On applications and limitations of one-dimensional capillarity formulations for media with heterogeneous wettability

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Force-balance-based one-dimensional algebraic formulations that are often used in characterizing the capillarity of a multi-component system (e.g., predicting capillary height rise in porous media) are discussed. It is shown that such formulations fail to provide accurate predictions when the distribution of wetting (or non-wetting) surfaces is not homogeneous. A more general mathematical formulation is suggested and used to demonstrate that for media with heterogeneous wettability, hydrophilic (or hydrophobic) surfaces clustered in groups will have less contribution to the overall capillarity of the system. © *2013 AIP Publishing LLC*. [http://dx.doi.org/10.1063/1.4811167]

Capillarity was first explored by measuring vertical fluid rise z in a capillary tube of fixed diameter d_{cap}, and relating it to the physical properties of the tube and fluid, eventually culminating in the Young–Laplace equation, or for height rise, Jurin's law[1]

$$z = \frac{4a^2 \cos\theta_{cap}}{d_{cap}}, \tag{1}$$

where θ_{cap} is the liquid–solid contact angle and $a = \sqrt{\sigma/\rho g}$ is equal to capillary length scale. σ, ρ, and g represent surface tension, density, and gravitational acceleration, respectively. The effect of capillarity is significant when d_{cap} is less than capillary length a.[2] Later, a dynamic model for 1-D Poiseuille flow to predict fluid height rise in a vertical capillary tube was devised,[3,4] the static (equilibrium) component of which becomes Eq. (1). This model has been adapted for modeling fluid transport in porous media as a series of aligned capillary tubes of a single equivalent diameter.[5] The same basis for derivation was later revisited by Marmur,[6] in which a model for predicting the radial horizontal spread of a fluid from an infinite reservoir of radius R_0 was developed, and later validated for spread in sheet papers.[7] A modified form of Marmur's equation was then presented in Ref. 8 as

$$\left(\frac{R}{R_0}\right)^2 \left(\ln\frac{R}{R_0} - \frac{1}{2}\right) + \frac{1}{2} = \frac{\sigma d_{cap}\cos\theta_{cap}}{12\mu R_0^2} t. \tag{2}$$

Equation (2), or any such equation derived based on a capillary-tube representation of a multi-component fibrous medium (medium having more than one fiber diameter and/or wall-contact angle), requires single numeric values for the diameter and contact angle of the capillary tube, d_{cap} and θ_{cap}. In this work, we discuss the applicability of the 1-D force-balance approach for obtaining d_{cap} and θ_{cap} for multi-component fibrous media using fiber bundles (media comprised of highly aligned fibers), as a special-case representation of a concept that can generally be applied to all systems in which capillary pressure is a driving mechanism, such as biological systems and capillary pumps.[9–11]

Let us consider a square array of four fibers as a unit cell in a bundle of vertically aligned fibers, as shown from overhead in Figure 1. Each fiber may be one of two materials, each of which with its own contact angle θ and fiber diameter d. The meniscus height z in such a medium can be described as

$$z = f(\alpha, d_1, d_2, \ldots, \theta_1, \theta_2, \ldots, n_1, n_2, \ldots), \tag{3}$$

where α is equal to solid volume fraction (SVF) of the medium, and d_i, θ_i, and n_i are, respectively, diameter, liquid–solid contact angle, and number fraction (between 0 and 1) for the ith fiber type. We can derive an expression for meniscus height rise based on the balance of forces across the meniscus as shown in Figure 1, with F_g and F_σ being gravity and capillary forces, respectively

$$A\rho g z_{\min} = C\sigma\cos\theta, \tag{4}$$

where A and C are total available fluid cross-sectional area and liquid–air–fiber interface perimeter, and z_{min} refers to the height of the bottom of the meniscus. Expanded in terms of Eq. (3) for a unit cell with two different fiber types, Eq. (4) becomes

$$z_{\min} = \frac{4\sigma(n_1 d_1\cos\theta_1 + n_2 d_2\cos\theta_2)}{\rho g(1/\alpha - 1)(n_1 d_1^2 + n_2 d_2^2)}. \tag{5}$$

It is worth mentioning that this equation simplifies to that of Princen[12] in the special case of one single fiber size and contact angle. From Eqs. (1) and (5), one obtains

$$\frac{\cos\theta_{cap}}{d_{cap}} = \frac{(n_1 d_1\cos\theta_1 + n_2 d_2\cos\theta_2)}{(1/\alpha - 1)(n_1 d_1^2 + n_2 d_2^2)}. \tag{6}$$

Examining Eq. (6) reveals that this equation is in fact comprised of two more familiar equations, a weighted averaging of cosines of the two contact angles for the cosine of

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