

Two phase flows in karstic geometry

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Abstract

Multiphase flow phenomena are ubiquitous. Common examples include coupled atmosphere and ocean system (air and water), oil reservoir (water, oil and gas), cloud and fog (water vapor, water and air). Multiphase flows also play an important role in many engineering and environmental science applications.

In some applications such as flows in unconfined karst aquifers, karst oil reservoir, proton membrane exchange fuel cell, multiphase flows in conduits and in porous media must be considered together. Geometric configurations that contain both conduit (or vug) and porous media are termed karstic geometry. Despite the importance of the subject, little work has been done on multi-phase flows in karstic geometry.

In this paper we present a family of phase field (diffusive interface) models for two phase flow in karstic geometry. These models together with the associated interface boundary conditions are derived utilizing Onsager's extremum principle. The models derived enjoy physically important energy laws. Uniquely solvable first and second order in time numerical schemes that preserve the associated energy law are presented as well.

1 Introduction

Multiphase flow phenomena are ubiquitous [1, 2, 3]. Common examples include coupled atmosphere and ocean system (air and water), oil reservoir

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(water, oil and gas), cloud and fog (water vapor, water and air). Many multiphase flows are important to us humans and to a lot of engineering processes. Therefore, there is a genuine need to understand various multiphase flow phenomena better.

Karst type geometry is a special type of configuration that consists of both conduit/channel (or vug or chamber) together with porous media. See Figure 1 below for an illustration. In many important applications such as contaminant transport in karst aquifer, oil recovery in karst oil reservoir, proton exchange membrane fuel cell technology, cardiovascular modeling, we must deal with karstic geometry. Despite the importance of the subject, little work has been done on multiphase flows in karstic geometry. Multiphase flows in karstic geometry pose additional challenges beyond the usual difficulties associated with multi-phase flows. The main goal of this manuscript is the derivation, based on Onsager's extremum principle, of a hierarchical family of diffuse interface models for two-phase flows in karstic geometry.

One of the most prominent and important example of two-phase flow in karstic geometry is flow in unconfined natural karst aquifers. A natural karst is a type of landscape that is formed by the dissolution of a layer or layers of soluble bedrocks, including carbonate rocks, limestone and dolomite. Karst regions usually contain aquifers that are capable of providing large supplies of water. A karst aquifer, in addition to a porous limestone or dolomite matrix, typically has large cavernous conduits that are known to have a great impact on groundwater flow and contaminant transport within the aquifer [4, 5].

Karst aquifers supply a significant portion of the drinking water in the United States (about 40%) and are particularly important in States like Florida for which karst aquifers provide more than 90% of the fresh water used [6]. Karst aquifers are susceptible to greater contamination than are non-karstic aquifers due to rapid transport processes and limited chemical filtering capacities, both of which quicken the spread of solutes [5, 7, 8]. During a high flow season, the water pressure in the conduits is larger than that in the ambient matrix so that conduit-borne contaminants can be driven into the matrix and the water table (the interface between water and air) rises. During dry seasons, the pressure differential reverses and contaminants long sequestered in the matrix can be released into the free flow in the conduits and exit through, e.g., springs and wells, into surface water systems [9]. This retention and release phenomenon induces an environmental issue in that sequestered contaminants may influence the quality of underground water sources for a long time and thus significantly decrease water availabil-

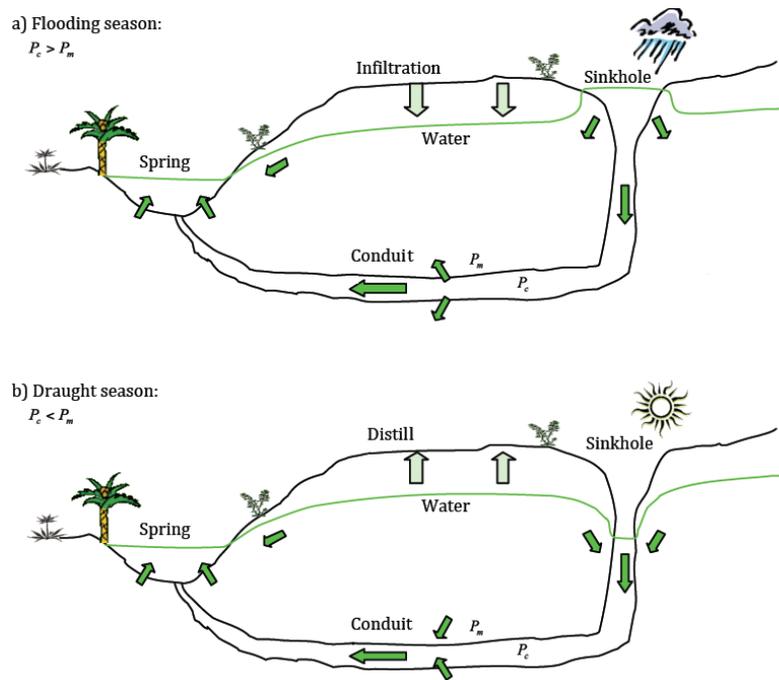


Figure 1: Schematic plot of an unconfined karst in flood and draught season

ity. Therefore the study of flows in karst aquifers is of great importance to us, especially since the aquifers are now being seriously threatened by over withdrawals and increasing contamination [5].

The mathematical study of flows in confined saturated karst aquifers is already a challenge due to the coupling of the flows in the conduits and the flows in the surrounding matrix which are governed by different physical processes, the complex geometry of the network of conduits, the vastly disparate spatial and temporal scales, the strong heterogeneity, and the huge associated uncertainty with the data. Even for a small lab size conceptual model with only one conduit (pipe) imbedded in a homogenous porous media (matrix), significant mathematically rigorous progress has been achieved only recently via the so-called coupled (Navier) Stokes-Darcy model with the classical Beavers-Joseph interface boundary condition [10] or various simplified interface conditions [11, 12, 13, 14, 15]. Existing mathematical work on flows in karst aquifers treats the case of confined saturated aquifer where only one type of fluid (water) occupies the whole region exclusively. However, many geologically important karst aquifers are unconfined and unsaturated which necessitates the study of two-phase flows (air and water in this case) instead of one single fluid (water in confined karst aquifer).

Multiphase flows in karst type domains are not restricted to flows in unsaturated karst aquifers. Besides groundwater study in karst regions that we mentioned above, multiphase flows in karstic geometry are also important in oil recovery in petroleum engineering in karst regions (two-phase flow of oil and water, or oil, water and gas, see for instance [16], <http://www.in.gov/nrc/2394.htm>, http://www.netl.doe.gov/technologies/oil-gas/petroleum/projects/ep/explor_tech/15504.htm, [17]), Polymer Electrolyte Membrane (or Proton Exchange Membrane) fuel cell technology (water management in PEM fuel cell [18]), as well as biomedical sciences (cardiovascular modeling and simulation, see for instance [19]). It is also relevant in CO_2 sequestration, and in assessing environmental impact on beaches after accidents like the Deepwater Horizon oil spill.

We will focus on essentially immiscible two phase fluids (like air and water, or oil and water for instance) in this paper for simplicity. There are two prevalent approaches to the study of two-phase immiscible flows.

The classical approach assumes that the fluids are completely immiscible. Therefore a sharp interface exists between the two fluids under investigation (see Fig.2b for an illustration). Sea surface is a well-known example of the interface between sea water and air, and water table is another example of the interface between air and water for flow in matrix (porous media).

The sharp interface model in porous media (matrix) is usually termed the Muskat problem [20, 21]. The two phase Muskat problem takes the form [22, 23]

$$\nabla \cdot \vec{u}_i = 0, \text{ in } \Omega_i, \vec{u}_i = -\frac{\Pi}{\eta_i} \nabla p_i, \text{ in } \Omega_i, (\vec{u}_1 - \vec{u}_2) \cdot \vec{n} = 0, \text{ on } \Gamma, p_2 - p_1 = \tau \kappa \text{ on } \Gamma, \quad (1)$$

where \vec{u}_i denotes the fluid velocity of the i^{th} fluid which occupies the region Ω_i , η_i is the viscosity of the i^{th} fluid, Π is the permeability of the porous media (matrix), p_i is the pressure, \vec{n} is the unit normal to the interface Γ (pointing from fluid 1 to fluid 2), κ is the (mean) curvature and τ is the dimensionless surface tension coefficient. The interface Γ moves with the speed $V_n = \vec{u}_1 \cdot \vec{n}$. In the case of water flow in unsaturated porous media (matrix), approximate models such as Richards equation may be utilized sometimes [24].

Likewise, the sharp interface model in the conduit or vug takes the form of the following two-phase Navier-Stokes equations [2, 3, 25, 26, 27, 28]

$$\begin{cases} \rho_i \left(\frac{\partial \vec{u}_i}{\partial t} + (\vec{u}_i \cdot \nabla) \vec{u}_i \right) - \nabla \cdot \mathbb{T}(\vec{u}_i, p_i) = 0, \text{ in } \Omega_i, \nabla \cdot \vec{u}_i = 0 \text{ in } \Omega_i, \\ \vec{u}_1 = \vec{u}_2, \text{ on } \Gamma, (\mathbb{T}(\vec{u}_1, p_1) - \mathbb{T}(\vec{u}_2, p_2)) \vec{n} = \tau \kappa \vec{n} \text{ on } \Gamma, \end{cases} \quad (2)$$

where ρ_i, \vec{u}_i denote the density and velocity of the i^{th} fluid which occupies the region Ω_i , $\mathbb{T}(\vec{u}_i, p_i) = 2\eta_i \mathbb{D}(\vec{u}_i) - p_i \mathbb{I}$ is the tress tensor, $\mathbb{D}(\vec{u}_i) = (\nabla \vec{u}_i + \nabla \vec{u}_i^T)/2$ is the rate of strain tensor, η_i is the viscosity of the i^{th} fluid, p_i is the pressure, \vec{n} is the unit normal to the interface Γ , κ is the (mean) curvature and τ is the dimensionless surface tension coefficient. The interface Γ moves with the speed $V_n = \vec{u}_1 \cdot \vec{n}$. When the Reynolds number is small, one can drop the total (material) derivative term in the momentum equation and arrive at the two-phase Stokes system.

