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Numerical modeling of unsaturated flow in porous media using a thermodynamical approach

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Abstract:
The Richards equation has been widely used to describe unsaturated flow in porous media, but its thermodynamical consistency has been scarcely investigated. In this paper, a thermodynamically consistent formulation of Richards equation is established on the basis of the free energy concept and the second law of thermodynamics. The capillary effect is described by an interfacial free energy and its corresponding chemical potential. The formulation takes the water saturation as the primary variable as well as chemical potential gradient as the primary driving force. An appealing feature is that the formulation follows an energy dissipation law, which implies the consistency to the second law of thermodynamics. Furthermore, a linearized and energy stable time discretized method is proposed for the model. Numerical results confirms the thermodynamical consistency of the formulation.

1. Introduction

Modeling of unsaturated flow in porous media has important applications in many fields including groundwater and oil recovery (DiCarlo, 2013; Cai et al., 2021; Vodák et al., 2022). A unsaturated porous medium usually stores multiple fluids in the pores, such as oil, water and gas (air). The interfacial tension between multiphase fluids and small pore scales generally result in capillarity effect, which is a particularly important fluid mechanics of unsaturated flow in porous media. Richards (1931) proposed the so-called Richards equation (RE), which has become a famous and simple mathematical model used to describe the unsaturated flow in porous media. Due to excellent insight into the imbibition processes, RE has been widely acknowledged and enormously applied to describe water flow in soils and oil reservoirs (Zha et al., 2013; Vodák et al., 2022; Stokke et al., 2023). The standard RE consists of a mass balance equation for water and Darcy's law for the water volumetric flux, which can be viewed as a simplification of the conventional model of immiscible and incompressible two-phase flow in porous media (Farthing and Ogden, 2017; Zha et al., 2019).

Despite the relative ease of its conventional derivation, the second law of thermodynamics has been scarcely taken into consideration. As a general and fundamental law obeyed by various physical processes, the second law of thermodynamics has been well recognized as a useful guideline for establishing reliable and complete mathematical models for a wide range of physical problems. In the isothermal context, it implies an energy dissipation law (Kou and Sun, 2018); that is, total free energy could decrease over time. Although this key law is particularly important, it has not received sufficient attention in the field of multiphase flow in porous media in the past. In recent works (Kou et al., 2022, 2023a, 2023b), thermodynamically consistent numerical modeling has been

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successfully established for incompressible, immiscible two-phase flow in porous media through introducing the novel concepts of free energies and chemical potentials to account for the conventional capillary effect. The development of energy stable numerical methods is also essential to various physical processes and has received great attention in many fields including flow in porous media (Qiao and Sun, 2014; Kou et al., 2022, 2023a; Feng et al., 2023). To our best knowledge, thermodynamically consistent RE and energy stable numerical methods have been scarcely explored in the past.

In this paper, a thermodynamically consistent formulation of RE is derived on the basis of free energy concept and the second law of thermodynamics. The new formulation takes the water saturation as the primary variable as well as chemical potential gradients as the primary driving force. An appealing feature of the new formulation is to follow an energy dissipation law, which yields the consistency to the second law of thermodynamics. To resolve the strong nonlinearity of RE in numerical simulation, a linearized and energy stable time discretized method is proposed for the model. Numerical results confirms the thermodynamical consistency of the formulation.

2. Model formulation

For the flow of water in partially saturated porous media, actually there exist two fluid phases, water and gas (air). The water phase is deemed to be active under the effects of capillarity and gravity, whereas the gas phase is passive in instantaneous response to the action of water, thereby approximately being neglected. The porosity and permeability of the porous material are independent of the fluid flow. The water saturation is denoted by s, which is the ratio of the volume occupied by water to the pore volume. Assume that $0 < s < 1$ for the unsaturated flow. The capillarity effect resulting from the interfacial tension between water and gas in the pores plays an important role in the migration of water. The logarithmic interfacial free energy f that characterizes the capillarity effect is expressed as (Kou et al., 2022, 2023a, 2023b):

$$f(s) = \alpha s[\ln(s)-1] + \beta(1-s)[\ln(1-s)-1] + \gamma s(1-s) + \varepsilon s \tag{1}$$

