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Non-equilibrium interphase heat and mass transfer during two-phase flow in porous media—Theoretical considerations and modeling

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ABSTRACT

Mass and heat transfer occurring across phase-interfaces in multi-phase flow in porous media are mostly approximated using equilibrium relationships or empirical kinetic models. However, when the characteristic time of flow is smaller than that of mass or heat transfer, non-equilibrium situations may arise. Commonly, empirical approaches are used in such cases. There are only few works in the literature that use physically-based models for these transfer terms. In fact, one would expect physical approaches to modeling kinetic interphase mass and heat transfer to contain the interfacial area between the phases as a variable. Recently, a two-phase flow and solute transport model was developed that included interfacial area as a state variable [36]. In that model, interphase mass transfer was modeled as a kinetic process.

In this work, we extend that model to account for kinetic heat transfer between two fluid phases as well as the solid phase. Therefore, we have introduced energy balances for both fluid phases and the solid phase and exchange terms that are proportional to specific interfacial areas.

We briefly discuss how these macro-scale energy balances are developed. The resulting macro-scale equation system for two-phase flow, including kinetic heat and mass transfer, is discussed and nondimensionalized. Based on the dimensionless equation system, possible simplifications are discussed. A numerical example illustrates a case where both kinetic interphase mass and heat transfer are relevant, and results are compared to those from a classical approach with equilibrium mass and heat transfer.

1. Motivation

Interphase mass and/or energy transfer in porous media are encountered in a number of applications. Typical practical non-equilibrium situations comprise CO_2 storage in the vicinity of injection wells (here, mass transfer kinetics is important), air or steam-air sparging (where kinetics of both interphase mass and energy transfer are crucial), drying of porous media in the food or textile industry (they are characterized by non-equilibrium heat transfer), degassing in fractures in the vicinity of radioactive waste disposal sites (which involves non-equilibrium mass transfer), enhanced oil recovery through injection of surfactants and DNAPL pool dissolution (the latter case is simpler as there is only one mobile phase). Commonly, these processes are modeled by equilibrium relationships. While an equilibrium assumption may be valid at the small scale (pore-scale), it is known that at larger scales it often fails. Non-equilibrium is always important in situations where the characteristic time of flow is small compared to that of mass or energy transfer, where the amount of interfacial areas separating the phases are low, or where—in the case of thermal non-equilibrium—thermal conductivities are low. So the question is how should one model non-equilibrium processes in a physically sound way.

Standard macro-scale (volume-averaged) two-phase flow models (without interphase mass or energy transfer) consist of a mass balance equation for each phase, extended Darcy's law as a simplified version of momentum balance equation, the saturation constraint, and the postulation that the difference between macro-scale non-wetting and wetting phase pressures is a function of saturation only, see e.g. [3,27,39,21]. This standard and widely applied model is not founded on an entirely sound physical basis for the following reasons:

- Darcy's law was empirically obtained by Darcy in 1856 for single-phase flow in a column filled by a homogeneous porous medium stating that the flux through that column is linearly related to the hydraulic head gradient. For the two-phase case, instead of considering other driving forces besides hydraulic head gradients, Darcy's law is "extended" by introducing some empirical function, called relative permeability, in order

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Nomenclature

Latin symbols

$a_{\alpha\beta}$	specific interfacial area of $\alpha\beta$-interface $\left(\frac{1}{\mathrm{m}}\right)$
a_{ij}	coefficients in interfacial area function (various)
b_i	coefficients (various)
$d^T_\alpha,\ d^T_{\alpha\beta}$	thermal diffusion length of phase α or $\alpha\beta$-interface, respectively (m)
d^κ	diffusion length of component κ (m)
$\underline{g}$	gravity $\left(\frac{\mathrm{m}}{\mathrm{s}^2}\right)$
h_α	specific enthalpy of phase α $\left(\frac{\mathrm{J}}{\mathrm{kg}}\right)$
$\underline{j}^\kappa_\alpha$	macro-scale diffusive flux of component κ in phase α $\left(\frac{\mathrm{kg\ m}^2}{\mathrm{s}}\right)$
$\underline{n}_{\alpha\beta}$	vector normal to $\alpha\beta$-interface pointing out of α into β (–)
p_α	pressure of phase α (Pa)
p_c	capillary pressure (Pa)
t	time (s)
$\underline{v}_\alpha,\ \underline{v}_{\alpha\beta}$	velocity of phase α or $\alpha\beta$-interface, respectively $\left(\frac{\mathrm{m}}{\mathrm{s}}\right)$
$A_{\alpha\beta}$	$\alpha\beta$-interface (m^2)
$C_{p,\alpha},\ C_{p,\alpha\beta}$	heat capacity of phase α or $\alpha\beta$-interface, respectively $\left(\frac{\mathrm{J}}{\mathrm{kg\ K}}\right)$
D^{th}_α	thermal dispersion tensor of phase α $\left(\frac{\mathrm{m}^2}{\mathrm{s}}\right)$
Da^κ	Damköhler number of component κ (–)
D^κ	micro-scale diffusion coefficient of component κ $\left(\frac{\mathrm{m}^2}{\mathrm{s}}\right)$
D^κ_α	macro-scale diffusion coefficient of component κ in phase α $\left(\frac{\mathrm{m}^2}{\mathrm{s}}\right)$
E_{wn}	production rate of specific interfacial area $\left(\frac{1}{\mathrm{m\ s}}\right)$
$G_\alpha,\ G_{\alpha\beta}$	Gibbs free energy density of phase α or $\alpha\beta$-interface, respectively $\left(\frac{\mathrm{m}^2}{\mathrm{s}^2}\right)$
$\underline{\underline{K}}$	intrinsic permeability tensor (m^2)
L	characteristic length (m)
L^{th}_α	characteristic thermal diffusion length of phase α (m)
M_α	mass ratio with respect to phase α (–)
$Nu_{\alpha\beta}$	Nusselt number for heat transfer from phase α to phase β (–)
Pe_α	Peclet number of phase α (–)
Q^κ_α	external source or sink of component κ in phase α $\left(\frac{1}{\mathrm{s}}\right)$
S_α	saturation of phase α (–)
T_α	temperature of phase α (K)
V	volume (m^3)
X^κ_α	mass fraction of component κ in phase α (–)
$X^\kappa_{\alpha,s}$	equilibrium mass fraction of component κ in phase α (–)