The sharp interface models have been very successful in explaining many physically interesting phenomena [2, 3, 29, 30, 31, 32, 33]. However, there are several known drawbacks associated with this sharp interface approach. In particular, this approach is not able to handle in an unambiguous fashion topological changes of the sharp interface (pinch-off and reconnection), singularity formation (breaking wave for instance), or moving contact lines. Moreover, there is no-known physically sound coupled two-phase models in karstic geometry in the literature to the best of our knowledge.

An alternative approach, the so-called diffuse-interface method (or phase-field method), recognizes the micro-scale mixing and hence treats the interface as a transition layer with small but non-zero width (see Fig.3a for an

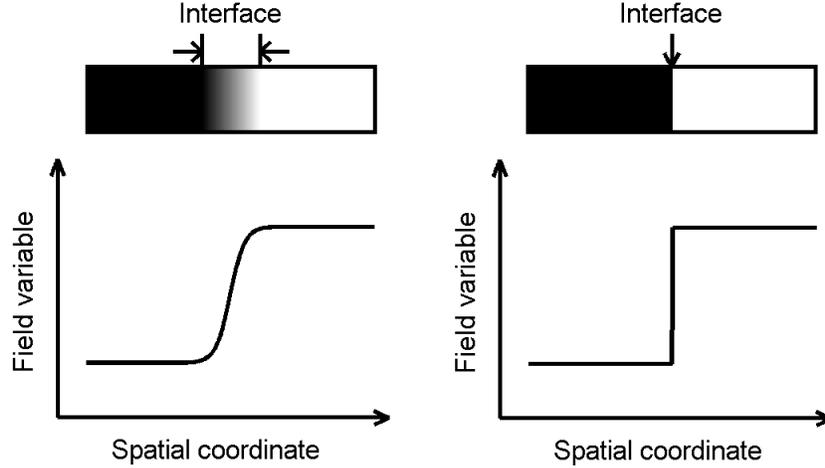


Figure 2: Left panel: diffusive interface; right panel: sharp interface

illustration) [34, 35, 36]. In the diffuse-interface approach (or phase-field method) that we have adopted here, we approximate the separating boundary between two (macroscopically) immiscible fluid phases using an order parameter ϕ (phase field variable) that continuously, and usually monotonically, varies from one value in phase A (water for instance), say $\phi = +1$, to another value in phase B (oil for instance), say $\phi = -1$, in a transition layer of small, but finite, thickness (see Fig. 2 for an illustration) [34, 35, 36, 37]. This idea can be traced back to van der Waals and Lord Rayleigh [38, 39]. This is in contrast to the sharp interface formulation that would employ a characteristic (or indicator) function description. In the diffuse interface approximation, the "location" of the interface can be recovered as the level surface $\phi = 0$.

This order parameter ϕ can be interpreted as volume fraction of fluids in the following way:

$$\begin{aligned} \text{volume fraction of phase } A &= (\phi + 1)/2, & \text{volume fraction of phase} \\ & & B = (1 - \phi)/2. \end{aligned}$$

In the case with matched density or when the Boussinesq approximation is applicable, the velocity \vec{u} of the mixture can be taken as incompressible [36], i.e., $\nabla \cdot \vec{u} = 0$. For the Boussinesq approximation, the density ρ of the mixture

is given by

$$\rho = \frac{(\rho_1 - \rho_2)\phi + \rho_1 + \rho_2}{2},$$

where ρ_1, ρ_2 are the densities of the two phases. The viscosity η of the mixture can be modelled as an appropriate smooth positive bounded function of the order parameter ϕ that satisfies $\eta(\phi) = \eta_1$, if $\phi = 1$; $\eta(\phi) = \eta_2$, if $\phi = -1$, where η_1, η_2 are the viscosities of the two fluids [28, 36, 40].

The diffuse-interface approach has the advantage that it can handle topological changes such as pinch-off and reconnection, moving contact lines seamlessly [36, 37, 41, 42]. Another advantage of the diffuse-interface approach is its relative easiness to handle the interface boundary condition between the matrix and the conduit as we will demonstrate below.

With the expected complex interfacial dynamics, including topological changes and interaction between the interface and the solid as well as the matrix-conduit/vug boundary, we propose to investigate two phase flows in karstic geometry utilizing a hierarchical family of physically motivated diffuse interface (phase field) models with increasing complexity that we derive in this manuscript.

The rest of the manuscript is organized as follows. In section 2 we derived the coupled Cahn-Hilliard-Stokes-Darcy model via Onsager's extremum principle. This new model enjoys a physically important energy law. Generalization of this model that inherits the energy law will be also presented. In section 3 we introduce and analyze two uniquely solvable numerical schemes, one first order and another one second order in time, for the Cahn-Hilliard-Stokes-Darcy model that preserve the energy law. In section 4 we provide concluding remarks.

2 The derivation of the models

The purpose of this section is the derivation of the thermal dynamically consistent Cahn-Hilliard-Stokes-Darcy (CHSD) model, and its generalization, based on Onsager's extremum principle. The family of models that we present here all enjoy physically important energy law. These energy laws are crucial to the analysis of, and the design of unconditionally stable numerical schemes for these models.

2.1 The conceptual domain

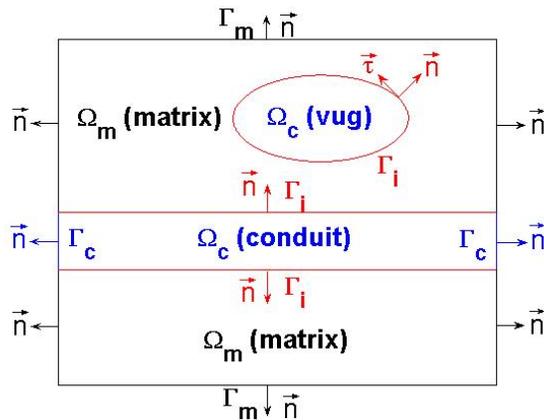


Figure 3: A conceptual karstic domain

Since a complete treatment of two-phase flow in karst region is out of the scope at this time even with diffuse-interface approach, we consider here a simple conceptual karstic domain where a horizontal conduit and one vug are embedded in a rectangular matrix (see Fig. 3). Such a simple geometry is easy to set-up in laboratory experiment. Here, Ω_c denotes the region occupied by the conduit or vug, Ω_m denotes region occupied by the matrix, Γ_i represents the interface between the matrix and the conduit or vug, $\Gamma_c = \partial\Omega_c \setminus \Gamma_i$ represents the boundary of the conduit/vug minus the conduit/vug-matrix interface, $\Gamma_m = \partial\Omega_m \setminus \Gamma_i$ represents the boundary of the matrix minus the conduit/vug-matrix interface, \vec{n} denotes the unit outer normal on $\partial\Omega = \Gamma_c \cup \Gamma_m$ as well as the unit normal on Γ_i pointing from Ω_c to Ω_m , $\vec{\tau}$ denotes a generic unit tangent vector to the conduit/vug-matrix interface Γ_i .

2.2 Derivation of the Cahn-Hilliard-Stokes-Darcy model via Onsager's extremum principle

Since there is no known coupled two-phase model for flows in karstic geometry in the literature, our first task is the derivation of physical models. We sketch here the derivation of the relative simple Cahn-Hilliard-Stokes-Darcy model under the matched density assumption utilizing Onsager's extremal principle

[43, 44, 45]. Onsager's principle itself is a generalization of Helmholtz's minimal dissipation principle [46]. Applications of Onsager's extremum principle to multiphase fluid problems can be found in [41, 47, 48, 49] among others.

2.2.1 Notations

We first introduce the following notations and assumptions in order to proceed.

- $\rho_0 = \rho_1 = \rho_2$: density of fluids (matched density);
- $\eta = \eta(\phi)$: viscosity of the mixture;
- χ : porosity of the matrix;
- Π : permeability of the matrix;
- $K = \frac{\Pi}{\eta}$: hydraulic conductivity of the fluid in the matrix;
- ϕ_m : order parameter (phase field variable) in matrix;
- \vec{u}_m : Darcy velocity in the matrix;
- p_m : (volume averaged) fluid pressure in the matrix;
- $\frac{1+\phi_m}{2}$: volume fraction of fluid A in the matrix;
- $\frac{1-\phi_m}{2}$: volume fraction of fluid B in the matrix;
- \vec{u}_c : fluid velocity in the conduit or vug;
- p_c : fluid pressure in the conduit or vug;
- $\mathbb{D}(\vec{u}) = \frac{\nabla\vec{u} + \nabla\vec{u}^T}{2}$: rate of strain tensor;
- $\mathbb{T}(\vec{u}, p) = 2\eta\mathbb{D}(\vec{u}) - p\mathbb{I}$: stress tensor;
- ϕ_c : order parameter (phase field variable) in the conduit or vug;
- $\beta(\phi_c) \geq 0$: slip coefficient of fluid along the interface Γ_i ;
- $\frac{1+\phi_c}{2}$: volume fraction of fluid A in the conduit or vug;
- $\frac{1-\phi_c}{2}$: volume fraction of fluid B in the conduit or vug;
- \vec{J}_m : chemical diffusive flux/current in the matrix;
- \vec{J}_c : chemical diffusive flux/current in the conduit/vug;
- ϵ : a small parameter proportional to the interface width in diffuse interface model (assumed to be the same for the matrix and the conduit for simplicity);
- f : Ginzburg-Landau type double-well Helmholtz free energy density, $f(\phi) = \frac{1}{\epsilon}f_0(\phi)$, $f_0(\phi) = \frac{1}{4}(1 - \phi^2)^2$;
- $F_i(\phi_i) = \gamma \int_{\Omega_i} [\epsilon|\nabla\phi_i|^2 + \frac{1}{\epsilon}f_0'(\phi_i)]$: total free energy in each domain ($i = m$ or c);
- γ : positive material parameter;
- $\mu = \gamma(-\epsilon\Delta\phi + f'(\phi))$: chemical potential;

$m(\phi) > 0$: mobility.

