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Modeling water imbibition into coated and uncoated papers

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HIGHLIGHTS

- Pore size distribution of coated/uncoated papers followed lognormal distribution.
- A critical-path-analysis model was proposed to estimate relative permeability k_{rw}.
- Comparing to simulations showed that k_{rw} was accurately estimated under imbibition.

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ABSTRACT

Modeling morphological and hydraulic properties of thin porous media, such as filter layers and papers is highly relevant to various industries. In our previous studies, the X-ray tomography and FIB-SEM methods were applied to capture micro- and nano-scale pores in uncoated paper and coated layer, respectively. Here, the reconstructed pore structures were used to investigate two-phase water imbibition in these porous media. The obtained pore size distributions showed a log-normal probability density function. Such a distribution, together with concepts from critical path analysis and percolation theory, was applied to calculate relative permeability over a wide range of water saturations. Comparison with pore-scale numerical simulations showed the capability of this method to estimate water relative permeability for coated and uncoated papers.

1. Introduction

Several different industries deal with thin porous media in their production processes. These include coating layers and papers is the printing industry, food packaging, and production of filters and membranes. The morphological and hydraulic properties of such thin layers are often critical in the process performance. Advanced high-resolution computed tomography provides a minimally-destructive and direct technique to determine pore space morphological and physical properties of thin porous media. Various algorithms have been developed to generate pore structures (Raoof and Hassanizadeh, 2012) or to analyze three-dimensional images (e.g., Lindquist et al., 1996; Silin et al., 2003; Øren and Bakke, 2003) to quantify pore space geometrical and topological properties. For example, Lindquist et al. (1996) introduced the medial axis as a technique to analyze the acquired geometric structure of pore space in porous media. Delerue et al. (1999) proposed a method based on skeletization to determine the void space from 3D images. In another study, Silin et al. (2003) proposed an algorithm in which the skeleton of the pore space is captured through maximal balls associated with each voxel. Those authors used the maximal ball distribution to simulate a dimensionless drainage capillary pressure curve and showed that their method provided realistic estimates of the number and shapes of pores and throats as well as the pore coordination number. More recently, Raoof and Hassanizadeh (2012) introduced a method to numerically generate pore structures with variable coordination number up to 26 connected neighbors at each pore.

During the printing process, liquid penetration into the paper (known as imbibition process) depends on several factors and mechanisms such as geometrical and morphological properties of pores (e.g., Ghassemzadeh et al., 2001), pore size distribution (Liu et al., 2017), and pore-solid interface roughness and wetting force (Liu et al., 2014a, 2014b). For instance, Ghassemzadeh et al. (2001) developed a new imbibition model of a coating fluid in a fibrous layer. The three-dimensional pore network of paper was represented by the interconnection of flow channels between fibers. Ghassemzadeh et al. (2001) found that the mean coordination number (i.e., the interconnectivity of the channels) and the average

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pore size of the paper strongly influenced imbibition of the coating fluid. Using a high-speed camera, Koivula et al. (2012) studied the influence of coating surface structure and pre-saturation state on the spreading of liquid. Results showed a high impact of pigment-based structure on the liquid distribution in both dry and pre-saturated structures. However, under the pre-saturated conditions, liquid-liquid interactions were the controlling mechanism. Koivula et al. (2012) showed the effectiveness of nano-size pores located in a calcium carbonate comprising base layer to increase capillarity absorption. In another study, Lamminmäki et al. (2011) investigated a set of critical parameters for print durability. In coated inkjet papers, the surface is treated based on pore-network of layer and addition of polymer binders to produce good ink fastness properties. Based on their study, low permeability of coating layer and bounding colorant part of ink by charge interactions could produce required print quality.

Pore-scale imaging has become a promising method to study fluid flow and transport in porous materials (see e.g., Raoof et al., 2013; Liu and Mostaghimi, 2017). Although there exist some challenges such as identifying a representative elementary volume (REV), needed to define macroscopic properties, and the resolution effect, there has been significant progress in three-dimensional imaging, especially in thin porous media. For instance, Huang et al. (2002) proposed a method based on X-ray micro-tomography imaging and determined porosity, pore size distribution, and specific surface area for fibers. Their results agreed reasonably well with the measured values using the mercury intrusion porosimetry method. More recent developments in pore-scale tomographic imaging of porous media can be found at Wildenschild and Sheppard (2013).

Pore-network models have also been used to study fluid flow in thin porous media. For example, Ghassemzadeh and Sahimi (2004a) carried out extensive computational simulations to investigate the effect of the microstructure of paper's pore space on the effective permeability tensor. They concluded that the distribution of fibers and consequently coordination number has a strong impact on fluid flow properties in fibrous layers. In another study, Ghassemzadeh and Sahimi (2004b) simulated the imbibition process of a coating fluid into a paper using a network of interconnected channels. Their results showed that the connectivity of the channels, the anisotropic structure of the paper's pore space, and the dynamic pressure distribution had strong effects on the imbibition process.

