International Journal of Heat and Mass Transfer 68 (2014) 310–323

Contents lists available at ScienceDirect

International Journal of Heat and Mass Transfer

journal homepage: www.elsevier.com/locate/ijhmt

Pore network study of slow evaporation in hydrophobic porous media

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ARTICLE INFO

Article history:
Received 5 May 2013
Received in revised form 16 September 2013
Accepted 18 September 2013
Available online 12 October 2013

Keywords:
Evaporation in porous media
Hydrophobic
Pore network model
Imbibition
Pore size distribution
Aspect ratio

ABSTRACT

A three-dimensional pore network model is developed in this paper to disclose the slow evaporation characteristics in various hydrophobic porous media. The constructed network is composed of large cubic pores connected by small throats of square cross section. During evaporation in the network, the two-phase flow is analogized as quasi-static imbibition, and water vapor transport is described as the diffusion process. Based on the developed model, parameter studies are performed to elucidate the effects on evaporation of the pore size distribution (PSD) and the aspect ratio (i.e. throat-to-pore ratio). In the wide PSD network, the drying induced two-phase displacement is a random process, and the impact of the aspect ratio is not significant. Two-phase displacement in the narrow PSD network is also a random process when the aspect ratio is high; but for the lower aspect ratio, the drying fronts are stably receded. In the case of the high aspect ratio, the evaporation rate with respect to network liquid saturation can be characterized by four periods in both the narrow and wide PSD networks: i.e. an initial drying period, a constant rate period, a falling rate period, and a receding front period, similar to that in the hydrophilic case.

1. Introduction

Evaporation in porous media is of great interest to numerous industrial applications, including, to name only a few, drying of many products, light oil recovery, and soil remediation. The porous media in these fields are generally hydrophilic, i.e. liquid is a wetting phase. The two-phase flow in these hydrophilic porous media during evaporation can be analogized as a drainage process of a non-wetting gas phase displacing a wetting liquid phase [1–3]. On the other hand, evaporation in the hydrophobic porous media also can be encountered. For example, in fields of proton exchange membrane fuel cells (PEMFCs), the gas diffusion layer is usually treated with PTFE to become hydrophobic so as to facilitate removal of liquid and obtain better water management. But, when the gas diffusion layer is completely flooded with liquid, dry gas is needed to purge into PEMFCs to eliminate liquid through the evaporation mechanisms [4]. This gas purge process is highly parasitic and consequently decreases efficiency of PEMFCs. To optimize the gas purge, it is needed to understand the detailed evaporation process in the hydrophobic porous gas diffusion layer.

Several experimental studies have been carried out to shed light on evaporation in the hydrophobic porous media. Chapuis et al. [4] fabricated a two-dimensional pore network composed of ducts of various widths in a hydrophobic PTFE plat and obtained the patterns of the drying fronts during evaporation. They found that the drying patterns are compact with the almost flat drying fronts. Sghaier and Prat [5] explored evaporation in a two-dimensional (2D) model porous network consisting of hydrophobic glasses. In their experiments, all the lateral sides of the fabricated network are open to the environment. The drying patterns were observed to be compact with no trappings. Eloukabi et al. [6] compared evaporation in two porous networks composed of monolayer of hydrophobic glasses and found that evolution of the drying fronts is largely affected by the network structures. Shokri et al. [7] analyzed the morphologies, scaling characteristics, and propagation dynamics of the drying fronts in a three-dimensional (3D) Hele–Shaw cell filled with hydrophobic sands. In their work, evolution of the drying fronts was recorded using nondestructive neutron radiography, and the fractal dimension and the roughness of the drying fronts were analyzed.

In addition to the experimental studies, pore network modeling has also been employed to understand the evaporation process in porous media. The basis of this approach is to convert the void spaces of a porous medium into a network composed of large pores and small throats. Since introduction of this approach to the evaporation fields by Prat [8], many complicated pore network models

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http://dx.doi.org/10.1016/j.ijheatmasstransfer.2013.09.042

Nomenclature

A	cross sectional area of the network (m^2)
$A_{pi(tij)}$	cross sectional area of pore i (throat tij) (m^2)
C_{df}	water vapor concentration at drying front (1.28 mol m^{-3})
$C_{pi}(_{tij})$	water vapor concentration in pore i (throat tij) (mol m^{-3})
C_{no}	water concentration at network open surface (mol m^{-3})
C_∞	water vapor concentration in surrounding air (0 mol m^{-3})
D	bulk water vapor diffusion coefficient (2.76×10^{-5} m^2 s^{-1})
D_e	effective diffusivity of water vapor in network (0.17×10^{-5} m^2 s^{-1})
f	fractional distance along the network thickness
J_{no}	evaporation rate at the network open side (mol s^{-1})
J_{df}	evaporation rate at the drying front (mol s^{-1})
l	distance between two neighboring pores (25 μm)
l_{tij}	length of throat connecting pores i and j (μm)
L	network thickness (6.25×10^{-4} m)
M_w	liquid molar mass (0.018 kg mol^{-1})
P_l	pressure in liquid phase (Pa)
P_g	pressure in gas phase (Pa)