where α, β, γ and ε are the energy parameters. The first two terms result from the ideal contributions and ensure $s \in (0,1)$, while the last two terms account for the water-gas and water-solid interactions. The chemical potential $\mu(s)$ is defined as the variation rate of the free energy f with respect to s, i.e., the derivative of f:

$$\mu(s) = \alpha \ln(s) - \beta \ln(1-s) + \gamma(1-2s) + \varepsilon \tag{2}$$

The traditional capillary pressure, denoted by p_c, can be related to the chemical potential as (Kou et al., 2023b):

$$p_c = -\mu(s) \tag{3}$$

The qualitative and quantitative study in (Kou et al., 2023b) demonstrates that Eq. (3) is in agreement with the capillary pressure experimental data, and consequently, the free energy and its corresponding chemical potential can characterize the capillarity effect.

The mass conservation equation of water is formulated as:

$$\frac{\partial(\phi s)}{\partial t} + \nabla \cdot \boldsymbol{u} = q \tag{4}$$

where ϕ is the porosity, $\boldsymbol{u}$ is the volumetric flux, and q stands for a water mass source (positive) or sink (negative).

Let Ω be a connected and smooth space domain. For the sake of simplicity, a no-flow boundary condition is taken as $\boldsymbol{u} \cdot \boldsymbol{n} = 0$ on the boundary $\partial\Omega$, where $\boldsymbol{n}$ is the normal unit outward vector to $\partial\Omega$. The cases with other boundary conditions can be similarly deduced. Total free energy ($\mathscr{E}$) within the fluid system consists of the interfacial free energy and the gravitational energy:

$$\mathscr{E}(t) = \mathscr{F}(t) + \mathscr{G}(t) \tag{5}$$

$$\mathscr{F}(t) = \int_\Omega \phi f(s) d\boldsymbol{x}, \quad \mathscr{G}(t) = \int_\Omega \phi s \rho g \ell d\boldsymbol{x} \tag{6}$$

where ρ represents the water (constant) density, g is the gravitational acceleration and ℓ is the elevation.

The total free energy generally varies with time. The variation equation of $\mathscr{F}$ with time is deduced using Eq. (4) as:

$$\begin{aligned}
\frac{\partial \mathscr{F}(t)}{\partial t} &= \int_\Omega \phi \frac{\partial f(s)}{\partial t} d\boldsymbol{x} \\
&= \int_\Omega \phi \mu \frac{\partial s}{\partial t} d\boldsymbol{x} \\
&= \int_\Omega \mu \frac{\partial(\phi s)}{\partial t} d\boldsymbol{x} \\
&= \int_\Omega \mu (q - \nabla \cdot \boldsymbol{u}) d\boldsymbol{x} \\
&= \int_\Omega \mu q d\boldsymbol{x} + \int_\Omega \boldsymbol{u} \cdot \nabla \mu d\boldsymbol{x}
\end{aligned}$$

The gravitational energy change with time is deduced as:

$$\begin{aligned}
\frac{\partial \mathscr{G}(t)}{\partial t} &= \int_\Omega \frac{\partial g \ell \phi s \rho}{\partial t} d\boldsymbol{x} \\
&= \int_\Omega \rho g \ell \frac{\partial(\phi s)}{\partial t} d\boldsymbol{x} \\
&= \int_\Omega \rho g \ell (q - \nabla \cdot \boldsymbol{u}) d\boldsymbol{x} \\
&= \int_\Omega \rho g \ell q d\boldsymbol{x} + \int_\Omega \boldsymbol{u} \cdot \rho g \nabla \ell d\boldsymbol{x}
\end{aligned} \tag{7}$$

According to the second law of thermodynamics, total free energy within the isothermal closed system should decrease with time. The closed system implies that $q = 0$ and $\boldsymbol{u} \cdot \boldsymbol{n} = 0$, and in this context, the variation equation of total free energy is obtained using Eqs. (7) and (7):

$$\frac{\partial \mathscr{E}(t)}{\partial t} = \int_\Omega \boldsymbol{u} \cdot (\nabla \mu + \rho g \nabla \ell) d\boldsymbol{x} \tag{8}$$

