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Thermodynamically Consistent Modeling and Energy Stable Numerical Simulation of Multicomponent Compressible Flow in Poroelastic Media

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Abstract. Modeling and numerical simulation of coupled poromechanical problems with multicomponent compressible flow are of particular importance in many fields including shale and natural gas engineering, carbon dioxide sequestration and geotechnical engineering. In this paper, using the second law of thermodynamics, we rigorously derive a thermodynamically consistent model for multicomponent compressible flow in deformable porous media coupled with poroelasticity. The model herein takes molar densities as the primary unknowns rather than pressure and molar fractions as well as introduces fluid and solid free energies, so that it naturally follows an energy dissipation law. Additionally, the Maxwell-Stefan model of multicomponent diffusion is generalized as a multicomponent fluid-solid coupling model accounting for the solid deformation, which not only satisfies Onsager's reciprocal principle but also yields a thermodynamically consistent poro-visco-elastic equation. For numerical simulation, we propose a novel energy stable and mass conservative numerical scheme for the model. We first design the semi-discrete time scheme using the stabilized energy factorization approach to deal with the multicomponent Helmholtz free energy as well as subtle semi-implicit treatments for the coupling between multicomponent fluids and solids. A nontrivial treatment is the use of the discrete Gibbs-Duhem equation substituting for the pressure gradient contributed by the multicomponent fluids in the solid mechanical balance equation, which establishes the thermodynamically consistent relation between fluids and solids at the discrete level. Based on the cell-centered finite

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volume method on staggered grids, the fully discrete scheme is constructed using the upwind strategy for both molar densities and porosity. The scheme is proved to preserve the discrete energy dissipation law and Onsager's reciprocal principle as well as to conserve the mass of fluid components and solids. Numerical experiments are performed to confirm our theories, especially to demonstrate the good performance of the proposed scheme in energy stability and mass conservation as expected from our theoretical analysis.

AMS subject classifications: 65M12, 65M08, 76S05

Key words: Multicomponent flow, poroelasticity, Maxwell-Stefan model, porous media, thermodynamic consistency, energy stability.

1 Introduction

Multicomponent and multiphase fluids flow through a deformable porous medium may trigger a response from the solid skeleton, thereby significantly changing the medium properties. For instance, in CO_2 geological storage, the injection of CO_2 could lead to the increase of pressure within reservoirs, which could cause rock deformation and rearrangement, thereby changing porosity and permeability [53, 56]. During the recovery of natural and shale gas, significant changes of the reservoir pressure often result in the non-negligible rock deformation and compaction [7,12,31,37,59], and in turn, the deformation of rock structure affects the gas production of shale reservoirs [13]. Therefore, incorporating the solid deformation into the modeling framework of multicomponent flow in porous media has potential applications in CO_2 geological storage, gas production and other gas flows in poroelastic media.

To account for the deformation of solid skeletons, a popular modeling approach is to adopt Biot's poroelasticity theory [3], which usually solves a solid mechanical equation to obtain the solid displacements and subsequently derives the porosity changes from the displacements. The models and numerical methods of poroelasticity have been extensively investigated and successfully applied in many fields, such as petroleum engineering and geomechanics [5,10,19,22,33,37,40,43,47,57,58]. Yotov et al. [19,40] developed efficient and accurate numerical methods for solving the single-phase Biot system of poroelasticity. Wu et al. [57, 58] proposed novel numerical manifold methods to simulate multiphase flow in heterogeneous, fractured, deformable or elasto-plastic porous media. In recent years, a number of works have focused on modeling and numerical simulation of coupled two-phase flow and poroelasticity. For the coupled two-phase flow and poroelasticity model, Shen and Riviere [47] proposed an accurate and robust discontinuous Galerkin method. Camargo et al. [5] proposed preconditioning approaches for poromechanical problems coupled with two-phase flow. Using the extended finite element method, Khoei and Mortazavi [22] presented a fully coupled thermo-hydro-mechanical model of two-phase flow and heat transfer in fractured porous media. It is