Drying of porous materials at pore scale using lattice Boltzmann and pore network models

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Abstract. Drying at macroscale shows a first drying period with constant drying rate followed by second drying period showing a receding moisture front, phenomena that can be tailored upon need. In order to study the drying of materials, we present a new hybrid computational method, where the dynamics of the liquid-vapor interfaces is modelled by lattice Boltzmann modelling (LBM) in the two-phase pores, while the single-phase flow in the pores filled solely by vapor or liquid is solved by pore network model (PNM). This hybrid method is validated by comparison with reference full LBM simulations. The hybrid method combines the advantages of both methods, i.e., accuracy and computational efficiency. LBM and the hybrid LBM-PNM method are used to study the drying of porous media at pore scale. We analyse two different pore structures and consider how capillary pumping effect can maximize the drying rate. Finally, we indicate how optimized drying rates are relevant when designing facade or pavement solutions that can mitigate higher surface temperatures in urban environments by evaporative cooling.

1. Introduction
Drying at macroscale shows a first drying period with constant drying rate followed by second drying period showing a receding moisture front. In order to improve the drying of materials, it is favorable to maintain the first drying period as long as possible. Large pores are known to be invaded first by the non-wetting fluid, namely air. When neighboring smaller pores remain filled by capillary pumping from larger pores, the liquid phase can remain connected to the surface maintaining high drying rates for longer periods. The mechanisms acting during drying can be optimized by varying the pore structures and pore size distribution of materials. Computational means can support such optimization.

Studying explicitly the configuration of the liquid-vapor interface, vapor and liquid movements at pore scale can yield insights not achievable with continuum methods. Thus different computational modeling approaches have been used to document the configuration of the liquid-air interface within the porous medium. For one, drying of porous materials has been studied by pore network models (PNM) using invasion percolation algorithms. However, it is known that the dynamics of the receding menisci in the pore structure can be better modelled by direct numerical methods at pore scale, such as lattice Boltzmann modelling (LBM). However, LBM still suffers from high computational costs.
We present a new hybrid method, where the dynamics of the liquid-vapor interfaces is modelled by lattice Boltzmann modelling (LBM) in the two-phase pores, while the single-phase flow in the pores filled solely by vapor or liquid is solved by pore network model (PNM). This hybrid method is validated by comparison with reference full LBM simulations. The hybrid method combines the advantages of both methods, i.e. accuracy and computational efficiency.

To demonstrate the capacities of LBM, we analyze the influence of different pore structures on the capillary pumping effect in order to maximize the drying rate. The hybrid LBM-PNM method is used to study the drying of porous media at pore scale. Finally, we indicate how optimized drying rates are relevant when designing facade or pavement solutions that can mitigate higher surface temperatures in urban environments by evaporative cooling.

2. Hybrid method coupling lattice Boltzmann method and pore network model

2.1. Lattice Boltzmann modelling

The lattice Boltzmann model has been widely utilized to study drying of liquid and colloidal suspension in different porous materials [1–8]. In this paper, we apply the entropic multiple-relaxation-time multi-range pseudo-potential LBM [9] to model isothermal liquid drying.

In a nutshell, LBM is a meso-scale model that uses density distribution, referred as $f$ here, in different fixed directions to represent the flow. It consists of two parts, where the collision part models the redistribution of $f$ at the current lattice, while streaming means the exchange of $f$ with neighboring lattices. The fluid-fluid and fluid-solid interactions in two-phase flows are modeled by adding additional force terms in the LB equation [10]. The macroscopic variables like density and momentum are obtained by weighted summation of $f$. Due to its kinematic nature, LBM can capture the liquid-vapor interface automatically without any interface tracking techniques, a major plus on many other computational approaches. Noteworthy, since a uniform Cartesian mesh is used, LBM can deal with arbitrary geometry accurately without simplification and is very efficient in parallel computation. To induce isothermal diffusive drying in our simulations, a smaller gas pressure is applied at the open boundary of the computational domain [11].