Darcy's law relates the volumetric flux $\boldsymbol{u}$ to the driving forces linearly. Furthermore, the second law of thermodynamics requires $\partial \mathscr{E}(t)/\partial t \le 0$, and as a result, $\boldsymbol{u}$ should take the form:

$$\boldsymbol{u} = -L(s)(\nabla \mu + \rho g \nabla \ell) \tag{9}$$

where $L(s) \ge 0$. The usual choice in unsaturated flow gives:

$$L(s)=\lambda(s)K \tag{10}$$

where $\lambda(s)$ is the water mobility depending on the water saturation and viscosity and K is the absolute permeability. Based on the above derivations, the chemical potential-based model of unsaturated flow in porous media is derived as:

$$\frac{\partial(\phi s)}{\partial t}+\nabla\cdot\boldsymbol{u}=q \tag{11a}$$

$$\boldsymbol{u}=-\lambda(s)K(\nabla\mu+\rho g\nabla\ell) \tag{11b}$$

Substituting Eq. (11b) into Eq. (8) yields an energy dissipation law:

$$\frac{\partial\mathscr{E}(t)}{\partial t}=-\int_{\Omega}\lambda(s)K|\nabla\mu+\rho g\nabla\ell|^{2}d\boldsymbol{x}\leq 0 \tag{12}$$

which shows that for the closed system, total free energy would decrease over time. Using Eq. (7) and Eq. (7), the general energy dissipation law at the presence of mass transfer between the system and outsides is deduced as:

$$\frac{\partial\mathscr{E}(t)}{\partial t}=\int_{\Omega}q(\mu+\rho g\ell)\,d\boldsymbol{x}-\int_{\Omega}\lambda(s)K|\nabla\mu+\rho g\nabla\ell|^{2}d\boldsymbol{x} \tag{13}$$

The above derivations show that the model Eq. (11) and the associated energy dissipation law actually hold for various feasible free energy functions besides the free energy given in Eq. (1).

3. Numerical method

Due to the nonlinearity of chemical potential and mobility, the model yields a nonlinear equation. Despite a great deal of effort to resolve the strong nonlinearity of RE in numerical simulation, the development of efficient stable numerical methods remains challenging so far (Farthing and Ogden, 2017; Zha et al., 2019; Stokke et al., 2023). The thermodynamical consistency explored herein sheds light on the construction of such methods. In this section, an efficient, linearized, energy stable numerical scheme is proposed for solving the model. Divide the total time interval $(0,T)$ into M time steps as $0=t_0<t_1<\cdots<t_M=T$ and denote the time step size by $\tau_k=t_{k+1}-t_k$. The superscript k is used to denote the approximation of any variable at the time t_k.

Applying approaches proposed by Wang et al. (2020) to treat the free energy yields the following linearized discrete chemical potential:

$$\begin{aligned}\mu^{k+1}=&\left(\frac{\alpha}{s^k}+\frac{\beta}{1-s^k}\right)s^{k+1}-\alpha-\beta\frac{s^k}{1-s^k}\\&+\alpha\ln\left(s^k\right)-\beta\ln\left(1-s^k\right)+\gamma\left(1-2s^k\right)+\varepsilon\end{aligned} \tag{14}$$

which satisfies the following energy inequality:

$$f(s^{k+1})-f(s^k)\leq\mu^{k+1}(s^{k+1}-s^k) \tag{15}$$

A semi-implicit time discretized scheme is proposed as follows:

$$\phi\frac{s^{k+1}-s^k}{\tau_k}+\nabla\cdot\boldsymbol{u}^{k+1}=q^{k+1} \tag{16a}$$

$$\boldsymbol{u}^{k+1}=-\lambda(s^k)K\left(\nabla\mu^{k+1}+\rho g\nabla\ell\right) \tag{16b}$$

where μ^{k+1} is given by Eq. (14). Substituting Eq. (16b) into Eq. (16a) yields a single equation:

$$\phi\frac{s^{k+1}-s^k}{\tau_k}-\nabla\cdot\lambda(s^k)K\left(\nabla\mu^{k+1}+\rho g\nabla\ell\right)=q^{k+1} \tag{17}$$

Since μ^{k+1} given in Eq. (14) is linear with respect to s^{k+1}, Eq. (17) is a linearized equation of s^{k+1} and thus easy to implement in practical simulation. Additionally, the scheme preserves the local mass conservation law.