The particular choice of total free energy F_i is crucial in the phase field model. The second term in the total free-energy is a double-well Ginzburg-Landau type energy expressing the hydrophobic part of the free-energy. It is this term, together with the small parameter ϵ , that models the essential immiscibility of the two fluids. The first term in the total free energy is a diffusion term that represents the hydrophilic part of the free-energy. This term penalizes sharp transition and helps to create the transition layer depicted in figure 2.

2.2.2 Preliminary consideration in terms of boundary and interfacial conditions

The following boundary and interfacial conditions follow from simple physical consideration:

$\vec{u}_c|_{\Gamma_c} = \vec{0}$: no-slip on Γ_c ;

$\vec{u}_m \cdot \vec{n}|_{\Gamma_m} = 0$: no-penetration on Γ_m ;

$\vec{J}_c \cdot \vec{n}|_{\Gamma_c} = 0$: chemical impermeability at the solid wall Γ_c ;

$\vec{J}_m \cdot \vec{n}|_{\Gamma_m} = 0$: chemical impermeability at the solid surface Γ_m ;

$\vec{J}_c \cdot \vec{n}|_{\Gamma_i} = \vec{J}_m \cdot \vec{n}|_{\Gamma_i}$: continuity of normal chemical flux across the interface.

Conservation of mass for each phase across the interface ($\rho_0 \frac{1+\phi_c}{2} \vec{u}_c \cdot \vec{n} = \rho_0 \frac{1+\phi_m}{2} \frac{\vec{u}_m}{\chi} \cdot \vec{n} \chi$, $\rho_0 \frac{1-\phi_c}{2} \vec{u}_c \cdot \vec{n} = \rho_0 \frac{1-\phi_m}{2} \frac{\vec{u}_m}{\chi} \cdot \vec{n} \chi$, where $\frac{\vec{u}_m}{\chi}$ is the seepage velocity in the matrix.) implies the following interfacial boundary conditions

$$\vec{u}_c \cdot \vec{n} = \vec{u}_m \cdot \vec{n}, \quad \phi_c = \phi_m, \quad \text{on } \Gamma_i.$$

Notice that these two interfacial boundary conditions on Γ_i and the continuity of the normal chemical current are consistent with phase conservation across the interface and the continuity equation for the order parameter

$$\frac{\partial \phi}{\partial t} + \vec{u} \cdot \nabla \phi = -\nabla \cdot \vec{J}.$$

2.2.3 Application of Onsager's extremum principle

In order to apply Onsager's extremum principle, we need to identify the total free energy in the matrix and in the conduit, and the total dissipation

functions for the matrix and the conduit. Here we utilize the free energy instead of the entropy as in Onsager's original setting since conditions of mechanical equilibrium necessarily enter the laws of irreversible processes [41, 44, 50]. Further explanation is provided below.

Recall that we have adopted the following choice of total free energy in each domain [28, 34, 35, 40]. For the conduit,

$$F_c(\phi_c) = \gamma \int_{\Omega_c} [\frac{\epsilon}{2} |\nabla \phi_c|^2 + f(\phi_c)] = \gamma \int_{\Omega_c} [\frac{\epsilon}{2} |\nabla \phi_c|^2 + \frac{1}{4\epsilon} (\phi_c^2 - 1)^2],$$

where γ is a positive material parameter. Similar formula holds for the matrix with the subscript c replaced by m .

Therefore, the variation of the total free energy in the conduit/vug is given by

$$\delta F_c(\phi_c) = \int_{\Omega_c} \mu_c \delta \phi + \gamma \left[\int_{\Gamma_c} \epsilon \frac{\partial \phi_c}{\partial n} \delta \phi + \int_{\Gamma_i} \epsilon \frac{\partial \phi_c}{\partial n} \delta \phi \right],$$

where $\mu_c = \gamma[-\epsilon \Delta \phi_c + f'(\phi_c)]$ is the chemical potential in Ω_c . Minimizing the total free energy in Ω_c yields the equilibrium conditions $\mu_c = \text{constant}$ in Ω_c and $\frac{\partial \phi_c}{\partial n} = 0$ on $\partial \Omega_c$ (ignoring the coupling with the matrix for the moment). This implies that deviations from the equilibrium may be measured by the "force" $\nabla \mu_c$ in the bulk, and $\gamma \epsilon \frac{\partial \phi_c}{\partial n}$ on the boundary. For small perturbations away from the equilibrium, the additional rate of dissipation arises from system responses that are linear in $\nabla \mu_c$ and $\gamma \epsilon \frac{\partial \phi_c}{\partial n}$. Such responses can be described in terms of the diffusive flux (current) \vec{J}_c in Ω_c and the time derivative of the order parameter ϕ_c on the boundary ($\frac{\partial \phi_c}{\partial t}$). The time derivative on the boundary is needed as a rate because the system is not equilibrium on the boundary for the order parameter ϕ_c since $\frac{\partial J_n}{\partial n} \neq 0$ on the boundary in general.

We notice that the rate of the change of the free energy in Ω_c can be written as

$$\begin{aligned} \dot{F}_c &= \int_{\Omega_c} \mu_c \frac{\partial \phi_c}{\partial t} + \gamma \epsilon \left[\int_{\Gamma_c} \frac{\partial \phi_c}{\partial n} \frac{\partial \phi_c}{\partial t} + \int_{\Gamma_i} \frac{\partial \phi_c}{\partial n} \frac{\partial \phi_c}{\partial t} \right] \\ &= \int_{\Omega_c} \mu_c (-\nabla \cdot \vec{J}_c - \vec{u}_c \cdot \nabla \phi_c) + \gamma \epsilon \left[\int_{\Gamma_c} \frac{\partial \phi_c}{\partial n} \frac{\partial \phi_c}{\partial t} + \int_{\Gamma_i} \frac{\partial \phi_c}{\partial n} \frac{\partial \phi_c}{\partial t} \right] \\ &= \int_{\Omega_c} [\nabla \mu_c \cdot \vec{J}_c - \mu_c \vec{u}_c \cdot \nabla \phi_c] + \gamma \epsilon \int_{\Gamma_c} \frac{\partial \phi_c}{\partial n} \frac{\partial \phi_c}{\partial t} + \int_{\Gamma_i} [\gamma \epsilon \frac{\partial \phi_c}{\partial n} \frac{\partial \phi_c}{\partial t} - \mu_c \vec{J}_c \cdot \vec{n}], \end{aligned}$$

where we have utilized the continuity equation for the order parameter ϕ_c , performed one integration by parts, and utilized the boundary conditions on the diffusion (chemical) current (flux). Likewise, the rate of change of the

free energy in Ω_m can be written as $\dot{F}_m = \int_{\Omega_m} [\nabla \mu_m \cdot \vec{J}_m - \mu_m \vec{u}_m \cdot \nabla \phi_m] + \int_{\Gamma_m} \gamma \epsilon \frac{\partial \phi_m}{\partial n} \frac{\partial \phi_m}{\partial t} - \int_{\Gamma_i} [\gamma \epsilon \frac{\partial \phi_m}{\partial n} \frac{\partial \phi_m}{\partial t} - \mu_m \vec{J}_m \cdot \vec{n}]$.

On the other hand, the dissipation function Φ_c for immiscible two phase flows in the conduit/vug can be identified as

$$\Phi_c = \int_{\Omega_c} [\eta \mathbb{D}(\vec{u}_c)|^2 + \frac{|\vec{J}_c|^2}{2m}] + \int_{\Gamma_i} \frac{\beta}{2} |\vec{u}_{c,\tau}|^2,$$

where the first term corresponds to viscous damping, the second term is the dissipation associated with the diffusive current (chemical flux), and the last term is related to dissipation due to slip on the matrix-conduit interface with $\vec{u}_{c,\tau}$ denoting the tangential component of \vec{u}_c on the conduit-matrix interface Γ_i . $\frac{\eta}{\beta}$ can be interpreted as the slip length. Slip along conduit-matrix interface is a well-known phenomenon. See for instance Beavers-Joseph [10]. Here m is a phenomenological parameter and will be identified as the mobility. We have ignored the potential damping due to the time-derivative of the order parameter ϕ_c (a term like $\int_{\partial\Omega_c} \frac{1}{2\Gamma} |\frac{\partial \phi_c}{\partial t}|^2$) since we assume instantaneous relaxation ($\Gamma = \infty$). See discussion below for dynamic boundary conditions.

Likewise, the dissipation function Φ_m for immiscible two-phase flows in the matrix can be identified as

$$\Phi_m = \int_{\Omega_m} [\frac{1}{2K} |\vec{u}_m|^2 + \frac{|\vec{J}_m|^2}{2m}]$$

where the second term is dissipation associated with the diffusive current in the bulk while the first term corresponds to Darcy damping. Here we have assumed the same mobility in the matrix as in the conduit for simplicity. The specific form of the Darcy damping utilized here can be deduced from the volume averaged Navier-Stokes equations in porous media, see for instance Le Bars and Worster [51] (equation 2.13) or Nield and Bejan [52].