In the literature, various theoretical approaches have been used to model water relative permeability in porous media. Some models were developed based on the parallel (e.g., Purcell, 1949; Burdine, 1953), series-parallel (e.g., Mualem, 1976; Kosugi, 1999), or tortuous parallel (e.g., Zheng et al., 2013; Zhang et al., 2017) capillary tubes approach. However, such models are distorted idealizations (Sahimi, 2011; Hunt et al., 2014), since pores in porous media exist neither in series nor in parallel, but are distributed throughout an interconnected and complex multi-scale network.

In addition to the bundle of capillary tubes model, effective-medium theory has been utilized to estimate the relative permeability k_r (see e.g., Petropoulos et al., 1989; Kainourgiakis et al., 1998; Ghanbarian et al., 2016a). For example, Ghanbarian et al. (2016a) assumed that the pore size distribution of porous media followed a power-law form and determined its parameters (including pore space fractal dimension) from the capillary pressure curve. Invoking Kirkpatrick's effective-medium theory, Ghanbarian et al. (2016a) estimated the relative permeability for water, k_{rw}, from measured capillary pressure data and found good agreement with experiments. However, those authors reported k_{rw} underestimations via effective-medium theory in porous media with broad pore size distribution.

Hunt (2001) was probably the first to apply concepts from critical path analysis (CPA) to model k_{rw} in porous media with broad hydraulic conductance (or pore size) distribution. Hunt (2001) combined CPA with the power-law pore size distribution whose parameters were determined from the capillary pressure curve. By comparison with experiments, Hunt (2001) showed that CPA accurately estimated k_{rw}, particularly at high water saturations. Years later, Ghanbarian-Alavijeh and Hunt (2012) combined CPA with the pore-solid fractal model and proposed a more general water relative permeability relationship. Results of Ghanbarian-Alavijeh and Hunt (2012), Ghanbarian et al. (2015a, 2016b), and Ghanbarian and Hunt (2017) indicated that the proposed general model estimated k_{rw} accurately.

Concepts from CPA and power-law pore size distribution have been applied to estimate k_{rw} from the measured capillary pressure curve. However, to the best of the authors' knowledge CPA has never been combined with the log-normal pore size distribution to predict k_{rw}. Nor has it been used to estimate k_{rw} directly from the pore size distribution and three-dimensional reconstructed pore structure derived from FIB-SEM imaging. Therefore, the main objectives of this study are: (1) to develop a theoretical k_{rw} model based on CPA and log-normal pore size distribution, and (2) to evaluate the proposed approach in the estimation of k_{rw} from measured pore size distribution for thin porous media like paper coating layers and uncoated papers.

2. Theory

2.1. Pore size distribution and capillary pressure curve

Thin porous media such as fibrous layers consist of solid matrix and pore space. The latter is formed of void regions of irregular shapes and various sizes spanning orders of magnitude from several nanometers to a few hundred micrometers. Similar to natural porous media such as rocks and soils, the geometrical definition of a single pore is ambiguous in fibrous layers and papers. This, accordingly, makes determination of the actual distribution of pore sizes difficult. Nonetheless, following Qin and Hassanizadeh (2014) and Qin et al. (2016), we assume that pore sizes in thin porous media conform to the following truncated log-normal probability density function $f(r)$

$$f(r) = \frac{A}{\sqrt{2\pi}\sigma r}\exp\left[-\left(\frac{\ln\left(\frac{r}{r_m}\right)}{\sqrt{2}\sigma}\right)^2\right], \quad r_{min} \leqslant r \leqslant r_{max} \tag{1}$$

in which,

$$A = \frac{2}{\mathrm{erf}\left(\frac{\ln\left(\frac{r_{max}}{r_m}\right)}{\sqrt{2}\sigma}\right) - \mathrm{erf}\left(\frac{\ln\left(\frac{r_{min}}{r_m}\right)}{\sqrt{2}\sigma}\right)} \tag{2}$$

where erf is the error function, r is the pore radius, r_{min} and r_{max} are the smallest and largest pore radii, respectively, representing the lower and upper bounds of the log-normal distribution, r_m is the geometric mean pore radius, and σ is the log-normal standard deviation. The value of r_m, r_{min}, r_{max}, and σ can be determined by directly fitting Eq. (1) to the pore size distribution derived from, e.g., tomography images.

Following Eq. (1), the porosity ϕ of the medium is

$$\begin{aligned}\phi &= \int_{r_{min}}^{r_{max}} s r^3 f(r)\mathrm{d}r + \theta_r \\ &= \frac{sAr_m^3}{2}\exp\left(\frac{9\sigma^2}{2}\right)\left[\mathrm{erf}\left(\frac{3\sigma^2 - \ln\left(\frac{r_{min}}{r_m}\right)}{\sqrt{2}\sigma}\right) - \mathrm{erf}\left(\frac{3\sigma^2 - \ln\left(\frac{r_{max}}{r_m}\right)}{\sqrt{2}\sigma}\right)\right] + \theta_r\end{aligned} \tag{3}$$