A pronounced feature of the proposed scheme is to inherit the energy dissipation law at the discrete level. In fact, the discrete total free energy is defined as:

$$\mathscr{E}^k=\mathscr{F}^k+\mathscr{G}^k \tag{18}$$

where:

$$\mathscr{F}^k=\int_{\Omega}\phi f(s^k)d\boldsymbol{x},\quad \mathscr{G}^k=\int_{\Omega}\phi s^k\rho g\ell d\boldsymbol{x} \tag{19}$$

The variations of $\mathscr{F}$ and $\mathscr{G}$ between two time steps are deduced using Eqs. (15) and (16a) as:

$$\begin{aligned}\frac{\mathscr{F}^{k+1}-\mathscr{F}^k}{\tau_k}&=\int_{\Omega}\phi\frac{f(s^{k+1})-f(s^k)}{\tau_k}d\boldsymbol{x}\\&\leq\int_{\Omega}\phi\mu^{k+1}\frac{s^{k+1}-s^k}{\tau_k}d\boldsymbol{x}\\&=\int_{\Omega}\mu^{k+1}(q^{k+1}-\nabla\cdot\boldsymbol{u}^{k+1})d\boldsymbol{x}\\&=\int_{\Omega}\mu^{k+1}q^{k+1}d\boldsymbol{x}+\int_{\Omega}\boldsymbol{u}^{k+1}\cdot\nabla\mu^{k+1}d\boldsymbol{x}\end{aligned} \tag{20}$$

$$\begin{aligned}\frac{\mathscr{G}^{k+1}-\mathscr{G}^k}{\tau_k}&=\int_{\Omega}\rho g\ell\phi\frac{s^{k+1}-s^k}{\tau_k}d\boldsymbol{x}\\&=\int_{\Omega}\rho g\ell(q^{k+1}-\nabla\cdot\boldsymbol{u}^{k+1})d\boldsymbol{x}\\&=\int_{\Omega}\rho g\ell q^{k+1}d\boldsymbol{x}+\int_{\Omega}\boldsymbol{u}^{k+1}\cdot\rho g\nabla\ell d\boldsymbol{x}\end{aligned} \tag{21}$$

The discrete energy dissipation law is obtained from Eqs. (20), (21) and (16b):

$$\begin{aligned}&\frac{\mathscr{E}^{k+1}-\mathscr{E}^k}{\tau_k}\\&\leq\int_{\Omega}(\mu^{k+1}+\rho g\ell)q^{k+1}d\boldsymbol{x}+\int_{\Omega}\boldsymbol{u}^{k+1}\cdot\left(\nabla\mu^{k+1}+\rho g\nabla\ell\right)d\boldsymbol{x}\\&=\int_{\Omega}(\mu^{k+1}+\rho g\ell)q^{k+1}d\boldsymbol{x}-\int_{\Omega}\lambda(s^k)K|\nabla\mu^{k+1}+\rho g\nabla\ell|^{2}d\boldsymbol{x}\end{aligned} \tag{22}$$

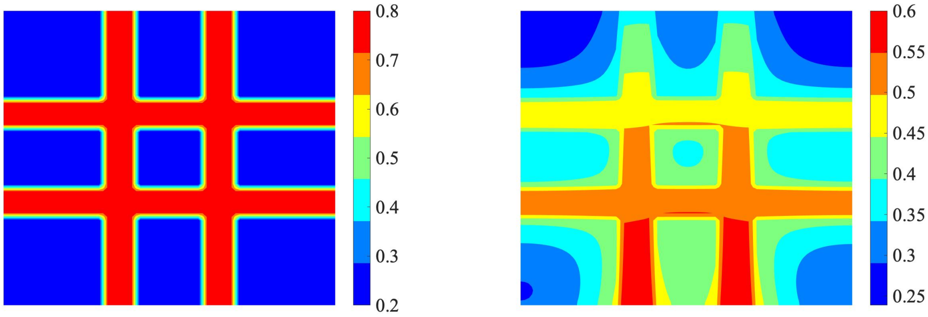
which means that the scheme Eq. (16) is energy stable. As a consequence, this method possesses the merit of using large time steps in the long time simulation.