2.2. Pore network model

Pore network models simulate fluid flow in simplified pore networks, which characteristics are extracted from porous media. As example, a two-dimensional (2D) porous medium is translated into a pore network in Figure 1 (a)-(c). Figure 1 (a) shows a 2D porous medium consisting of circular solid particles. Using the watershed method, the pore space is decomposed into pore regions, shown in different colors in Figure 1 (b). The different pore regions are connected with narrow interfaces. The simplified pore network can be extracted based on the pore regions distribution, as shown in Figure 1 (c). Each pore body corresponds to one pore region and the connection of neighboring pore regions is extracted as throat bond. One pore body in the PNM would require hundreds to thousands lattices for a simulation with LBM. Therefore, in PNM, the computational cost is dramatically reduced compared to LBM.

For single-phase flow in the pore network, the pressure and velocity distribution can be calculated by solving the mass balance equations in all the pore bodies for a given boundary condition, while the mass flow rate through a throat bond between two pore bodies under a certain pressure difference is determined by the throat conductance. Therefore, the accuracy of the single-phase pore network model strongly depends on the accuracy of predicting the throat conductance. Different methods have been proposed to improve the accuracy of pore network model by coupling with LBM [12–14]. We have evaluated four different pore network models to simulate single-phase flow in porous media and the improved pore network model which retains the actual pore-throat-pore geometry is shown to be sufficiently accurate to describe single-phase flow in porous media [13].

2.3. Hybrid LBM-PNM method
For liquid drying in porous media, both liquid and vapor phases coexist in the pore space. One example is shown in Figure 1 (d), where the red and blue colors represent the liquid and vapor phases, respectively. The liquid-vapor interface has a significant influence on the drying process as there is a pressure drop between the liquid and vapor phases at this position, known as capillary pressure. In addition, the liquid drying rates at different positions of the interface may be different. Therefore, accurate characterization of the movement of the two-phase interface and of the surrounding fluid flows is the key issue in modeling drying in porous media, thus the critical task of interface movement is performed here by LBM. For the single-liquid and single-vapor phase flows far away from the two-phase interfaces, the improved pore network model as described above [13] is used to calculate the pressure and velocity distributions, as such this strategy saves computational cost.

To implement this strategy, we proposed a hybrid method coupling LBM and PNM, as shown in Figure 1 (d)-(f). Figure 1 (d) shows the liquid-vapor two-phase distribution at a certain drying state. By mapping the phase distribution onto the pore regions distribution shown in Figure 1 (b), the pore regions can be classified into four types: (1) the two-phase pores shown in yellow which include the two-phase interfaces. (2) The single-liquid phase pores shown in red which only include liquid phase. (3) The single-vapor phase pores shown in light blue which only include vapor phase. (4) The buffer pores shown in green, located between the two-phase pores and single-phase pores. Similarly, the pore bodies and throat bonds in the extracted pore network can be also divided into the above four types, as shown in Figure 1 (f). We note that buffer pores are introduced to increase the accuracy of the LBM simulations [14].

In one simulation step, the pseudo-potential LBM is used to simulate liquid drying in the two-phase and buffer pores. The volume-averaged liquid or vapor pressures in the buffer pores are calculated in LBM, which act as pressure boundary conditions in the PNM simulations. Combined with the inlet/outlet boundary conditions of the pore network, the pressure distributions in single-liquid phase and single-vapor phase are calculated. In a next simulation step, the pressure distributions obtained by PNM simulation in turn provide the boundary conditions for the LBM simulation at the interfaces between buffer pores and single-phase pores. The above-described pore-type classification step and hybrid simulation step are repeated until the liquid phase dried out of the porous media. The accuracy and efficiency of the hybrid method is shown in section 3.2 below.

![Figure 1](image_url)

**Figure 1.** Schematic of liquid drying simulation in a 2D porous medium with the hybrid LBM-PNM method. (a) Example of a 2D porous medium, where black indicates solids and white the pores. (b) Pore regions decomposition based on watershed method, where different random colors represent different pore regions. (c) Extracted pore network with color indicating the pore/throat sizes in number of pixels. (d) Hybrid LBM-PNM method result showing liquid-vapor distribution at a certain drying state. Red and blue represent liquid and vapor phases, respectively. (e) Pore-type distribution for the phase distribution shown in (d). (f) Different types of pore bodies and throat bonds distribution for the phase distribution.
shown in (d). In figures (e) and (f), red and light blue indicate single-liquid phase and single-vapor phase pores, respectively. Yellow indicates two-phase pores and green buffer pores.

