Lattice Boltzmann Simulations for Micro-Macro Interactions during Isothermal drying of capillary porous media

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Abstract
Drying of capillary porous media involves coupled heat and mass transfer in complex void space geometry which makes it difficult to model and estimate drying rates accurately. The intricate dynamics of invasion patterns lead to phenomena like Haines jumps and capillary pumping resulting existence of drying front for a longer period. Hence, it plays a vital role in alteration of drying rates. So far, modeling of drying was done using continuum models or more popularly, Pore Network Models (PNM). However, reconstructed geometry in PNM lack in representing actual void space which plays a role in invasion patterns in drying phenomena. Alternatively, Lattice Boltzmann method (LBM) can be used which automatically track the interface and simulate multiphase model with such an irregularity in geometry. In this work, Lattice Boltzmann method has been used to simulate invasion patterns of a monodispersed capillary porous media and the corresponding drying rates were estimated.

Keywords: Lattice Boltzmann Method, Drying Kinetics, Haines jumps, Micro-Macro Interactions

Nomenclature
Abbreviations
LBM: Lattice Boltzmann Method
PNM: Pore Network Model
PDF: Particle Distribution Function
BGK: Bhatnagar-Gross-Krook

Alphabets
c: Discrete speed
f: Particle distribution Function variable
u: Macroscopic velocity
w: Lattice Weights
F: Force
G: Inter-particle forcing parameter

Greek Symbols
ρ: Macroscopic Density
τ: Relaxation Time
ψ: Effective Mass

Subscripts/Superscripts
eq: Equilibrium
i: Discrete Particle Moments
int: Inter-particle

1. Introduction
One of the recurrent phenomena occur in our daily life is drying and yet one of the most challenging problem to many environmental and engineering applications ranging from weathering of monuments and building and soil evaporation, to serve as a common unit operation in food processing, wood, and pharmaceutical industries. Drying rates of porous media exhibit intricate dynamics due to its complex geometry causing consequential transmutations in internal transport mechanisms i.e. capillary pumping and sudden jumps in fluid-fluid interface i.e. Haines jumps [1]. This is the main reason of the subsistence of percolating drying front at microscale in a capillary porous media which directly affects the macroscale drying rate.

Thus far, modeling of drying was done using either continuum models or Pore network models (PNM) [2]–[4] both of which have some limitations on representing the void space and underlying intricate transport mechanisms. To be precise, the reconstructed void spaces lack in representing cluster formations and dynamic invasion patterns which play an important role in the determination of drying kinetics of the porous media. Alternatively, meso-simulation such as the Lattice Boltzmann Method (LBM) [5]–[8] can be used to execute drying phenomena as it can easily track the invasion patterns in any intricate geometry presented. Moreover, intermolecular forces which play an important role in drying phenomena are also incorporated in the model.

Very few researchers have reported simulations in drying of capillary porous media using the Lattice Boltzmann method (LBM)[5],[6]. Recently, Zachariah et. al. [11] presented invasion patterns in different geometries of capillary porous media and discussed the prevailing cluster formations leading to drying front using Shan Chen Lattice Boltzmann method. The present work explains how the Lattice Boltzmann method can be used to simulate micro-macro interactions in capillary porous media, i.e. Invasion patterns corresponding drying kinetics for the monodispersed void space.

2. Lattice Boltzmann Methods
2.1. General Lattice Boltzmann Methods
In general, LBM is a meso-simulation strategy where the motion of fluid is described by particle distribution function (PDF) which quantifies number of particles spatially as well as momentarily. The evolution of PDF with time is described by Boltzmann Equation given by:

$$\frac{\partial f_i}{\partial t} + c_i \frac{\partial f_i}{\partial x} = \Omega_i(\mathbf{f}) + F_i$$  \hspace{1cm} (1)

Where, $f_i$ is the particle distribution function in the $i^{th}$ direction, $c_i$ is the velocity in the $i^{th}$ direction, $F_i$ is the forcing term and $\Omega_i$ is the collision operator (BGK collision operator) given by

$$\Omega_i(\mathbf{f}) = -\frac{1}{\tau}(f_i - f_i^{\text{eq}})$$  \hspace{1cm} (2)
Where, $\tau$ is the relaxation time and $f_i^{eq}$ is the equilibrium distribution function given by the Maxwell Boltzmann Distribution, which can be approximated into the following simple form:

$$f_i^{eq}(x,t) = p\omega_i(1 + 3c_iu + \frac{9}{2}(c_iu)^2 - \frac{3}{2}u^2)$$  \hspace{1cm} (3)

Discretizing explicitly Eq. (1) with respect to space, time and velocity will obtain Lattice Boltzmann Equation given by:

$$f_i(x + c_i\Delta t, t + \Delta t) = f_i(x, t) + \Omega_i(x, t)$$ \hspace{1cm} (4)

The LBE can be decomposed into two steps i.e. collision and streaming steps given by:

1. Collision:

$$f_i^*(x, t) = f_i(x, t) - \frac{\Delta t}{\tau}(f_i(x, t) - f_i^{eq}(x, t))$$ \hspace{1cm} (5)

2. Streaming:

$$f_i(x + c_i\Delta t, t + \Delta t) = f_i^*(x, t)$$ \hspace{1cm} (6)

Where $f_i^*(x, t)$ are PDF of just collided particles.