Greek and other symbols

α	dispersivity (m)
$\lambda_\alpha,\ \lambda_{\alpha\beta}$	thermal conductivity of phase α or $\alpha\beta$-interface, respectively $\left(\frac{\mathrm{W}}{\mathrm{m\ K}}\right)$
μ_α	dynamic viscosity of phase α (Pa s)
ϕ	porosity (–)
ρ_α	density of phase α $\left(\frac{\mathrm{kg}}{\mathrm{m}^3}\right)$
$\underline{\tau}_\alpha,\ \underline{\tau}_{\alpha\beta}$	friction forces acting on phase α, or $\alpha\beta$-interface, respectively $\left(\frac{\mathrm{kg}}{\mathrm{m}^2\ \mathrm{s}^2}\right)$
τ	tortuosity (–)
$\Gamma_{\alpha\beta}$	areal mass density of $\alpha\beta$-interface $\left(\frac{\mathrm{kg}}{\mathrm{m}^2}\right)$
$\langle\cdot\rangle$	averaged quantity
$'$	deviation quantity

Subscripts

c	capillary
n	non-wetting
s	solid
w	wetting
$wn,\ tot$	total *wn*-interfaces
L	longitudinal
R	reference
T	transversal
α	phase
$\alpha\beta$	interface
$\alpha,\ s$	equilibrium value in phase
$\alpha,\ Q$	external source property of phase α

Superscripts

a	air
sat	saturation
w	water
th	thermal
T	thermal
κ	component
$*$	(indicates dimensionless quantity)

to maintain the linear relationship between flux and hydraulic head gradient. It has been shown that these empirical relative permeability functions may depend, in addition to saturation, on a list of parameters, such as boundary conditions, pressure gradient, flow rate, and temperature, see e.g. [31,10,1,2,28,23,29]. This makes the concept of relative permeability problematic.

- Capillary pressure has a clear definition on the pore-scale: it is defined by the Young–Laplace equation as the interfacial tension divided by the mean radius of curvature. The equilibrium of forces at the interface shows (see e.g. [19]) that the pore-scale capillary pressure is equal to the difference in fluid pressures across a fluid–fluid interface. On the macro-scale, however, the concept of capillary pressure is not clear. The standard approach is to assume that macro-scale capillary pressure is a function of saturation. Then, it is assumed that the pore-scale equilibrium also holds on the macro-scale; the difference between bulk non-wetting and wetting phase pressures is assumed to be equal to the macro-scale capillary pressure. This is an ad-hoc approach and it leads to hysteresis in capillary pressure, and to the fact that the standard model is, strictly speaking, only valid for equilibrium conditions, i.e. for steady-state flow or when there is no flow.

Including interphase mass and/or heat transfer further increases the challenge: because mass and energy are transferred across phase-interfaces, they are highly dependent on interfacial areas, at least, as long as local equilibrium is not reached. Unfortunately, interfacial areas do not appear as variables in standard two-phase flow models. Therefore, these standard models either are only applicable to equilibrium situations with respect to mass and energy transfer, or have to employ some empirical transfer relationships, where a kinetic transfer coefficient is obtained by fitting to experimental data. In conclusion, there is a strong need for physically motivated models for two-phase flow that include interfacial areas, thus allowing to properly account for non-equilibrium interphase mass and heat transfer. Fig. 1 illustrates this situation: on the pore-scale, mass is transferred across the fluid–fluid interface and energy is transferred between all three phases. Phases are denoted by α and may be the wetting fluid phase (index w), the non-wetting fluid phase (index n), or the solid phase