3. Results

3.1. Effects of capillary pumping during drying studied by LBM

In this part, we study in 2D the drying of a bi-modal porous system to better illustrate capillary pumping effects, a main mechanism at play in the redistribution of the liquid phase within a drying porous medium. As shown in Figure 2 (a), the lower and upper sections of the system have a higher porosity, namely 89.6%, while the central section has a smaller porosity of 76.7%. Pores are larger in the higher porosity sections and lower in the middle section. The contact angle of the liquid in this system is set to 60°. The left, top and bottom sides are set as solid walls while on the right side a smaller gas pressure is applied to allow drying to the open atmosphere.

Figure 2. Sequential liquid configurations during drying of a bi-modal porous system obtained with LBM.

From the drying process in Figure 2 (b-h), we can see that the large pores at top and bottom of high porosity regions are invaded by the gas phase first, because they correspond to a smaller capillary pressure. Meanwhile, the liquid-vapor interfaces in the smaller pore section remain almost unchanged, showing only a slight receding. The capacity of the porous medium to retain liquid in the smaller pores is due to the capillary pumping as discussed next.

Figure 3 shows an intermediate state of the drying process which happens between the states (d) and (e) of Figure 2. We superimpose streamlines on the liquid-vapor configuration to indicate both
the liquid flow by capillary pumping and the vapor diffusion to the open atmosphere. We consider five specific menisci, which are named A to E. At the large interfaces of A and B in the high porosity regions, the liquid is transported from these menisci to smaller interfaces in the high porosity region, as shown by streamlines connecting A to C and B to D and E. These streamlines show that such liquid flows can occur both in the high porosity region (A-C, B-D) and between high and low porosity regions (B-E). At the smaller interfaces C and D in the high porosity regions, the pumping effect is weaker than the local drying rate, thus these interfaces will recede due to dominant drying rate. On the other hand, at the small interface E, the pumping effect is slightly stronger than or equivalent to the local drying rate, making the interface to stay pinned until all the large pores are invaded by air. After the high porosity regions are invaded, which occur from Figure 2 (i) on, the liquid cluster in the small porosity region starts to shrink, since no capillary pumping can supply liquid anymore. In Figure 2 (j-l), the cluster breaks into smaller clusters until complete drying.

![Figure 3. Detailed analysis of capillary pumping effects occurring during one instance of drying of a bi-modal porous system.](image)

### 3.2. Evaluation of the hybrid LBM-PNM method to capture liquid-vapor interface during drying

In this section, the hybrid method is used to simulate the liquid drying process in the porous medium shown in Figure 1 (a). At initial condition, most of the pore space is saturated with liquid phase, shown in red in Figure 4 (a). The right boundary of the computational domain allows vapor to escape from the porous medium while all the other boundaries are vapor-tight solid walls. A low constant vapor pressure is assigned at the right boundary to drive the drying process. To evaluate the accuracy and efficiency of the hybrid method, the same setup is also used for a whole-domain LBM simulation to provide the reference results.

Figure 4 (a) shows 12 states of the two-phase distributions during the whole drying process. As can be seen from these figures, the drying process is dominated by capillary pressure as the vapor phase always seeks to invade the largest available pore region, i.e. where the smallest capillary pressure occurs. The whole-domain LBM simulation results are almost the same as the hybrid method and, to quantitatively verify the accuracy of the hybrid method, the relationship between liquid saturation and simulation steps (time) obtained by the two methods are plotted in Figure 4 (b). As drying proceeds, the drying rate gradually decreases which can be characterized by the slope of the curve. This is mainly because the two-phase interfaces invade deeper into the porous medium and the vapor leaving the interfaces is transported over a longer distance in order to reach the outlet. The simulation results of the hybrid method match quite well with those of the whole-domain LBM simulation, which demonstrates the accuracy of the hybrid method. As the hybrid method only implements the computationally expensive LBM simulations in the two-phase pores and buffer
pores, the computational time is significantly reduced, as shown in Figure (c). For the given porous medium, the hybrid method saves more than 2/3 computational time compared with the whole-domain LBM simulation. For a larger porous medium, the hybrid method could save even more computational time as the proportion of the computational domain that contains two-phase and buffer pores becomes smaller with respect to the single-phase pores.