P_{tt}	threshold entry pressure of the partially filled throat (Pa)
P_{tp}	threshold entry pressure of the partially filled pore (Pa)
$q_{pi,tij}$	diffusive rate from pore i to throat connecting pores i and j (mol s^{-1})
$q_{ti,\infty}$	diffusive rate from throat i to environment (mol s^{-1})
Q_{lc}	drying rate of a liquid cluster (mol s^{-1})
r_p	pore radius (μm)
r_t	throat radius (μm)
s	network liquid saturation
t_c	time to completely evaporate available element (s)
V_{al}	volume of liquid in available element (m^3)
z_{df}	distance from drying front to network open surface (m)

Greek symbols

ϕ	aspect ratio
σ	surface tension (0.072 Nm^{-1})
θ	contact angle taken in gas (wetting) phase (60°)
δ	thickness of external diffusion layer (12.5 μm)
ρ_w	liquid density (1000 kg m^{-3})
ε_{no}	network surface porosity

have been developed to account for the viscous effects [9–11], gravity effects [12,13], thermal effects [14–16], topological effects [17–21], and liquid film effects [22,23]. Two types of pore network models, i.e. quasi-static and dynamic, can be found in literatures. In the quasi-static models, the two-phase flow during evaporation is dominated by the capillary forces, and the viscous effects are ignored, whereas both the capillary and viscous forces must be considered in the dynamic models. Most of the current pore network studies on the problems of evaporation in porous media are based on the quasi-static models and are focused on the hydrophilic cases.

The first work for pore network modeling of evaporation in the hydrophobic porous media is carried out by Chapuis and Prat [24]. In their work, a 2D square network, which consists of ducts of various sizes, was constructed. The evaporation process in this network was simulated by combining the quasi-static imbibition rule for the liquid flow and Fick's law for gas transport (the imbibition process represents displacement of a non-wetting phase by a wetting phase). The authors found that the drying fronts are flat, and dimensionless average overall drying time tends toward 0.93 as the network size increases (dimensionless average overall drying time is defined as the ratio of time to empty the network obtained from the pore network model to that gained from the theoretical model). Chraibi et al. [25] performed the pore network simulations on evaporation in a 2D network composed of the hydrophobic cylinders. For such network, three basic types of local instability of the drying fronts can be distinguished: i.e. burst, touch, and overlap. They revealed that evolution of the drying fronts in the hydrophobic network is dominated by the overlap mechanism. More recently, Wu et al. [26] studied evaporation in a hydrophobic gas diffusion layer (GDL) of PEMFCs using a 3D quasi-static pore network model. In their model, the GDL surface is partially screened by the land of the bipolar plate. The authors disclosed that the evaporation process in the GDL consists of two steps: through-plane evaporation under the channel of the bipolar plate and in-plane evaporation under the land of the bipolar plate. It was revealed that the evaporation rate with respect to network liquid saturation can be characterized by four periods: a rapid drop period, a slow drop period, a constant rate period, and a further falling period.

From the above literature reviews, we can know that two-phase displacement in a hydrophobic network during slow evaporation can be described using the quasi-static imbibition rule. It has been revealed that the imbibition process is significantly affected by network morphology [27–29]. For instance, Lenormand [27] found that two-phase displacement during imbibition is controlled by the throat-to-pore ratio (i.e. the aspect ratio). In this regard, it can be inferred that for evaporation in a hydrophobic network, the drying patterns, which determine the drying characteristics, are significantly dependent on the network structures. That is to say, revealing the influences of the network structures is critical to understanding of evaporation in the hydrophobic porous media. However, to our best knowledge, no work has been performed to address this fundamental issue.

The objective of this study is to disclose the effects of the network structures, i.e. the pore size distribution and the aspect ratio, on slow evaporation in the hydrophobic porous media using a 3D pore network model. In what follows, pore network construction is described, and the procedures to describe two-phase transport during evaporation are illustrated. Then, how the network structures affect the evaporation characteristics in the hydrophobic porous media is discussed in Section 3. Finally, in Section 4, some interesting conclusions are drawn, and the future work is presented.

2. Pore network model

As we mentioned, the purpose of the present work is to explore the effects of the network structures on slow evaporation in the purely hydrophobic porous media based on the pore network modeling approach. As in Ref. [30], a three-dimensional (3D) pore network model is employed in this contribution. The constructed network consists of large cubic pores connected by small square cross-sectional throats, as schematically illustrated in Fig. 1a. The pores represent the large void regions in porous media, and the