Combining everything together, we see that for immiscible two-phase flows Onsager's variational principle may be expressed in terms of the functional

$$\begin{aligned} & \Phi + \dot{F} \\ &= \int_{\Omega_c} [\eta \mathbb{D}(\vec{u}_c)|^2 + \frac{|\vec{J}_c|^2}{2m}] + \int_{\Gamma_i} \frac{\beta}{2} |\vec{u}_{c,\tau}|^2 + \int_{\Omega_m} [\frac{1}{2K} |\vec{u}_m|^2 + \frac{|\vec{J}_m|^2}{2m}] \\ &+ \int_{\Omega_c} [\nabla \mu_c \cdot \vec{J}_c - \mu_c \vec{u}_c \cdot \nabla \phi_c] + \gamma \epsilon \int_{\Gamma_c} \frac{\partial \phi_c}{\partial n} \frac{\partial \phi_c}{\partial t} + \int_{\Omega_m} [\nabla \mu_m \cdot \vec{J}_m - \mu_m \vec{u}_m \cdot \nabla \phi_m] + \int_{\Gamma_m} \gamma \epsilon \frac{\partial \phi_m}{\partial n} \frac{\partial \phi_m}{\partial t} \\ &+ \int_{\Gamma_i} [\gamma \epsilon \frac{\partial \phi_c}{\partial n} \frac{\partial \phi_c}{\partial t} - \mu_c \vec{J}_c \cdot \vec{n} - \gamma \epsilon \frac{\partial \phi_m}{\partial n} \frac{\partial \phi_m}{\partial t} + \mu_m \vec{J}_m \cdot \vec{n}]. \end{aligned}$$

The two-phase immiscible flow model in karst geometry according to Onsager's extremum principle is then derived by minimizing $\Phi + \dot{F}$ with respect to the rates $\{\vec{u} = (\vec{u}_m, \vec{u}_c), \vec{J} = (\vec{J}_m, \vec{J}_c), \frac{\partial \phi}{\partial t}|_{boundary} = (\frac{\partial \phi_m}{\partial t}|_{\Gamma_m, \Gamma_i}, \frac{\partial \phi_c}{\partial t}|_{\Gamma_c, \Gamma_i})\}$. Therefore, we deduce that the two-phase flow model in karstic geometry is the following coupled **Cahn-Hilliard-Stokes-Darcy system** which consists of the *Cahn-Hilliard-Darcy system* [37, 53, 54, 55, 56, 57, 58]

$$\begin{aligned} \frac{\eta}{\mu} \vec{u}_m + \nabla p_m - \mu_m \nabla \phi_m &= 0, \quad \nabla \cdot \vec{u}_m = 0, \quad \text{in } \Omega_m, \\ \frac{\partial \phi_m}{\partial t} + \vec{u}_m \cdot \nabla \phi_m &= \nabla \cdot (m \nabla \mu_m), \quad \mu_m = \gamma[\frac{1}{\epsilon} f'_0(\phi_m) - \epsilon \Delta \phi_m], \quad \text{in } \Omega_m, \\ \frac{\partial \phi_m}{\partial n}|_{\Gamma_m} &= 0, \quad \frac{\partial \mu_m}{\partial n}|_{\Gamma_m} = 0, \quad \vec{u}_m \cdot \vec{n}|_{\Gamma_m} = 0, \end{aligned} \quad (3)$$

in the matrix, coupled with the *Cahn-Hilliard-Stokes system* [34, 35, 36, 59]

$$\begin{aligned} -\nabla \cdot \mathbb{T}(\vec{u}_c, p_c) - \mu_c \nabla \phi_c &= 0, \quad \nabla \cdot \vec{u}_c = 0, \quad \text{in } \Omega_c, \\ \frac{\partial \phi_c}{\partial t} + \vec{u}_c \cdot \nabla \phi_c &= \nabla \cdot (m \nabla \mu_c), \quad \mu_c = \gamma[\frac{1}{\epsilon} f'_0(\phi_c) - \epsilon \Delta \phi_c], \quad \text{in } \Omega_c, \\ \frac{\partial \phi_c}{\partial n}|_{\Gamma_c} &= 0, \quad \frac{\partial \mu_c}{\partial n}|_{\Gamma_c} = 0, \quad \vec{u}_c|_{\Gamma_c} = 0, \end{aligned} \quad (4)$$

in the conduit, through the following interface boundary conditions on Γ_i ,

$$\begin{aligned} \vec{u}_m \cdot \vec{n} &= \vec{u}_c \cdot \vec{n}, \quad \phi_m = \phi_c, \quad \mu_m = \mu_c, \quad \frac{\partial \phi_m}{\partial n} = \frac{\partial \phi_c}{\partial n}, \quad \nabla \mu_m \cdot \vec{n} = \nabla \mu_c \cdot \vec{n}, \\ \vec{n} \cdot \mathbb{T}(\vec{u}_c, p_c) \vec{n} &= -p_m, \quad \vec{\tau} \cdot \mathbb{T}(\vec{u}_c, p_c) \vec{n} = -\beta \vec{\tau} \cdot \vec{u}_c. \end{aligned} \quad (5)$$

Here the pressures p_m and p_c also serve as the Lagrangian multiplier for the incompressibility constraint in the matrix and conduit respectively. The last velocity interface boundary condition is exactly the Beavers-Joseph-Saffman-Jones interface boundary condition [10, 12, 14, 15, 60, 61, 62, 63, 64, 65] with the slip coefficient β equal to the Beavers-Joseph-Saffman-Jones coefficient α_{BJSJ} . The Cahn-Hilliard-Stokes system can be viewed as the low Reynolds number approximation of the better-known Cahn-Hilliard-Navier-Stokes system for two phase flow [28, 35, 34, 36, 40, 66, 67, 68, 69, 70].

The derivation above indicates that the interface boundary conditions (except for the three obtained via conservation of mass consideration) are in fact variational interface boundary conditions. In the one phase case, Onsager's variation principle reduces to Helmholtz's minimal dissipation principle, and these interface boundary conditions reduce to the well-known Beavers-Joseph-Saffman-Jones interface boundary conditions that have been used in groundwater study and blood filtration [11, 13, 14, 15, 19, 62, 64, 65, 71, 72, 73, 74]. The Beavers-Joseph-Saffman-Jones type interface boundary conditions can be also derived via homogenization consideration under appropriate assumptions [75] in the one phase case.

2.2.4 Consistency with thermodynamics

We can now observe the consistency of the current formulation with the laws of thermodynamics as long as we identify entropy and work appropriately following [41]. The laws of thermodynamics [76] dictate $\dot{F} = -T\dot{S} + \dot{W}$ where F is the total free energy, T is the temperature, S the entropy and W the work. Recall that

$$\dot{F} = \dot{F}_c + \dot{F}_m = \int_{\Omega_c} [\nabla\mu_c \cdot \vec{J}_c - \mu_c \vec{u}_c \cdot \nabla\phi_c] + \int_{\Omega_m} [\nabla\mu_m \cdot \vec{J}_m - \mu_m \vec{u}_m \cdot \nabla\phi_m].$$

Since F is the free energy associated with the order parameter ϕ , the entropy part $-T\dot{S}$ should be from the chemical diffusion in the bulk and relaxation on the boundary or interface, and the work rate \dot{W} is due to the work done by the flow to the (diffuse) interface. That is

$$-T\dot{S} = \int_{\Omega_c} \nabla\mu_c \cdot \vec{J}_c + \int_{\Omega_m} \nabla\mu_m \cdot \vec{J}_m, \quad \dot{W} = \int_{\Omega_c} [-\mu_c \nabla\phi_c \cdot \vec{u}_c] + \int_{\Omega_m} [-\mu_m \nabla\phi_m \cdot \vec{u}_m].$$

Therefore, $-\mu\nabla\phi$ is identified as a force which can be interpreted as the "elastic" force (or Korteweg force) exerted by the (diffusive) interface on the flow. This "elastic" force converges to the surface tension at sharp interface limit at least heuristically [28, 36, 37]. The total free energy in each domain also converges to the corresponding interfacial energy for the sharp interface model [77, 78].

2.2.5 Energy law

An immediate consequence of this variational approach is the following **energy law** associated with the Cahn-Hilliard-Stokes-Darcy system with matched density. The equations (3)-(4) under the interface boundary condition (5) satisfy the energy law

$$\begin{aligned} & \frac{d}{dt}(F_m(\phi_m) + F_c(\phi_c)) \\ = & - \int_{\Omega_m} \left[\frac{\eta}{\Pi} |\vec{u}_m|^2 + m |\nabla\mu_m|^2 \right] - \int_{\Omega_c} [2|\sqrt{\eta}\mathbb{D}(\vec{u}_c)|^2 + m |\nabla\mu_c|^2] - \int_{\Gamma_i} |\sqrt{\beta}\vec{u}_{c,\tau}|^2 \end{aligned} \quad (6)$$

We remark that more general systems with dynamic boundary conditions can be derived if we take into consideration within the dissipation function quadratic forms in the rate $\frac{\partial\phi}{\partial t}$. More specifically, we could include the following terms in the total dissipation function Φ : $\int_{\Gamma_c} \frac{1}{2\gamma_c} \left| \frac{\partial\phi_c}{\partial t} \right|^2 +$

$\int_{\Gamma_m} \frac{1}{2\gamma_m} \left| \frac{\partial \phi_m}{\partial t} \right|^2 + \int_{\Gamma_i} \frac{1}{2\gamma_{ic}} \left| \frac{\partial \phi_c}{\partial t} \right|^2 + \int_{\Gamma_i} \frac{1}{2\gamma_{im}} \left| \frac{\partial \phi_m}{\partial t} \right|^2$. We could also include the following surface free energy terms in the total free energy $\int_{\Gamma_c} \left[\frac{\sigma_c}{2} |\nabla_\tau \phi_c|^2 + \gamma_{fsc}(\phi_c) \right] + \int_{\Gamma_m} \left[\frac{\sigma_m}{2} |\nabla_\tau \phi_m|^2 + \gamma_{fsm}(\phi_m) \right] + \int_{\Gamma_i} \left[\frac{\sigma_{ic}}{2} |\nabla_\tau \phi_c|^2 + \gamma_{fsic}(\phi_c) \right] + \int_{\Gamma_i} \left[\frac{\sigma_{im}}{2} |\nabla_\tau \phi_m|^2 + \gamma_{fsim}(\phi_m) \right]$, where ∇_τ represents tangential gradient on the appropriate surface. Such kind of consideration can potentially better represent the interaction of the system with the walls and the interface due to the surface energy terms and surface diffusion terms. This formulation leads to the so-called dynamic boundary condition since the boundary (and interface) conditions will involve time derivative of the order parameter ϕ . See for instance [41, 79, 80, 81]. We focus on the instantaneous relaxation case (formally $\gamma_c = \gamma_m = \gamma_{ic} = \gamma_{im} = \infty$) for simplicity. Domain dependent ϵ, γ, m can be considered as well.

