the basic method presented here may be extended to more complicated situations, such as the cases in which the solid matrix changes its volume and shape with the temperature and moisture varied, and/or the total pressure is not uniform inside the medium. For actual modeling, there are difficulties in two respects: one of which is how to determine the transport properties of the porous media, including the minimum gradient (capillary hysteresis characteristic), and the other is how to solve the governing differential equations. For the former, some progress had been made [17–19], and some problems still exist. For the latter, the obstacle lies on the contradiction to judge the flow condition and determining the finite time step in numerical solutions of governing equations. It is believed that, with the practical solution of the relevant problems, improving techniques will be further advanced to predict the actual processes of complex heat and mass transfer of unsaturated moist porous media more reasonably and more precisely, so as to promote the progress in all the relevant respects of theories and applications.

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