4. Numerical results

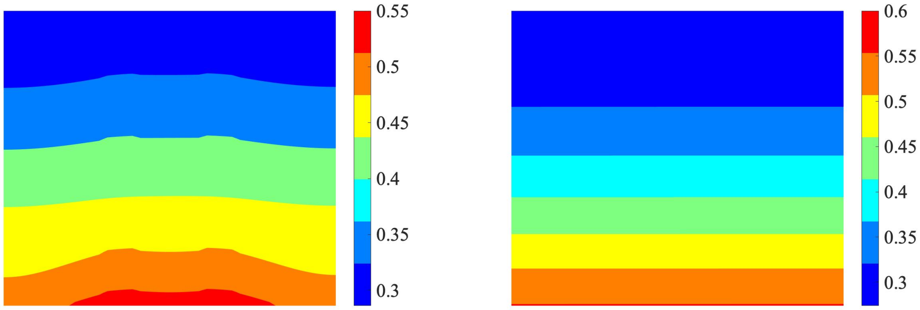
In this section, numerical experiments are conducted to validate the features of the model and numerical scheme. The water relative permeability is expressed as:

$$\lambda(s)=\frac{s^3}{\eta_w} \tag{23}$$

where η_w is the water viscosity. Here, we take $\eta_w=1$ cP.

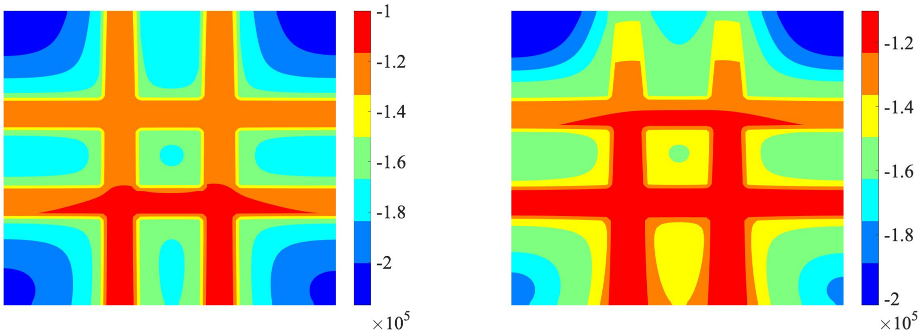


(a) Initial (b) $t = 6$ days

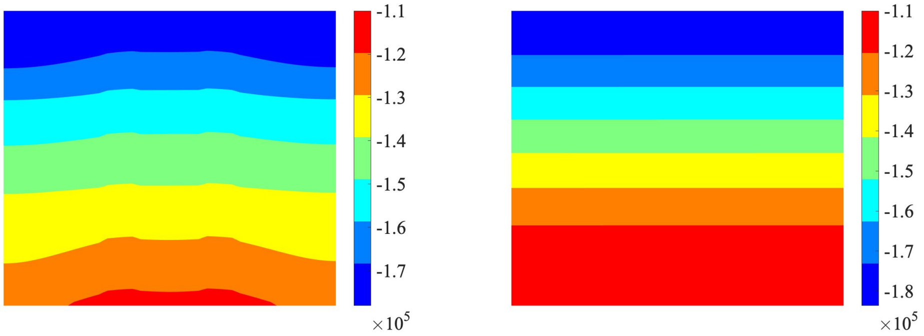


(c) $t = 18$ days (d) $t = 60$ days

Fig. 1. Saturation distributions at different times in Example 1.



(a) $t = 3$ days (b) $t = 6$ days



(c) $t = 18$ days (d) $t = 60$ days

Fig. 2. Chemical potential distributions at different times in Example 1.

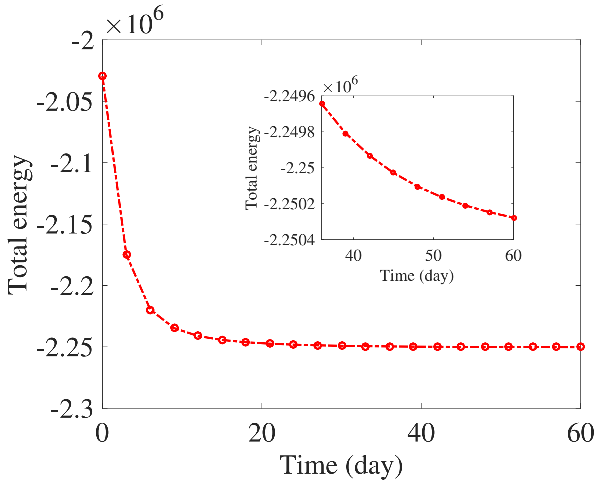


Fig. 3. Energy dissipation profile (the energy unit is Pa) in Example 1.