We would like to emphasize that although the Cahn-Hilliard-Darcy (3) and Cahn-Hilliard-Stokes (4) models derived above are not new, the coupling of the two systems with the interface boundary conditions derived from Onsager's variational principle is novel. This new system forms the foundation of our future study of two phase flows in karstic geometry.

Alternative derivations of two phase flows (in conduit) via other variational principles or rational mechanics considerations are also possible [34, 35, 36, 37, 40, 49]. However, we are not aware of any systematic derivation of hydrodynamic model with interface boundary conditions for two-phase flows in karstic geometry. We also remark that the derivation above based on Onsager's extremum principle will not lead to Cahn-Hilliard-Navier-Stokes-Darcy type system directly since Onsager's principle is applicable to system near equilibrium only. On the other hand, most processes in karstic region do evolve near equilibrium and hence the Cahn-Hilliard-Stokes-Darcy model is expected to be applicable most of the time.

2.3 Generalizations of the Cahn-Hilliard-Stokes-Darcy system

The basic Cahn-Hilliard-Stokes-Darcy system that we derived above via Onsager's extremum principle can be generalized to handle situations that requires other physical factors.

The first important generalization is the following **Cahn-Hilliard-Stokes-Darcy-Boussinesq system** that deals with system with mismatched den-

sity under the Boussinesq assumption.

$$\begin{aligned}
& \frac{\eta}{\Pi} \vec{u}_m + \nabla p_m - \mu_m \nabla \phi_m = -\rho(\phi_m) g \vec{k}, \quad \nabla \cdot \vec{u}_m = 0, \quad \text{in } \Omega_m, \\
& \frac{\partial \phi_m}{\partial t} + \vec{u}_m \cdot \nabla \phi_m = \nabla \cdot (m \nabla \mu_m), \quad \mu_m = \gamma \left[\frac{1}{\epsilon} f'_0(\phi_m) - \epsilon \Delta \phi_m \right], \quad \text{in } \Omega_m, \\
& -\nabla \cdot \mathbb{T}(\vec{u}_c, p_c) - \mu_c \nabla \phi_c = -\rho(\phi_c) g \vec{k}, \quad \nabla \cdot \vec{u}_c = 0, \quad \text{in } \Omega_c, \\
& \frac{\partial \phi_c}{\partial t} + \vec{u}_c \cdot \nabla \phi_c = \nabla \cdot (m \nabla \mu_c), \quad \mu_c = \gamma \left[\frac{1}{\epsilon} f'_0(\phi_c) - \epsilon \Delta \phi_c \right], \quad \text{in } \Omega_c
\end{aligned} \tag{7}$$

equipped with the same interface boundary conditions (5) and boundary conditions as for the Cahn-Hilliard-Stokes-Darcy system. Here \vec{k} is the unit vector pointing upward. This model is consistent with the quasi-incompressible models in each subdomain under Boussinesq approximation [36, 37].

This Cahn-Hilliard-Stokes-Darcy-Boussinesq system (7) has the advantage that it can handle fluids with close but different densities (oil and water for instance). It also enjoys the following *energy law* which will be crucial to the analysis, design and implementation of effective numerical schemes.

$$\begin{aligned}
& \frac{d}{dt} (F_m(\phi_m) + F_c(\phi_c)) \\
& = - \int_{\Omega_m} \left[\frac{\eta}{\Pi} |\vec{u}_m|^2 + m |\nabla \mu_m|^2 \right] - \int_{\Omega_c} [2 |\sqrt{\eta} \mathbb{D}(\vec{u}_c)|^2 + m |\nabla \mu_c|^2] - \int_{\Gamma_i} |\sqrt{\beta} \vec{u}_{c,\tau}|^2 \\
& - \int_{\Omega_c} \rho(\phi_c) g \vec{u}_c \cdot \vec{k} - \int_{\Omega_m} \rho(\phi_m) g \vec{u}_m \cdot \vec{k}.
\end{aligned}$$

The second is the following **Cahn-Hilliard-Stokes-Darcy-Boussinesq system with velocity time derivative**:

$$\begin{aligned}
& \frac{\rho_0}{\chi} \frac{\partial \vec{u}_m}{\partial t} + \frac{\eta}{\Pi} \vec{u}_m + \nabla p_m - \mu_m \nabla \phi_m = -\rho(\phi_m) g \vec{k}, \quad \nabla \cdot \vec{u}_m = 0, \quad \text{in } \Omega_m, \\
& \frac{\partial \phi_m}{\partial t} + \vec{u}_m \cdot \nabla \phi_m = \nabla \cdot (m \nabla \mu_m), \quad \mu_m = \gamma \left[\frac{1}{\epsilon} f'_0(\phi_m) - \epsilon \Delta \phi_m \right], \quad \text{in } \Omega_m, \\
& \rho_0 \frac{\partial \vec{u}_c}{\partial t} - \nabla \cdot \mathbb{T}(\vec{u}_c, p_c) - \mu_c \nabla \phi_c = -\rho(\phi_c) g \vec{k}, \quad \nabla \cdot \vec{u}_c = 0, \quad \text{in } \Omega_c, \\
& \frac{\partial \phi_c}{\partial t} + \vec{u}_c \cdot \nabla \phi_c = \nabla \cdot (m \nabla \mu_c), \quad \mu_c = \gamma \left[\frac{1}{\epsilon} f'_0(\phi_c) - \epsilon \Delta \phi_c \right], \quad \text{in } \Omega_c,
\end{aligned} \tag{8}$$

equipped with the same interface boundary conditions (5) and boundary conditions as for the Cahn-Hilliard-Stokes-Darcy system. The inclusion of the time derivative of the velocity heuristically provides better approximation to the physics when the system is not in equilibrium. This Cahn-Hilliard-Stokes-Darcy-Boussinesq system with explicit velocity time derivative also enjoys an *energy law* in the form of

$$\begin{aligned}
& \frac{d}{dt} (F_m(\phi_m) + F_c(\phi_c) + \int_{\Omega_c} \frac{\rho_0}{2} |\vec{u}_c|^2 + \int_{\Omega_m} \frac{\rho_0}{2\chi} |\vec{u}_m|^2) \\
& = - \int_{\Omega_m} \left[\frac{\eta}{\Pi} |\vec{u}_m|^2 + m |\nabla \mu_m|^2 \right] - \int_{\Omega_c} [2 |\sqrt{\eta} \mathbb{D}(\vec{u}_c)|^2 + m |\nabla \mu_c|^2] - \int_{\Gamma_i} |\sqrt{\beta} \vec{u}_{c,\tau}|^2 \\
& - \int_{\Omega_c} \rho(\phi_c) g \vec{u}_c \cdot \vec{k} - \int_{\Omega_m} \rho(\phi_m) g \vec{u}_m \cdot \vec{k}.
\end{aligned}$$

In the case with relatively high velocity in the conduit, one can even use the Cahn-Hilliard-Navier-Stokes system in the conduit and vug [28, 34, 35, 40, 41], and we arrive at the following **Cahn-Hilliard-Navier-Stokes-Darcy system** with Boussinesq approximation:

$$\begin{aligned}
\frac{\rho_0}{\chi} \frac{\partial \vec{u}_m}{\partial t} + \frac{\eta}{\Pi} \vec{u}_m + \nabla p_m - \mu_m \nabla \phi_m &= -\rho(\phi_m) g \vec{k}, \quad \nabla \cdot \vec{u}_m = 0, \quad \text{in } \Omega_m, \\
\frac{\delta \phi_m}{\delta t} + \vec{u}_m \cdot \nabla \phi_m &= \nabla \cdot (m \nabla \mu_m), \quad \mu_m = \gamma \left[\frac{1}{\epsilon} f'_0(\phi_m) - \epsilon \Delta \phi_m \right], \quad \text{in } \Omega_m, \\
\rho_0 \left(\frac{\partial \vec{u}_c}{\partial t} + (\vec{u}_c \cdot \nabla) \vec{u}_c \right) - \nabla \cdot \mathbb{T}(\vec{u}_c, p_c) - \mu_c \nabla \phi_c &= -\rho(\phi_c) g \vec{k}, \quad \nabla \cdot \vec{u}_c = 0, \quad \text{in } \Omega_c, \\
\frac{\delta \phi_c}{\delta t} + \vec{u}_c \cdot \nabla \phi_c &= \nabla \cdot (m \nabla \mu_c), \quad \mu_c = \gamma \left[\frac{1}{\epsilon} f'_0(\phi_c) - \epsilon \Delta \phi_c \right], \quad \text{in } \Omega_c.
\end{aligned} \tag{9}$$

In this case, it may be useful to employ the so-called Lions interface boundary condition [13, 73, 82, 83, 84]

$$\vec{n} \cdot \mathbb{T}(\vec{u}_c, p_c) \vec{n} - \frac{\rho_0}{2} |\vec{u}_c|^2 = -p_m$$

instead of the original balance of normal force

$$\vec{n} \cdot \mathbb{T}(\vec{u}_c, p_c) \vec{n} = -p_m$$

if we are interested in a relatively simple energy law that has the potential to lead to a global in time well-posed problem. Indeed, with this new alternative interface boundary condition, we maintain the same energy law (9) as in the case of Cahn-Hilliard-Stokes-Darcy-Boussinesq model with explicit velocity time derivative. Such a modification of the interface boundary condition is quite natural since all we did is to have the static pressure p_c replaced by the total pressure (static plus dynamic) as suggested by the Bernoulli equation. This quadratic correction term $\frac{\rho_0}{2} |\vec{u}_c|^2$ can be neglected as a higher order effect if the velocity is small (near equilibrium) and we recover the original interface force balance condition.

