



Modeling two-fluid-phase flow and species transport in porous media



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SUMMARY

The thermodynamically constrained averaging theory (TCAT) is used to formulate a modeling framework for mechanistic models of species transport in multiphase porous medium systems containing two fluid phases and a solid phase. Primary restrictions guide the selection of entities and the set of conservation and balance equations needed to formulate an augmented entropy inequality (EI). Classical irreversible thermodynamics is upscaled from the microscale to the macroscale and used to provide a connection among material derivatives that arise from the conservation and balance equations under near-equilibrium conditions. An essentially exact constrained EI (CEI) is derived to approach the force-flux form of the EI that is desired. A set of approximations is applied to the CEI to produce a non-unique simplified EI (SEI), which is in the strict force-flux form needed to guide the formulation of closure relations.

Sets of secondary restrictions are applied to the general SEI to form simpler subsets of the general SEI that apply for the local thermal equilibrium and isothermal cases. The SEI is then used to constrain the permissible form of the closure relations and to formulate a set of low-order closure relations. A specific model instance is formulated in closed form by specifying a complete set of conservation equations and closure relations. Many other model instances can be derived from the general modeling framework presented, and these potential extensions are discussed.

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1. Introduction

Multiphase flow and transport processes in porous medium systems are important for a wide range of environmental, industrial, and biological applications, such as groundwater contamination, carbon storage and sequestration, design of filters and insulators, enhanced gas and oil recovery, transport of nutrients in natural tissues, and biofilm growth (Aziz and Settari, 1979; Helmig, 1997; Lake, 1989; Nordbotten and Celia, 2012; Vafai, 2011; Wakeman and Tarleton, 2005).

Processes important in these applications evolve on multiple length and time scales, contributing to the complexity of these systems. One contributing factor to this complexity is the existence of multiple classes of entities, which include phases, interfaces between phases, and common curves that form at the boundary between three phases. Accounting for interfaces and common curves in the model formulation provides a higher fidelity representation of the underlying system compared to formulations based upon conservation equations for phases alone. This is so because many processes happen across interfaces and along

common curves, e.g., transport of chemical species, momentum, and energy. Surfactants are known to accumulate at interfaces, altering the interfacial tension and the morphology of the boundary between phases. Although these facts are widely acknowledged, traditional approaches (Bear, 1972; Freeze and Cherry, 1979; Helmig, 1997) do not account for these lower dimensional entities explicitly in the formulation. Instead, traditional models of two-fluid-phase porous medium systems are closed using *ad hoc* closure relations that must implicitly be dependent on the unresolved entities through parametric dependence of constitutive relations. However, these extensions do not have a rigorous basis and as a consequence often lead to a non-physical behavior of the system, such as apparent hysteretic behavior.

The classical approach to apply Fick's law for modeling species transport in porous medium systems (Bird et al., 2002; Helmig, 1997), according to which the dispersive mass flux is proportional to the concentration gradient and independent of the concentration itself, is successful for dilute solutions and homogeneous porous media. For some applications the concentration of dissolved substances is indeed low. However, many porous medium systems are non-dilute and not sufficiently homogeneous for a Fickian approximation to be accurate, e.g., brines in aquifers above salt formations, radioactive waste disposal in salt domes, evaporative salt precipitation, and transport in fractured porous media (Berkowitz

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Nomenclature

Roman letters

\hat{A}^α	interfacial velocity coefficient related to velocity of fluid phase α
\hat{B}^α	common curve velocity coefficient related to velocity of fluid phase α
b	entropy body source density
\mathbf{C}	Green's deformation tensor
\hat{c}	closure coefficient
$\hat{\mathbf{D}}$	dispersion tensor
\mathbf{d}	rate of strain tensor, $\mathbf{d} = [\nabla\mathbf{v} + (\nabla\mathbf{v})^T]/2$
E	internal energy density
\bar{E}	partial mass energy
$\mathcal{E}_{**}^{\bar{x}}$	macroscale entity-based total energy conservation equation, Eq. (3)
f	general scalar function
\mathbf{G}	geometric orientation tensor, $\mathbf{G}_\alpha = \mathbf{I} - \mathbf{I}'_\alpha$ for $\alpha \in \mathcal{J}_1$, $\mathbf{G}_{wns} = \mathbf{I} - \mathbf{I}''_{wns}$
$G_0^{\kappa \rightarrow \alpha}$	macroscale transfer rate of potential energy due to variability of mass exchange per volume
$\mathcal{G}_{**}^{\bar{x}}$	macroscale entity-based body force potential balance equation, Eq. (5)
\mathbf{g}	body force per unit mass, gravity
\bar{H}	partial mass enthalpy
$h_{\bar{x}}$	energy source density
$h_0^{\bar{x}}$	macroscale energy source density for entity α due to body force and velocity fluctuations
\mathbf{I}	identity tensor
\mathbf{I}'	unit tensor in a surface, $\mathbf{I}'_\alpha = \mathbf{I} - \mathbf{n}_\beta \mathbf{n}_\beta$ for $\alpha \in \mathcal{J}_1$, $\beta \in \mathcal{J}_{c\alpha}^+$
\mathbf{I}''	unit tensor in a common curve, $\mathbf{I}''_{wns} = \mathbf{I}_{wns} \mathbf{I}_{wns}$
$\mathbf{I}^{(n)}$	unit tensor associated with 3 – n -dimensional entity where (n) is the number of primes used
\mathcal{J}	set of entity indices
\mathcal{J}_C	set of common curve entities
$\mathcal{J}_{c\alpha}$	connected set of indices for entity α , $\mathcal{J}_{c\alpha} = \mathcal{J}_{c\alpha}^+ \cup \mathcal{J}_{c\alpha}^-$
$\mathcal{J}_{c\alpha}^+$	connected set of indices of one dimension higher than entity α
$\mathcal{J}_{c\alpha}^-$	connected set of indices of one dimension lower than entity α
\mathcal{J}_f	set of fluid-phase indices
\mathcal{J}_I	set of interface indices
\mathcal{J}_P	set of phase indices
\mathcal{J}_s	set of species indices
$\mathcal{J}_{s \setminus N}$	set of species indices except species N
$\mathcal{J}_{\setminus S}$	set of entity indices except the solid phase
$J_\alpha^{\alpha\beta}$	macroscale surface curvature, $J_\alpha^{\alpha\beta} = \langle \nabla' \cdot \mathbf{n}_\alpha \rangle_{\Omega_{\alpha\beta}, \Omega_{\alpha\beta}}$ for $\alpha, \beta \in \mathcal{J}_f$
j	Jacobian
K_E	kinetic energy per mass due to velocity fluctuations
\hat{K}_M	mass transfer coefficient
$\hat{\mathbf{K}}_\theta$	heat conductivity tensor
\hat{k}_{wn}	parameter for rate of relaxation of interfacial area
\hat{k}_1^{wn}	parameter for rate of relaxation of interfacial area
\hat{k}_{wns}	parameter for rate of relaxation of common curve length
\mathbf{l}	unit vector tangent to a common curve
$M^{i\kappa \rightarrow i\alpha}$	macroscale transfer rate of mass of species i in entity κ to species i in entity α per volume
$\mathcal{M}_{**}^{\bar{x}}$	macroscale species mass conservation equation, Eq. (1)
N	number of chemical species
\mathbf{n}	unit normal vector
$\mathcal{P}_{**}^{\bar{x}}$	macroscale entity-based momentum conservation equation, Eq. (2)

