A2: The optimal drying of porous materials

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Abstract

This study models convective drying at the pore scale using a two-component two-phase pseudopotential lattice Boltzmann model (LBM). Layered porous media with varying pore sizes and contact angles are designed based on the capillary pumping principle, ensuring effective capillary transport to the surface even at low saturation levels. This promotes high drying rates and shortens the drying period. In the optimal scenario, a narrow drying front quickly penetrates toward the bottom of the porous medium and then expands horizontally, followed by layer-by-layer drying from the bottom up to the surface. These findings offer valuable insights into the rational design of innovative porous materials with controlled drying behavior, paving the way for enhanced drying processes in various applications.

Keywords: Drying, Porous Media, Pore scale, Lattice Boltzmann Modelling

1. Drying of porous media at the pore scale influenced by capillary pumping

The main goal of this study is to design new porous materials optimizing their drying behavior. The key idea is the exploitation of capillary pumping to allow water to be transported to the surface of the material where it evaporates, referred to as self-pumping. Laplace's law shows that capillary transport occurs from large to small pores, and from surfaces with high to low contact angle. Figure 1a shows, as an example, the schematic of a dual-porosity porous medium used in Lattice Boltzmann model (LBM) simulations of convective drying. The domain, with a uniform contact angle, features large pores in the middle and small pores along the sides [1]. During convective drying, the gas phase penetrates first into the large pores in the middle region. The fine pores at the

side regions remain saturated due to capillary pumping of water from the central large-pore region (Fig. 1b). The evaporation from the water-filled pores at the surface generates a high drying rate (Fig 1c).

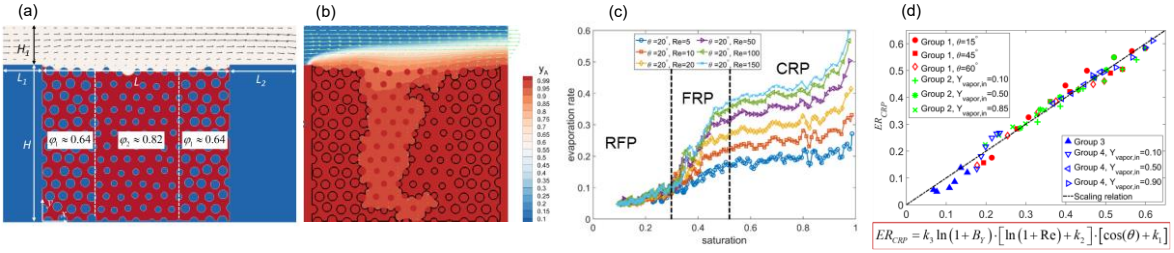
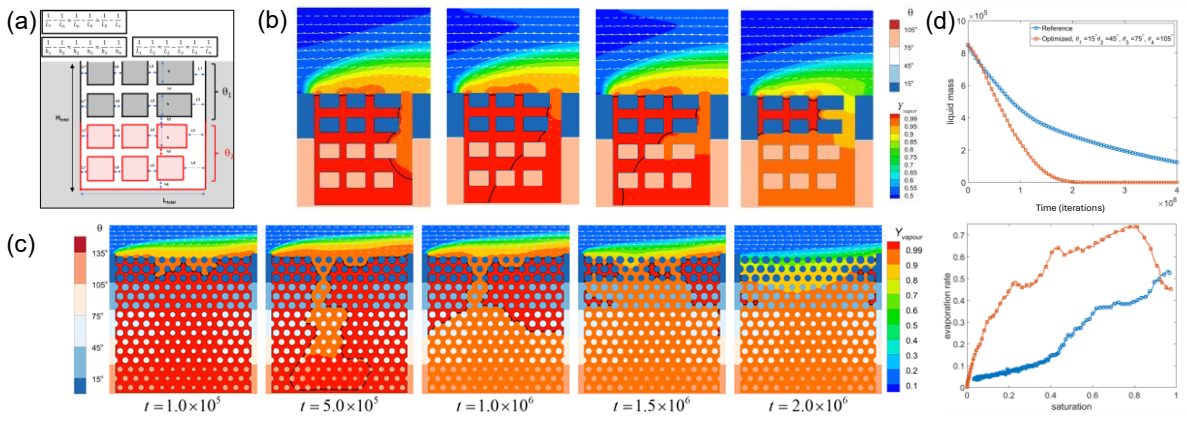


Figure 1. (a) Dual-porosity porous medium for LBM simulations of convective drying. (b) Snapshot of vapor concentration field, liquid configuration and velocity vectors at a selected time step. (c) Evaporation rate versus saturation degree for different Re numbers. (d) Universal scaling of evaporation rate in the first drying period.