3 Time Discretization of Cahn-Hilliard-Stokes-Darcy

The purpose of this section is to present two time-discretization of the Cahn-Hilliard-Stokes-Darcy system, one first order and another second order, that preserve the energy law. We also prove that the semi-discrete in time schemes are uniquely solvable. The discrete energy law and unique solvability make

the schemes desirable in terms of numerical simulation and numerical analysis. The main idea behind is the so-called convex splitting [85]. Applications to the Cahn-Hilliard-Darcy, Cahn-Hilliard-Stokes, and models of thin film epitaxial growth can be found at [55, 59, 86] among others.

3.1 Time discretization

For systems like (3)-(5) that contains a small parameter and describes physical phenomena with very large spatial derivative, it is of great importance to derive numerical schemes that are unconditionally stable so that the stiffness can be handled with ease without resolving all the small scales. For system that enjoys variational structure, a key idea in the development of unconditionally stable schemes is convex splitting (see [55, 85, 86, 87] among many others). Indeed, the convex splitting idea has already been applied to the Cahn-Hilliard-Darcy model [55] and Cahn-Hilliard-Stokes model [59] to generate unconditionally stable (with discrete energy law) schemes. Here we combine the ideas and propose the following convex splitting scheme for the coupled Cahn-Hilliard-Stokes-Darcy system (3)-(4) with appropriate interface boundary conditions (5).

More specifically, denoting $k = \Delta t := \frac{T}{N}$ for a large positive integer N , a time discretization of the Cahn-Hilliard-Darcy system (3) is given by

$$\begin{aligned}
& \frac{\eta(\phi_m^n)}{\Pi} \bar{u}_m^{n+1} + \nabla p_m^{n+1} - \mu_m^{n+1} \nabla \phi_m^n = 0, \text{ in } \Omega_m, \\
& \nabla \cdot \bar{u}_m^{n+1} = 0, \text{ in } \Omega_m, \\
& \frac{\phi_m^{n+1} - \phi_m^n}{k} + \bar{u}_m^{n+1} \cdot \nabla \phi_m^n = \nabla \cdot (m(\phi_m^n) \nabla \mu_m^{n+1}), \text{ in } \Omega_m, \\
& \mu_m^{n+1} = \gamma \left[\frac{1}{\epsilon} f'_0(\phi_m^{n+1}, \phi_m^n) - \epsilon \Delta \phi_m^{n+1} \right], \\
& \frac{\partial \phi_m^{n+1}}{\partial n} \Big|_{\Gamma_m} = 0, \\
& \frac{\partial \mu_m^{n+1}}{\partial n} \Big|_{\Gamma_m} = 0, \\
& \bar{u}_m^{n+1} \cdot \bar{n} \Big|_{\Gamma_m} = 0,
\end{aligned} \tag{10}$$

while a time-discretization of the Cahn-Hilliard-Stokes is formulated as

$$\begin{aligned}
& \nabla \cdot \mathbb{T}(\bar{u}_c^{n+1}, p_c^{n+1}) + \mu_c^{n+1} \nabla \phi_c^n = 0, \text{ in } \Omega_c, \\
& \nabla \cdot \bar{u}_c^{n+1} = 0, \text{ in } \Omega_c, \\
& \frac{\phi_c^{n+1} - \phi_c^n}{k} + \bar{u}_c^{n+1} \cdot \nabla \phi_c^n = \nabla \cdot (m(\phi_c^n) \nabla \mu_c^{n+1}), \text{ in } \Omega_c, \\
& \mu_c^{n+1} = \gamma \left[\frac{1}{\epsilon} f'_0(\phi_c^{n+1}, \phi_c^n) - \epsilon \Delta \phi_c^{n+1} \right], \\
& \frac{\partial \phi_c^{n+1}}{\partial n} \Big|_{\Gamma_c} = 0, \\
& \frac{\partial \mu_c^{n+1}}{\partial n} \Big|_{\Gamma_c} = 0, \\
& \bar{u}_c^{n+1} = 0, \text{ on } \Gamma_c.
\end{aligned} \tag{11}$$

On Γ_i ,

$$\begin{aligned}
\bar{u}_m^{n+1} \cdot \bar{n} &= \bar{u}_c^{n+1} \cdot \bar{n}, \\
\phi_m^{n+1} &= \phi_c^{n+1}, \\
\mu_m^{n+1} &= \mu_c^{n+1}, \\
\frac{\partial \phi_c^{n+1}}{\partial n} &= \frac{\partial \phi_m^{n+1}}{\partial n}, \\
\nabla \mu_m^{n+1} \cdot \bar{n} &= \nabla \mu_c^{n+1} \cdot \bar{n}, \\
\bar{n} \cdot \mathbb{T}(\bar{u}_c^{n+1}, p_c^{n+1}) \bar{n} &= -p_m^{n+1}, \\
\bar{\tau} \cdot \mathbb{T}(\bar{u}_c^{n+1}, p_c^{n+1}) \bar{n} &= -\beta \bar{\tau} \cdot \bar{u}_c^{n+1}.
\end{aligned} \tag{12}$$

A convex-splitting of F [55, 59, 85, 87] leads to

$$f_0(\phi^{n+1}, \phi^n) = (\phi^{n+1})^3 - (\phi^n). \tag{13}$$

It can be verified by Taylor's expansion that

$$f_0(\phi^{n+1}) - f_0(\phi^n) \leq f_0'(\phi^{n+1}, \phi^n)(\phi^{n+1} - \phi^n). \tag{14}$$

3.2 Unique solvability and discrete energy law for the first order scheme

3.2.1 Weak formulation

The discretization in time above is given in its strong form. It is convenient to write a weak formulation of (10)-(12), especially when one considers finite element or spectral discretization in space of the scheme.

Assume $\Omega = \Omega_m \cup \Omega_c$ is a bounded connected open set of \mathbb{R}^3 (\mathbb{R}^2 , resp.) with Lipschitz boundary $\partial\Omega$. The L^2 inner product in Ω (Ω_m and Ω_c resp.) is denoted by $(\cdot, \cdot)_\Omega$ ($(\cdot, \cdot)_m$ and $(\cdot, \cdot)_c$ resp.). For a given integer m , $H^m(\Omega)$ denotes the classical Sobolev space. One also recalls

$$\dot{L}^2(\Omega) = \left\{ v \in L^2(\Omega); \int_\Omega v = 0 \right\}.$$

and defines $\dot{H}^1(\Omega) := H^1(\Omega) \cap \dot{L}^2(\Omega)$. Then for our problem with two subdomains, we propose

$$\mathbf{H} := \{ \vec{v} \in \mathbf{L}^2(\Omega); \nabla \cdot \vec{v} = 0; \vec{v} \cdot \bar{n} = 0 \text{ on } \partial\Omega \}, \tag{15}$$

$$\mathbf{H}_{c,div} := \{ \vec{v} \in \mathbf{H}^1(\Omega_c); \nabla \cdot \vec{v} = 0; \vec{v} = 0 \text{ on } \Gamma_c \}, \tag{16}$$

$$\mathbf{X} := \{ \vec{v} \in \mathbf{H}; \vec{v}_c := \vec{v}|_{\Omega_c} \in \mathbf{H}_{c,div} \}. \tag{17}$$

The norm on the exotic space \mathbf{X} is defined as

$$\|\vec{v}\|_{\mathbf{X}} = \|\vec{v}_c\|_{H^1(\Omega_c)} + \|\vec{v}_m\|_{L^2(\Omega_m)}.$$

For functions in $\mathbf{H}_{c,div}$, there holds the Korn's inequality (cf. [88])

$$\|\mathbf{v}\|_{H^1(\Omega_c)} \leq C\|\mathbb{D}(\mathbf{v})\|_{L^2(\Omega_c)}, \forall \vec{v} \in \mathbf{H}_{c,div}, \quad (18)$$

with the constant C depending only on Ω_c , provided that Γ_c has positive measure within $\partial\Omega_c$.