3.3. Optimization of drying rate, with application to urban pavement

The intent of the developments presented above is to support the design and optimization of porous media with known transport properties. The capacity of the hybrid method to consider and document drying in all its intricacies can be harnessed to evolve designs of porous media, e.g. how the drying rate of urban pavement can be maximized. For this purpose, we are currently developing a two-component (air-water) two-phase (liquid-vapor) non-isothermal hybrid LBM model to model convective drying of porous media at pore scale including evaporative cooling. In recent work [15, 16], we have considered the use of porous pavements as sources of evaporative cooling in the urban environments, to counter the urban heat island, particularly during heat waves.

We have documented the environmental behavior of an urban street while varying the porous pavements, playing with porosity and with layering of fine and coarse porous materials. We found that, under dry conditions, the retained porous pavements yielded higher surface temperatures compared to conventional impervious concrete. Porous media have a smaller thermal diffusivity than more compact materials. As a result, higher porosity pavements show larger surface temperatures compared to lower porosity materials. In contrast, more interestingly, when the porous media have been wetted, the permeable pavements yield lower surface temperatures than those of
impervious pavements. This cooling effect is due to evaporation and thus depends on material transport properties, on the availability of water at or near the surface and on the rate of evaporation. We found that permeable porous pavements have a significantly longer first drying phase that conventional concrete pavements have. The second drying phase of such almost impermeable pavements is onset almost immediately after the end of a rain event. A combination of high albedo and coarse permeable pavements is shown to reduce urban surface temperatures, increase thermal comfort conditions in urban streets and squares and mitigate urban heat island. Thus, new porous cement or asphalt porous concrete solutions that meet the requirements of the pavements used in the simulation can be developed, providing the needed long first drying phase by combining porosity and layering. The hybrid LB-PNM method presented above can uniquely support such material design and development endeavour.

4. Conclusion
The two-phase LBM and the hybrid LBM-PNM methods allow to investigate and document transport in porous media at pore scale. In the first part of this paper, we used LBM to simulate the drying of a bi-modal porous system. Modeling the liquid and gas phases explicitly within the porous medium provides insightful information. For example, we showed that the large pore regions are invaded first, followed by small pore regions until complete drying. To explain this hierarchy, streamlines indicating flow from large pores to smaller ones can be analyzed and the capillary pumping effect can be seen in action.

As a direct numerical method, LBM simulates fluid flow directly in the digitalized porous geometry, which is accurate in characterizing the detailed pore structure and the inside flow information. However, it usually requires large computational resources. Through simplifying the actual pore structures into regular pore bodies and throat bonds, fluid flow in porous media can be modeled by the PNM. PNM is a very computationally efficient pore-scale model. On the other hand, it cannot capture the detailed pore structure information determining the detailed pore scale flow. In the second part of this paper, in order to combine the accuracy of LBM and the efficiency of PNM, a hybrid algorithm coupling these two methods is presented to simulate drying in porous media. The porous medium is firstly decomposed into pore regions based on watershed method. According to the liquid-vapor two-phase distribution, the pore regions are classified into four types, namely the two-phase pores, buffer pores, single-liquid phase and single-vapor phase pores. Then the LBM is only used to simulate liquid drying near the two-phase interfaces in the two-phase and buffer pores, while the PNM is used to simulate the pressure distribution in the buffer pores and single-phase pores. The two methods are coupled through exchange boundary information in the buffer pores. The hybrid method is used to simulate liquid drying in a porous medium and its accuracy and efficiency are verified by comparing with the whole-domain LBM reference simulation results.

In the near future, we will use LBM and hybrid LB-PNM methods to study and develop new porous materials, that could provide evaporative cooling pavement solutions for urban environments at stress during heat waves. As the hybrid simulations were in the work presented here simulated in 2D, in next steps, we will extend the modeling framework to 3D. Also, as future extension, for taken into non isothermal drying processes, we will follow the approach developed in our previous work [2].

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