p	pressure
$Q_1^{\kappa \rightarrow \alpha}$	macroscale transfer rate of internal energy from entity κ to entity α per volume
$Q_0^{\kappa \rightarrow \alpha}$	macroscale energy exchange between entities which dimensionalities differ by two
\mathbf{q}	non-advective energy flux
\mathbf{q}_{g0}	non-advective energy flux associated with mechanical processes
$\hat{\mathbf{R}}$	resistance tensor
r	mass production rate density
$\mathcal{S}_{**}^{\bar{x}}$	macroscale entity-based entropy balance equation, Eq. (4)
s	saturation
$T_0^{\kappa \rightarrow \alpha}$	macroscale transfer rate of momentum from entity κ to entity α per volume
$\mathbf{T}^{\kappa \rightarrow \alpha}$	macroscale momentum exchange between entities which dimensionalities differ by two
$\mathcal{T}_*^{\bar{x}}$	macroscale Euler equation, Eq. (6), for all entities except solid, and Eq. (7) for solid phase
$\mathcal{T}_{\mathcal{G}^*}^{\bar{x}}$	macroscale body source potential balance equation, Eq. (8)
\mathbf{t}	stress tensor
t	time
$\mathcal{U}_{**}^{\bar{x}}$	macroscale entity-based internal energy equation, Eq. (64)
\mathbf{u}	diffusion/dispersion velocity, $\mathbf{u}_{i\alpha} = \mathbf{v}_{i\alpha} - \mathbf{v}_\alpha$, $\mathbf{u}_{i\alpha}^{\bar{x}} = \mathbf{v}_{i\alpha}^{\bar{x}} - \mathbf{v}_\alpha^{\bar{x}}$
\mathcal{V}	set of variables
\mathbf{v}	velocity
W	weighting function for averaging
\mathbf{w}	velocity of a domain boundary

Greek letters

γ	interfacial or common curve lineal tension
ϵ	porosity
$\epsilon^{\bar{x}}$	specific entity measure
η	entropy density
$\bar{\eta}$	partial mass entropy
θ	temperature
κ_G	geodesic curvature, $\kappa_{Gwns} = \mathbf{l}_{wns} \cdot \nabla'' \mathbf{l}_{wns} \cdot \mathbf{n}_{ws}$
κ_N	normal curvature, $\kappa_{Nwns} = \mathbf{l}_{wns} \cdot \nabla'' \mathbf{l}_{wns} \cdot \mathbf{n}_s$
\mathcal{A}	entropy production rate
λ	vector Lagrange multiplier
λ	scalar Lagrange multiplier
μ	chemical potential
ρ	mass density
σ	Lagrangian solid-phase stress tensor
$\Phi_0^{\kappa \rightarrow \alpha}$	macroscale transfer rate of entropy from entity κ to entity α per volume
$\Phi^{\kappa \rightarrow \alpha}$	macroscale entropy exchange between entities which dimensionalities differ by two
φ	non-advective entropy flux
$\varphi^{\overline{ws,wn}}$	macroscale measure of contact angle
$\gamma_{s^{\bar{x}}}$	fraction of the solid surface in contact with fluid phase α , $\gamma_{s^{\bar{x}}} = \epsilon^{\bar{x}s} / (\epsilon^{\bar{x}s} + \epsilon^{\bar{x}ns})$, $\alpha \in \mathcal{J}_f$
Ψ	body force potential density
ψ	body force potential per mass
Ω	spatial domain
ω	mass fraction

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