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Thermodynamically constrained averaging theory approach for modeling flow and transport phenomena in porous medium systems: 3. Single-fluid-phase flow

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Abstract

This work is the third in a series of papers on the thermodynamically constrained averaging theory (TCAT) approach to modeling flow and transport phenomena in multiscale porous medium systems. Building upon the general TCAT framework and the mathematical foundation presented in previous works in this series, we demonstrate the TCAT approach for the case of single-fluid-phase flow. The formulated model is based upon conservation equations for mass, momentum, and energy and a general entropy inequality constraint, which is developed to guide model closure. A specific example of a closed model is derived under limiting assumptions using a linearization approach and these results are compared and contrasted with the traditional single-phase-flow model. Potential extensions to this work are discussed. Specific advancements in this work beyond previous averaging theory approaches to single-phase flow include use of macroscale thermodynamics that is averaged from the microscale, the use of derived equilibrium conditions to guide a flux–force pair approach to simplification, use of a general Lagrange multiplier approach to connect conservation equation constraints to the entropy inequality, and a focus on producing complete, closed models that are solvable.

Keywords: Porous medium models; Averaging theory; TCAT; Single-phase flow

1. Introduction

This paper is the third in a series of efforts designed to yield complete, rigorous, closed models that describe transport phenomena in multiscale porous medium systems using the thermodynamically constrained averaging theory (TCAT) approach. Work to date has outlined a general TCAT approach that can be used to generate such models [20] and laid a mathematical foundation upon which these models can be constructed [25]. We will build on these results in the current and subsequent papers to construct closed models for important systems, to compare and contrast these models with conventional models in use for similar purposes, and to compare these new models with highly resolved sub-scale simulations and experimental observations. The present paper is focused on single-fluid-phase flow in porous media. This system has been chosen because it provides a relatively simple setting in which to demonstrate the application of the TCAT approach and to illustrate that putting even this well-studied system on firm theoretical footing illuminates some important intrinsic assumptions in conventional models.

The traditional model for single-phase flow is derived typically by (1) writing an equation of mass conservation for a fluid phase; (2) using Darcy's law as an approximate momentum equation to remove the superficial velocity vector from the conservation equation; (3) assuming a simple equation of state for the fluid phase that relates its density and pressure; (4) assuming that spatial gradients in density are small; and (5) approximating the compressibilities of

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Nomenclature

Roman letters

b	external entropy source per unit volume
$\mathbf{C}$	Greens' deformation tensor
$\hat{c}$	compressibility parameter
$\mathbf{d}$	rate of strain tensor
E	internal energy per unit volume
$\hat{E}$	Young's modulus
E_{T}	total energy per unit volume
$\mathscr{E}$	the set of entities in the model
$\mathcal{E}$	conservation of energy equation
$\mathscr{E}_{\mathrm{c}}$	connected set of entities
$\hat{E}_v$	variable grouping defined by Eq. (114)
$\mathbf{e}$	solid-phase Eulerian strain tensor
e^s_{zz}	macroscale solid-phase Eulerian strain tensor diagonal component for the vertical direction
$\mathbf{F}$	thermodynamic force tensor
$\mathbf{F}$	thermodynamic force vector
F	thermodynamic force scalar
$\mathscr{F}$	set of all thermodynamic forces
$\mathbf{G}$	geometric orientation tensor for an interface
$\mathbf{g}$	gravitational acceleration vector
g	magnitude of gravitational acceleration
H	hydraulic head
h	heat source per unit volume
$\mathbf{I}$	identity tensor
$\mathbf{I}'$	surface identity tensor
$\mathscr{J}$	index set of entities
$\mathscr{J}_{\mathrm{c}}$	index set of connected entities
$\mathscr{J}_{\mathrm{p}}$	index set of phase entities
$\mathbf{J}$	thermodynamic flux tensor
$\mathbf{J}$	thermodynamic flux vector
J	thermodynamic flux scalar
$\mathfrak{J}$	set of all thermodynamic fluxes
j	solid-phase Jacobian
$\hat{\mathbf{K}}$	hydraulic conductivity tensor
$\hat{\mathbf{K}}_q$	second-rank, symmetric, positive semi-definite heat conduction tensor
K_{E}	kinetic energy per unit mass due to microscale velocity fluctuations
$\hat{K}_{\mathrm{S}}$	bulk modulus of the solid phase
$\hat{K}_{\mathrm{T}}$	bulk modulus of the skeleton
$\mathbf{k}$	unit Cartesian vector oriented vertically upward
$\hat{k}_m$	non-negative interfacial mass transfer parameter
$\hat{k}_q$	non-negative interfacial heat transfer parameter
$\mathscr{M}$	conservation of mass equation
$\overset{\kappa\to\iota}{M}$	transfer of mass from the κ to the ι entity
$\overset{\kappa\to\iota}{M}_{\mathrm{E}}$	transfer of energy from the κ to the ι entity resulting from mass transfer
$\overset{\kappa\to\iota}{\mathbf{M}}_v$	exchange of momentum from the κ to the ι entity resulting from mass transfer
$\overset{\kappa\to\iota}{M}_\eta$	exchange of entropy from the κ to the ι entity resulting from mass transfer
$\mathbf{n}_\iota$	outward normal vector from entity ι
$\mathcal{P}$	conservation of momentum equation
$\mathscr{P}_i$	general microscale property
p	fluid pressure
$\overset{\kappa\to\iota}{Q}$	transfer of energy from the κ to the ι entity resulting from phase change, interfacial stress, and heat transfer
$\mathbf{q}$	heat flux vector
$\hat{\mathbf{R}}$	symmetric, positive semi-definite second-rank momentum resistance tensor
$\mathscr{S}$	entropy balance equation
$\hat{S}_{\mathrm{s}}$	specific storage coefficient
$\mathscr{T}$	CIT-based thermodynamic equation for material derivative of internal energy
$\overset{\kappa\to\iota}{\mathbf{T}}$	transfer of momentum from the κ to the ι entity
$\overset{\kappa\to\iota}{T}_v$	transfer of energy from the κ to the ι entity resulting from interfacial stress
$\mathbf{t}$	stress tensor
t	time
$\mathscr{V}$	the set of unknown variables requiring closure relations
$\mathbf{v}$	velocity vector
$\mathbf{v}^{\bar{\iota},\bar{s}}$	mass-averaged velocity of the ι entity relative to the mass-averaged velocity of the s entity
w	weighting function in averaging operator
$\mathbf{X}$	position vector in the solid phase initially
$\mathbf{x}$	position vector in the solid phase

Greek letters

$\hat{\alpha}$	Biot coefficient
$\hat{\beta}$	compressibility parameter
Γ	boundary of domain of interest
γ	interfacial tension
ϵ^ι	specific measure of the ι entity
η	entropy per unit volume
θ	temperature
Λ	entropy production per unit volume
$\boldsymbol{\lambda}$	vector of Lagrange multipliers
λ	Lagrange multiplier
μ	chemical potential
$\hat{\nu}$	Poisson's ratio
ρ	density
$\boldsymbol{\sigma}$	solid-phase Lagrangian stress tensor
$\boldsymbol{\tau}$	effective solid-phase stress tensor
$\overset{\kappa\to\iota}{\Phi}$	transfer of entropy from the κ to the ι entity
$\boldsymbol{\varphi}$	entropy flux vector
ψ	gravitational potential
Ω	spatial domain
$\overline{\Omega}$	closed domain