Now we are ready to reformulate our scheme (10)-(12) in the following weak form: For a given $\phi^n \in H^2(\Omega)$, find $\phi^{n+1} \in H^2(\Omega)$, $\mu^{n+1} \in H^1(\Omega)$, $\vec{u}^{n+1} \in \mathbf{X}$ that solve the following nonlinear elliptic system

$$(\phi - \phi^n, v)_{\Omega} = -k \left[(m \nabla \mu, \nabla v)_{\Omega} + (\vec{u} \cdot \nabla \phi^n, v)_{\Omega} \right], \quad \forall v \in H^1(\Omega), \quad (19)$$

$$(\mu, \varphi)_{\Omega} = \gamma \left[\left(\frac{1}{\epsilon} f'_o(\phi, \phi^n), \varphi \right)_{\Omega} + \epsilon (\nabla \phi, \nabla \varphi)_{\Omega} \right], \quad \forall \varphi \in H^1(\Omega), \quad (20)$$

$$(2\eta \mathbb{D}(\vec{u}_c), \mathbb{D}(\vec{v}_c))_c + \left(\frac{\nu}{\Pi} \vec{u}_m, \vec{v}_m \right)_m + (\beta \vec{u}_c \cdot \vec{\tau}, \vec{v}_c \cdot \vec{\tau})_{\Gamma_i} = (\mu \nabla \phi^n, \vec{v})_{\Omega}, \quad \forall \vec{v} \in \mathbf{X}. \quad (21)$$

where we have omitted the dependence of ϕ, μ, \vec{u} on $n+1$ and of the coefficients m, η, ν, β on ϕ^n for notational simplicity. Here $\vec{u}_m := \vec{u}|_{\Omega_m}$, $\vec{u}_c := \vec{u}|_{\Omega_c}$ (similarly for \vec{v}_m, \vec{v}_c).

Notice that the interface boundary conditions

$$\begin{aligned} \vec{u}_m \cdot \vec{n} &= \vec{u}_c \cdot \vec{n}, \\ \phi_m &= \phi_c, \\ \mu_m &= \mu_c, \end{aligned}$$

are enforced strongly by requiring $\vec{u} \in \mathbf{X}$ and $\phi \in H^1(\Omega)$, $\mu \in H^1(\Omega)$, whereas the rest of the interface boundary conditions are satisfied as a result of the weak formulation (19)-(21).

3.2.2 Unique solvability of the first order scheme

Here we show the unique solvability of the weak form of (10)-(12) as formulated in (19)-(21).

Theorem 1. *Suppose that $\phi^n \in H^2(\Omega)$. The numerical scheme (10)-(12) is uniquely solvable in the weak sense of (19)-(21).*

Proof 1. *In order to show that our scheme (19)-(21) is the Euler-Lagrange equation associated with an appropriate strictly convex variational problem, we introduce a bilinear form $a(\mu, \chi)$ on $\dot{H}^1(\Omega)$ as*

$$a(\mu, \chi) = k(m\nabla\mu, \nabla\chi)_\Omega + k(\vec{u}_\mu \cdot \nabla\phi^n, \chi)_\Omega, \quad (22)$$

where \vec{u}_μ is the unique solution of

$$(2\eta\mathbb{D}(\vec{u}_{\mu,c}), \mathbb{D}(\vec{v}_c))_c + \left(\frac{\nu}{\Pi}\vec{u}_{\mu,m}, \vec{v}_m\right)_m + (\beta\vec{u}_{\mu,c} \cdot \vec{\tau}, \vec{v}_c \cdot \vec{\tau})_{\Gamma_i} = (\mu\nabla\phi^n, \vec{v})_\Omega, \quad \forall \vec{v} \in \mathbf{X}. \quad (23)$$

The left-hand side of the above equation defines a continuous bilinear form on \mathbf{X} that is coercive by Korn's inequality (18). Thus for given $\mu \in \dot{H}^1(\Omega)$ and $\phi^n \in H^2(\Omega)$, the existence and uniqueness of the solution \vec{u}_μ follows from the classical Lax-Milgram theorem. Moreover, one has

$$\|\vec{u}_\mu\|_{\mathbf{X}} := \|\vec{u}_{\mu,c}\|_{\mathbf{H}^1} + \|\vec{u}_{\mu,m}\|_{\mathbf{L}^2} \leq C\|\mu\|_{\dot{H}^1}. \quad (24)$$

It follows that $a(\mu, \chi)$ is a continuous bilinear functional on $\dot{H}^1(\Omega)$, which gives rise to a continuous linear operator $\mathcal{L} : \dot{H}^1(\Omega) \rightarrow (\dot{H}^1(\Omega))'$ defined as

$$\langle \mathcal{L}(\mu), \chi \rangle := a(\mu, \chi), \quad \forall \chi \in \dot{H}^1. \quad (25)$$

Now consider equation (23) with source χ and take the test function $\vec{v} = \vec{u}_\mu$. It is then easy to see that $a(\mu, \chi)$ can be formulated as

$$a(\mu, \chi) = k(m\nabla\mu, \nabla\chi)_\Omega + (2\eta\mathbb{D}(\vec{u}_{\mu,c}), \mathbb{D}(\vec{u}_{\chi,c}))_c + \left(\frac{\nu}{\Pi}\vec{u}_{\mu,m}, \vec{u}_{\chi,m}\right)_m + (\beta\vec{u}_{\mu,c} \cdot \vec{\tau}, \vec{u}_{\chi,c} \cdot \vec{\tau})_\Gamma. \quad (26)$$

It follows that $a(\mu, \chi)$ is symmetric and coercive on $\dot{H}^1(\Omega)$, i.e.

$$a(\mu, \chi) = a(\chi, \mu), \quad a(\mu, \mu) \geq C\|\nabla\mu\|_{L^2(\Omega)}^2. \quad (27)$$

Thus the operator \mathcal{L} is invertible. One can then define the inner product in $(\dot{H}^1(\Omega))'$ as: for $f, g \in (\dot{H}^1(\Omega))'$

$$(f, g)_{\mathcal{L}^{-1}} := a(\mathcal{L}^{-1}f, \mathcal{L}^{-1}g). \quad (28)$$

And the associated norm in $(\dot{H}^1(\Omega))'$ is then given as

$$\|f\|_{\mathcal{L}^{-1}} = \sqrt{(f, f)_{\mathcal{L}^{-1}}} = \sqrt{a(\mathcal{L}^{-1}f, \mathcal{L}^{-1}f)}. \quad (29)$$

If further $f, g \in \dot{L}^2(\Omega)$, one has

$$(f, g)_{\mathcal{L}^{-1}} = (f, \mathcal{L}^{-1}g)_{L^2} = (\mathcal{L}^{-1}f, g)_{L^2}. \quad (30)$$

Consider the functional

$$G(\phi) = \frac{1}{2}\|\phi - \phi^n\|_{\mathcal{L}^{-1}}^2 + \int_{\Omega} \left\{ \frac{1}{4\epsilon}\phi^4 + \frac{\epsilon}{2}|\nabla\phi|^2 - \frac{1}{\epsilon}\phi^n\phi \right\} dx \quad (31)$$

It is clear that G is a strictly convex and coercive functional on the admissible set

$$\mathcal{A} := \{\phi \in H^1(\Omega); (\phi - \phi^n, 1)_{L^2} = 0\}. \quad (32)$$

Thus G has a unique minimizer $\phi \in \mathcal{A}$ (cf. [89, 90]), in particular, ϕ is the weak solution of the associated Euler-Lagrange equation

$$\mathcal{L}^{-1}(\phi - \phi^n) = -\mu + C, \quad \text{with } \mu = \frac{1}{\epsilon}(\phi^3 - \phi^n) - \epsilon\Delta\phi, \quad (33)$$

where $C = \bar{\mu} = \frac{1}{|\Omega|} \int_{\Omega} \mu dx$ such that $-\mu + C \in \dot{H}^1(\Omega)$.

The equivalence of (33) and (19)-(21) can be verified if one takes in (33) the test function P_0v for any $v \in H^1(\Omega)$ with P_0 the projection onto $\dot{L}^2(\Omega)$.

Since the left-hand-side of (33) belongs to H^1 , this implies that $\mu \in H^1$, which further implies that $\phi \in H^2$ by elliptic regularity result in convex domain (cf. [91]). This ends the proof of Theorem 1.

The proof presented here follows closely those in [55, 56]. Alternative proof that does not rely on the variational structure, but on the monotonicity is also possible. The alternative approach via Browder-Minty monotone operator approach allows us to treat the case of Cahn-Hilliard-Navier-Stokes-Darcy system. Details will be reported elsewhere.

3.2.3 Discrete energy law for the first order scheme

We are now ready to verify the discrete associated with the semi-discrete in time scheme (19)-(21). More specifically, we have

Theorem 2. *The scheme (19)-(21) enjoys the following discrete energy law*

$$\begin{aligned} F(\phi^{n+1}) - F(\phi^n) &\leq -k \int_{\Omega} m |\nabla \mu^{n+1}|^2 dx - k \int_{\Omega_c} 2\eta |\mathbb{D}(\bar{u}_c^{n+1})|^2 dx - k \int_{\Omega_m} \frac{\nu}{\Pi} |\bar{u}_m^{n+1}|^2 dx \\ &- k \int_{\Gamma_i} \beta |\bar{u}_c^{n+1} \cdot \bar{\tau}|^2 dS - \gamma \frac{\epsilon}{2} \int_{\Omega} |\nabla \phi^{n+1} - \nabla \phi^n|^2 dx. \end{aligned} \quad (34)$$

Proof 2. *Taking the test function $v = \mu^{n+1}$ in (19), one has*

$$(\phi^{n+1} - \phi^n, \mu^{n+1})_{\Omega} = -k \int_{\Omega} m |\nabla \mu^{n+1}|^2 dx - k (\bar{u}^{n+1} \cdot \nabla \phi^n, \mu^{n+1})_{\Omega}. \quad (35)$$

Next, one takes $\varphi = -(\phi^{n+1} - \phi^n)$ in (20) to get

$$-(\mu^{n+1}, \phi^{n+1} - \phi^n)_{\Omega} + \gamma \left[\left(\frac{1}{\epsilon} f'_o(\phi^{n+1}, \phi^n), \phi^{n+1} - \phi^n \right)_{\Omega} + \epsilon (\nabla \phi^{n+1}, \nabla \phi^{n+1} - \nabla \phi^n)_{\Omega} \right] = 0. \quad (36)$$

Recall the inequality (14) and the following identity

$$a(a - b) = \frac{1}{2} [a^2 - b^2 + (a - b)^2].$$

Equation (36) becomes

$$-(\mu^{n+1}, \phi^{n+1} - \phi^n)_{\Omega} + F(\phi^{n+1}) - F(\phi^n) \leq -\gamma \frac{\epsilon}{2} \int_{\Omega} |\nabla \phi^{n+1} - \nabla \phi^n|^2 dx. \quad (37)$$

where one may recall the definition $F(\phi) = F_m(\phi_m) + F_c(\phi_c)$. Last, choosing $\vec{v} = k\vec{u}$ in (21), one obtains

$$k \int_{\Omega_c} 2\eta |\mathbb{D}(\bar{u}_c^{n+1})|^2 dx + k \int_{\Omega_m} \frac{\nu}{\Pi} |\bar{u}_m^{n+1}|^2 dx + k \int_{\Gamma_i} \beta |\bar{u}_c^{n+1} \cdot \bar{\tau}|^2 dS = k (\mu^{n+1} \nabla \phi^n, \bar{u}^{n+1})_{\Omega}. \quad (38)$$

One then adds equations (35)-(38) together and arranges terms appropriately to conclude the proof.