2.2. Shan Chen Lattice Boltzmann Methods

To incorporate multiphase model, Shan Chen LBM was incorporated by altering the forcing term in Eq. (1) given by:

$$F_{int}(x) = -G\psi(x)\sum_{i=1}^{9} w_i\psi_i(x + c_i)\xi_i$$ \hspace{1cm} (7)

Where $G$ is the interparticle force parameter and $\psi$ is the effective mass. This is responsible for innate characteristic of LB model to incorporate intermolecular forces at ease as the effective mass depends on local spaces. Similar approach is established for adhesive forces with the solid which inherently takes all fluid-solid interactions into considerations.

### 2.3. Quantification of Macroscopic Properties

The macroscopic density and velocity at each lattice cell are given by:

$$\rho = \sum_{i=1}^{9} f_i$$ \hspace{1cm} (8)

$$\rho u = \sum_{i=1}^{9} c_i f_i$$ \hspace{1cm} (9)

The lattice quantities are converted to real quantities using reduced properties of gases. The drying rate is given by:

$$M_v = -\frac{A\delta}{L} \frac{\mu R}{\beta RT} \ln\frac{P_g - P_{v_1}}{P_g - P_{v_2}}$$ \hspace{1cm} (10)

**Fig. 1.** (A) Drying rate curve for monomodal capillary porous media (B-I) Timeline of invasion patterns in the drying simulation
3. Results and Discussions

In this study, we simulated the drying of capillary porous media with monodispersed void space consists of throat radius ranging from 28 \( \mu m \) to 52 \( \mu m \) (normally distributed with mean radius 40 \( \mu m \)). The throats are equally spaced of 100 \( \mu m \) intersecting to form irregular pores. Figure 1 represents the simulated micro-macro interactions of the monodispersed capillary porous media using Lattice Boltzmann method. Fig 1A represents macroscale drying kinetics. The absence of macro throats in monodispersed porous media, the first drying period is very small. However, sooner, the gradual emptying of surface throats leads to drastic fall of drying rates. The prolonged constant drying period with gradual fall at the end is largely dependent upon the micro-intricate dynamics of invasion transport in the pores and throats. Two prominent phenomena that are usually observed which plays an important role in the drying of monodispersed capillary porous media are: (i) fast invasion causing Haines jumps in adjacent throats (ii) surface tension which prevents the invasion of pore even when the adjoining pores are invaded. Haines jumps occur when the interface experiences an instability in contact angle which intrigues the interface to move, in order to attain stability. Such a fast invasion causes pumping of surrounding liquid which fills the adjoining narrow throats. Such effect is shown in Fig 1C and D where the fast invasion of pores (blue square) lead to filling of the narrower throat (red square).

Apart from geometry point of view, the surface tension is also responsible for the constant rate period attainment as shown in Fig 1F. The throat does not invade for a considerable amount of time even when its neighboring throats are invading. As discussed earlier, the invasion of pores causes instability in the interface. The unstable intermediate interfaces are due to the high surface energy contained at the interface. Hence, to invade, the surface energy must be greater than or equal to the intermediate interface energy. This is usually attained by reduction of pressure above the interface resulting in an increase in surface tension and energy. Hence, the throats are not invaded until it reaches a threshold value.

4. Conclusion

Drying simulation was achieved successfully using Pore Network model in the past. The exclusion of intricate dynamics of capillary porous media made PNM to fail in achieving the accurate drying kinetics. Hence, we used a meso-simulation approach i.e. Lattice Boltzmann Method with certain modification in the attraction parameters to make it stable at high density ratios and minimization of spurious currents. Moreover, the drying rate for the monodispersed porous media has been estimated. The following key observations are drawn from our simulations:

(i) The absence of macro-throats in monodispersed porous media causes the first drying period to be very small. Moreover, emptying of surface throats lead to drastic fall in the drying rate.

(ii) Later, the prolonged uniform drying rate is due to micro-complex transmutation dynamics of the capillary porous media, namely, Haines jumps and surface energy.

(iii) Haines jumps lead to sudden jumps in intermediate throats leading to longer period of invasion of the throat.

(iv) Surface energy of the interface plays an important role in the decision making of which pore to invade early.

The prospects of the venture are to develop bigger networks of bi-dispersed and monodispersed porous media and predict the drying kinetics with respect to micro-intricate transmutation dynamics, that are usually observed in capillary porous media. It can be concluded that the Lattice Boltzmann method is the best alternative to continuum and Pore Network model in executing drying simulation in porous media.

5. References