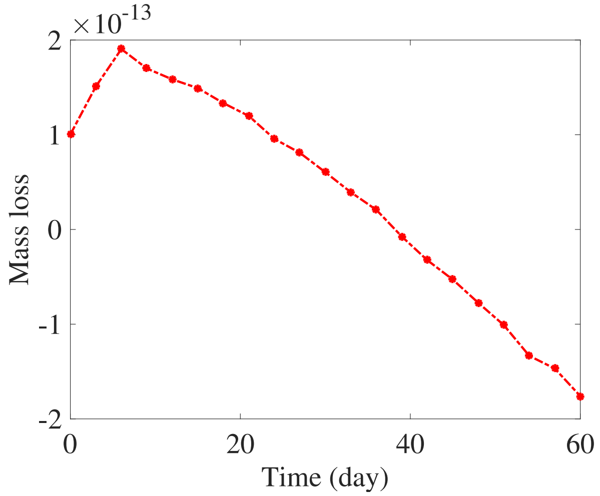


Fig. 4. Total mass conservation in Example 1.

4.1 Example 1

This example showcases a redistribution process taking place in a closed porous medium. The spatial domain is $\Omega = [0,\ 10\ \text{m}]^2$. The porosity and absolute permeability are taken as $\phi = 0.2$ and $K = 100$ md. The energy parameters are taken as $\alpha = 1.86$ bar, $\beta = 0.16$ bar, $\gamma = 1.15$ bar and $\varepsilon = 0$. The medium is homogeneous at the initial time. The initial distribution of the water saturation is illustrated in Fig. 1(a). The water density is $\rho = 1000$ kg/m^3 and the gravitational acceleration is $g = 10$ m/s^2. The elevation is taken as $\ell = 0$ on the bottom boundary. We take $q = 0$ and the boundary conditions $\boldsymbol{u} \cdot \boldsymbol{n} = 0$ on the entire boundary, where $\boldsymbol{n}$ is the normal unit outward vector to the boundary. The total time length is 60 hours and a large time step size is taken as $\tau_k = 3$ hours.

Fig. 1 illustrates the changes of the water saturation with time. Fig. 2 shows the variation of the chemical potential (representing the capillarity effect) with time. Due to the actions of capillarity and gravity, the water saturation varies from the initial heterogeneous state to an equilibrium state. At the equilibrium state, the balance between capillarity and gravity would be achieved. As a result, a grading distribution of water appears at the finial time.

Fig. 3 depicts the energy dissipation profile, which clearly shows that the total free energy is rapidly diminishing at the very early stage of the dynamical process, but after which it is still dissipated with time even at the later time. Therefore, the energy dissipation law is validated.

To examine the accuracy as well as verify the mass conservation of the scheme, it is necessary to define the relative error of total water content as:

$$\Delta s^k = \frac{\int_\Omega \phi s^k dx - \int_\Omega \phi s^0 dx}{\int_\Omega \phi s^0 dx} \tag{24}$$

Fig. 4 depicts the values of Δs^k with time, which demonstrates that the discrete errors are very small and vary tinily with time. Consequently, the scheme can not only conserve total mass but also perform well in the simulation of long-term dynamics.

4.2 Example 2

An imbibition process in a random porous medium is simulated in this example. The spatial domain is $\Omega = [0,\ 10]^2$ with the length unit meter. The porosity and absolute permeability are shown in Fig. 5. The energy parameters are taken as $\alpha = 1.86/\sqrt{K}$ bar, $\beta = 0.16/\sqrt{K}$ bar, $\gamma = 1.15/\sqrt{K}$ bar and $\varepsilon = 0$, where the unit of K is md. The boundary conditions are imposed as:

$$s(0,y,t) = 0.99, \quad 0 \le y \le 10, \quad t > 0 \tag{25}$$

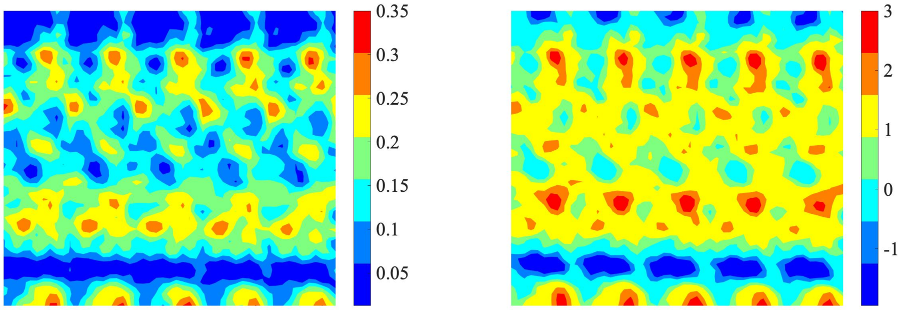
$$s(10,y,t) = 0.01, \quad 0 \le y \le 10, \quad t > 0 \tag{26}$$

There are no additional sources of water, i.e., $q = 0$. The gravity is ignored in this example. The time length is 1 year and the time step size is taken as $\tau_k = 3.65$ days.

During the imbibition process, water continuously migrates from the left boundary to the medium driven by the capillary force. Fig. 6 showcases this process through plotting the contours of the water saturation at different times. The water flow exhibits substantial randomness due to the random heterogeneity of the medium and the resulting differences of capillary forces in different regions.

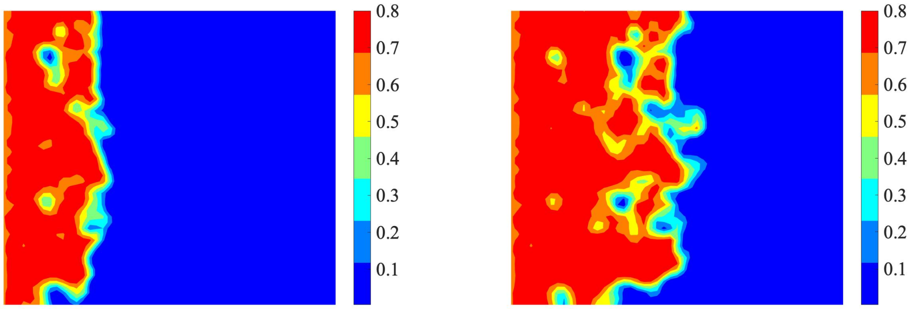
5. Conclusions

A thermodynamically consistent formulation of the Richards equation that describes unsaturated flow in porous media has been established through introducing the free energy concept. The capillarity resulting from the interfacial tension at the pore scales and significantly affecting unsaturated flow is characterized by an interfacial free energy and its corresponding chemical potential. The formulation is proved to follow an energy dissipation law, which implies the consistency to the second law of thermodynamics. Incorporating the free energy concept and the second law of thermodynamics into the modeling framework of unsaturated flow in porous media can not only establish a theoretical foundation for the

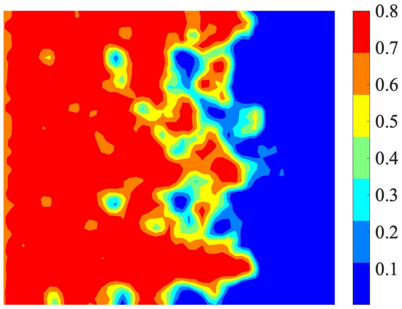


(a) Porosity (b) Permeability ($\log_{10}(K)$)

Fig. 5. Porosity and permeability ($\log_{10}(K)$, the md of K is md) in Example 2.



(a) $t = 0.3$ year (b) $t = 0.6$ year



(c) $t = 1$ year

Fig. 6. Saturation distributions at different times in Example 2.

mathematical modeling but also provide an essential criterion for the development of effective numerical methods; that is, the energy dissipation law (standing for the second law of thermodynamics in the isothermal context) should be preserved at the discrete level so as to guarantee the long-time stability and accuracy in numerical simulation.

To overcome the strong nonlinearity of the model, a linearized and energy stable time discretized method is proposed based on the semi-implicit discrete chemical potential. Numerical examples are conducted to validate the thermodynamical consistency of the model and numerical scheme. Compared to the existing numerical methods, the proposed numerical scheme inherits energy stability by a linearized way and therefore does not require any nonlinear iterative solvers and computational cost. Certainly, it has the first-order time approximate accuracy only, so it could be interesting future work to design energy stable high-order time discretized schemes.

Conflict of interest

The authors declare no competing interest.

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