The discrete energy law plays a central role in the proof of the existence of solution to the coupled Cahn-Hilliard-Stokes-Darcy system (3)-(5). Details will be reported elsewhere.

3.3 A second order scheme

A second order scheme that is unconditionally energy stable (with discrete energy law), and uniquely solvable for the Cahn-Hilliard-Stokes-Darcy system can be constructed by combining ideas from previous works, especially those from [59, 55]. More specifically, we propose the following algorithm

$$\begin{aligned} \frac{\phi_c^{k+1} - \phi_c^k}{\delta t} &= \nabla \cdot (m(\tilde{\phi}_c^{k+\frac{1}{2}}) \nabla \mu_c^{k+\frac{1}{2}} - \tilde{\phi}_c^{k+\frac{1}{2}} \vec{u}_c^{k+\frac{1}{2}}), \\ \mu_c^{k+\frac{1}{2}} &= \gamma \left[\frac{1}{2\epsilon} ((\phi_c^{k+1})^2 + (\phi_c^k)^2) \phi_c^{k+\frac{1}{2}} - \frac{1}{\epsilon} \tilde{\phi}_c^{k+\frac{1}{2}} - \epsilon \Delta \phi_c^{k+\frac{1}{2}} \right], \\ -\nabla \cdot (\eta(\tilde{\phi}_c^{k+\frac{1}{2}}) \mathbb{D}(\vec{u}_c^{k+\frac{1}{2}})) &= -\nabla p_c^{k+\frac{1}{2}} + \nabla \tilde{\phi}_c^{k+\frac{1}{2}} \mu_c^{k+\frac{1}{2}}, \quad \nabla \cdot \vec{u}_c^{k+\frac{1}{2}} = 0, \end{aligned} \quad (39)$$

coupled with

$$\begin{aligned} \frac{\phi_m^{k+1} - \phi_m^k}{\delta t} &= \nabla \cdot (m(\tilde{\phi}_m^{k+\frac{1}{2}}) \nabla \mu_m^{k+\frac{1}{2}} - \tilde{\phi}_m^{k+\frac{1}{2}} \vec{u}_m^{k+\frac{1}{2}}), \\ \mu_m^{k+\frac{1}{2}} &= \gamma \left[\frac{1}{2\epsilon} ((\phi_m^{k+1})^2 + (\phi_m^k)^2) \phi_m^{k+\frac{1}{2}} - \frac{1}{\epsilon} \tilde{\phi}_m^{k+\frac{1}{2}} - \epsilon \Delta \phi_m^{k+\frac{1}{2}} \right], \\ \vec{u}_m^{k+\frac{1}{2}} &= -\frac{\Pi}{\eta(\tilde{\phi}_m^{k+\frac{1}{2}})} (\nabla p_m^{k+\frac{1}{2}} - \nabla \tilde{\phi}_m^{k+\frac{1}{2}} \mu_m^{k+\frac{1}{2}}), \quad \nabla \cdot \vec{u}_m^{k+\frac{1}{2}} = 0, \end{aligned} \quad (40)$$

with $\phi^{k+\frac{1}{2}} = \frac{\phi^{k+1} + \phi^k}{2}$, $\tilde{\phi}^{k+\frac{1}{2}} = \frac{3\phi^k - \phi^{k-1}}{2}$, $\mu^{k+\frac{1}{2}} = \frac{\mu^{k+1} + \mu^k}{2}$ and $\vec{u}^{k+\frac{1}{2}} = \frac{\vec{u}^{k+1} + \vec{u}^k}{2}$. The coupled system is also equipped with the following interface boundary condition on Γ_i

$$\begin{aligned} \vec{u}_m^{k+1} \cdot \vec{n} &= \vec{u}_c^{k+1} \cdot \vec{n}, \quad \phi_m^{k+1} = \phi_c^{k+1}, \quad \mu_m^{k+1} = \mu_c^{k+1}, \quad \nabla \phi_c^{k+1} \cdot \vec{n} = \nabla \phi_m^{k+1} \cdot \vec{n}, \quad \nabla \mu_c^{k+1} \cdot \vec{n} = \nabla \mu_m^{k+1} \cdot \vec{n}, \\ \vec{n} \cdot \mathbb{T}(\vec{u}_c^{k+1}, p_c^{k+1}) \vec{n} &= -p_m^{k+1}, \quad \vec{\tau} \cdot \mathbb{T}(\vec{u}_c^{k+1}, p_c^{k+1}) \vec{n} = -\beta(\tilde{\phi}_c^{k+\frac{1}{2}}) \vec{u}_c^{k+1} \cdot \vec{\tau}. \end{aligned} \quad (41)$$

It can be shown that this scheme is **unconditionally stable** in the sense that the following discrete energy law is satisfied for any time-step δt .

$$\begin{aligned} (F_m(\phi_m^{k+1}) + F_c(\phi_c^{k+1})) - (F_m(\phi_m^k) + F_c(\phi_c^k)) &= -\delta t \int_{\Omega_m} [|\sqrt{\frac{\eta(\tilde{\phi}_m^{k+\frac{1}{2}})}{\Pi}} \vec{u}_m^{k+\frac{1}{2}}|^2 + |\sqrt{m(\tilde{\phi}_m^{k+\frac{1}{2}})} \nabla \mu_m^{k+\frac{1}{2}}|^2] \\ -\delta t \int_{\Omega_c} [|\sqrt{\eta(\tilde{\phi}_c^{k+\frac{1}{2}})} \mathbb{D}(\vec{u}_c^{k+\frac{1}{2}})|^2 + |\sqrt{m(\tilde{\phi}_c^{k+\frac{1}{2}})} \nabla \mu_c^{k+\frac{1}{2}}|^2] &- \delta t \int_{\Gamma_i} |\sqrt{\beta(\tilde{\phi}_c^{k+\frac{1}{2}})} \vec{u}_c^{k+\frac{1}{2}}|^2. \end{aligned} \quad (42)$$

This scheme also preserves the total mass in the sense that $\int_{\Omega_c} \phi_c^k + \int_{\Omega_m} \phi_m^k$ is independent of k .

4 Concluding Remarks

We have derived a thermodynamical consistent phase field model, the Cahn-Hilliard-Stokes-Darcy (CHSD) system, for two-phase flow in karstic geometry

utilizing Onsager's extremum principle. The CHSD system enjoys a physically important energy law. Generalizations of this model are also introduced. These generalized models also possess appropriate energy laws.

We have also proposed novel time-discretizations of the CHSD model. It is shown that the numerical schemes are uniquely solvable and inherit the energy law. The existence of discrete energy laws implies the unconditional stability of the schemes which is a highly desirable feature for stiff systems like this.

There are many additional issues to be investigated. The first is the well-posedness of this novel system. Although the well-posedness of both the Cahn-Hilliard-Stokes and the Cahn-Hilliard-Darcy systems are known [28, 40, 57, 58, 92, 93, 94], the well-posedness of the novel coupled systems has not been explored so far. The mathematical study of the coupled systems could be much more difficult than the study of each individual subsystems (fluid-structure interaction for example). Fortunately, the new models enjoy corresponding energy laws which can be exploited and further developed to investigate the mathematical validity of the new systems. These energy laws themselves are not sufficient to guarantee well-posedness due to the strong nonlinearity of the "elastic" force even in the slow flow regime (Stokes-Darcy). For instance the scaling argument presented in [57] indicates the challenge with the three-dimensional Cahn-Hilliard-Darcy model. The second theoretical issue is to identify the corresponding sharp interface model and verify the consistency of the new model with the corresponding sharp interface model by investigating the sharp interface limit. The sharp interface limit problem is a challenge due to the singular nature of the limit and the strong nonlinearity. The rigorous sharp interface limit within the Cahn-Hilliard-Navier-Stokes model has been established recently [93]. The rigorous justification in the case of Cahn-Hilliard-Darcy system is still open although the varifold approach can be adopted here. The third is more efficient numerical schemes. Numerical methods are mandatory for complex models like the ones that we have proposed here in order to make quantitative predictions and to make comparison to lab experiments. The numerical simulation will not be easy since the physical problem involves different physical properties (in matrix and in conduit, fluid A and fluid B), disparate spatial and time scales (slow motion in matrix versus fast motion in conduit, large spatial structure in matrix versus small spatial structure in conduit), disparate viscosities, as well as the stiffness that is associated with the thin diffuse-interface. Moreover, the associated physical processes usually occur on very long time scale.

Therefore, efficient and long-time stable algorithms are highly desirable. The semi-discrete in time scheme that we proposed here is the first step in this direction. Last but not the least, we need to compare our result with experiments to calibrate the parameters and validate the models. This requires expertise outside mathematical sciences.

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