LBM is an attractive simulation approach allowing automatic tracking of the interface between liquid water and water vapor, called meniscus, at the pore scale during the drying process. The authors developed an in-house isothermal two-component two-phase pseudopotential LBM code for simulation of the convective drying process at the pore scale. Two lattice Boltzmann equations are solved, one for water including phase transition from liquid to vapor and one for dry air. Water vapor is assumed to be well-mixed with dry air forming wet air. The cascaded collision operator is used to simulate the gas mixture of dry air and water vapor within a wide range of dry air/vapor mixture ratios. Using Chapman-Enskog multi-scale analysis, the model correctly recovers the macroscopic governing equations of convection-diffusion, where the binary diffusion of vapor and air in the gas phase follows Fick's law [1]. The model is verified by comparing with a two-component Stefan problem where the obtained binary diffusivity is consistent with theoretical analysis [1]. It is validated against a microfluid drying experiment, showing good agreement with observed drying dynamics [2]. Notably, the model successfully captures the development of the vapor boundary layer above the porous material (Fig. 1b). Simulation results reproduce the typical transition from the first drying period with almost constant high evaporation rate (referred to as the constant rate period CRP) at large liquid saturation to the second drying period, consisting of a falling rate period (FRP) at intermediate saturation and a receding front period (RFP) at small saturation (Fig. 1c). The transition from the first to the second drying period is observed when capillary pumping from large pores to fine pores diminishes, reducing water availability at the surface and thus lowering the evaporation rate. A parametric study is conducted to investigate the effect of environmental conditions, like inflow air speed (Reynolds number Re) and inflow vapor concentration (relative humidity RH), on the drying rate during the CRP. The results showed a universal scaling law that allows to predict the drying rate during CRP for varying environmental conditions (Fig. 1d) [2]. We showed in this study that the drying rate during CRP also depends on the contact angle, with lower contact angles resulting in higher drying rates due to enhanced capillary pumping.

2. Optimal drying of a porous material at the pore scale

Using LBM simulations at the pore scale, we developed a methodology for designing porous materials with controlled drying pattern and rate. In the first step, we design a two-dimensional network of channels based on the capillary pumping principle following Laplace's law. As illustrated in Fig. 2a, the channel width decreases from right to left side allowing capillary pumping from right to left during drying. Additionally, the channel width on the right-side increases from top to bottom to allow a fast penetration of the drying front to the bottom at the onset



of the drying process. The channels in the bottom half show a higher contact angle than those in the top half, generating capillary pumping from bottom to top. In the second step, we simulate the drying process by LBM and optimize the network geometry, the number of channel layers and the contact angle of the different layers (Fig. 2b). In the third step, the optimal channel network is transformed into a 2D porous medium, with both pore size and contact angle increasing from top to bottom. Moreover, the pores in the middle region are larger than those at the sides. In the fourth step, we extend the design to a 3D porous medium and simulate the drying process by LBM (Fig. 2c) [3]. The drying rate of the porous medium is optimized with respect to pore size, contact angle and number of layers. Fig. 2d top compares the drying rate versus saturation degree of the reference and optimized porous material with 4 layers and contact angles ranging from 15° to 105° downwards [3]. The results show that, in the optimized case, the porous medium dries five times faster than the reference sample to reach a saturation of S=0.05 (Fig. 2d bottom). This example shows the potential of the proposed methodology for designing porous materials with targeted drying behavior. In future, we will design new porous materials with optimal drying behavior, test them using microfluid experiments, extend to 3D structures, and evaluate their evaporative cooling potential for urban heat mitigation.

Figure 2. Design methodology. (a) Design of a 2D channel network. (b) Snapshots of the drying process simulated by LBM. (c) Simulation of the drying process simulated by LBM. (d) Curves of liquid mass versus time and evaporation rate versus degree of saturation for reference and optimized porous media [3].

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