

Improved Computational Procedure for Retention Relations of Immiscible Fluids Using Pressure Cells

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ABSTRACT

The capillary pressure–saturation relation, or the capillary pressure head–volumetric fluid content relation, is of widespread interest in modeling and predicting multiphase fluid flow. A common procedure to determine this relation is to use a pressure cell and assume uniform distributions of capillary pressure and volumetric fluid contents at static equilibrium. The pressure cell method, however, yields inaccurate results for certain combinations of multiphase fluids and porous media. The sensitivity analysis in this study shows that the pressure cell height, the positions of the pressure measuring devices, which can coincide with the in- and outflow ports, and the relative density difference of the fluids, can give rise to considerable errors in the determination of capillary pressure head–volumetric fluid content relations by the standard procedure using pressure cells. We, therefore, propose a curve-fitting method that considers nonuniform distributions of capillary pressure and volumetric fluid content of multiphase fluids. The method uses the same input data as commonly used procedures.

ACCURATE DETERMINATION of the capillary pressure (P_c)–saturation (S) relation, or the capillary pressure head (h_c)–volumetric fluid content (θ) relation, is important for modeling multiphase fluid flow. The relation between S and θ is $S = \theta/\phi$, where ϕ is the porosity of the porous medium. Pressure cells are often used to determine this relation (Lin et al., 1982; Lenhard and Parker, 1987; Turrin, 1988; Kuepper et al., 1989; Demond and Roberts, 1991). This procedure, however, can give inaccurate results for multiphase fluids with small interfacial tensions (Dane et al., 1992). An improved experimental method to determine this relation, using a gamma radiation technique, was developed by Dane et al. (1992). In this study, we propose a computational procedure to determine the capillary pressure–saturation relation for multiphase fluids using commonly obtained pressure cell data.

THEORY

One important reason for a $P_c(S)$ relation, determined with a pressure cell, to be inaccurate is the nonuniform distributions of P_c and S (or h_c and θ) of the fluids. As an example, consider the determination of the $P_c(S)$ relation for a wetting fluid in a two-phase fluid system with the pressure cell depicted in Fig. 1. At static conditions, the value for the average saturation \bar{S} (or the average volumetric fluid content $\bar{\theta}_w$) of the wetting fluid is measured as a function of the pressure difference between the nonwetting fluid with reference pressure \bar{P}_n ($M L^{-1} T^{-2}$), determined by the pressure at position z_n , and the wetting fluid with reference pressure \bar{P}_w ($M L^{-1} T^{-2}$), determined by the pressure at position z_w . The reference pressures \bar{P}_n and \bar{P}_w can be measured with hydrophobic and hydrophilic

tensiometers, respectively (Lenhard and Parker, 1987), or they can be measured directly at the in- and outflow ports located at the top and bottom of the pressure cell (Fig. 1). It should be mentioned that for $\rho_n > \rho_w$, the nonwetting fluid should enter the pressure cell from the bottom, while for $\rho_n < \rho_w$ it should enter from the top. For $\rho_n = \rho_w$ it can enter from either the top or the bottom. The hydrophilic porous plate should always be located where the wetting fluid enters or exits the pressure cell.

The measured reference pressures are commonly used to represent some sort of average values in the pressure cell. In this study, we assume the pressure measurement locations, z_n and z_w , to be at arbitrary elevations between the bottom and top of the pressure cell. In the standard procedure, the experimental relation between $\bar{P}_c = \bar{P}_n - \bar{P}_w$ and \bar{S} is considered to be the capillary pressure–saturation relation for the particular fluids and porous medium in the pressure cell. One should keep in mind, however, that this $\bar{P}_c(\bar{S})$ is an average relation for the sample as a whole. Dane et al. (1992) showed that under certain conditions a considerable difference exists between this relation and the one determined at a given point. In the computational scheme we propose, we make use of the local distributions of P_c (or h_c) and S (or θ) of the wetting fluid in the pressure cell. At hydraulic equilibrium, the local wetting fluid pressure, P_w ($M L^{-1} T^{-2}$), and the local nonwetting fluid pressure, P_n ($M L^{-1} T^{-2}$), at any elevation within the pressure cell (Fig. 1) can be expressed as:

$$P_w(z) = \bar{P}_w - \rho_w g(z - z_w) \quad [1]$$

$$P_n(z) = \bar{P}_n - \rho_n g(z - z_n) \quad [2]$$

where g is the gravitational field strength ($L T^{-2}$), ρ_n and ρ_w are the density of the nonwetting and wetting fluids ($M L^{-3}$), respectively, and z is the distance from the datum.

The local capillary pressure at elevation z is

$$P_c(z) = P_n(z) - P_w(z) \quad [3]$$

Substituting Eq. [1] and [2] into [3], and defining capillary pressure heads by

$$h_c = \frac{P_c}{\rho_w g} \quad [4]$$

$$\bar{h}_c = \frac{\bar{P}_c}{\rho_w g} = \frac{\bar{P}_n - \bar{P}_w}{\rho_w g} \quad [5]$$

we obtain:

$$h_c = \bar{h}_c + A + Bz \quad [6]$$

where

$$A = z_n \frac{\rho_n}{\rho_w} - z_w \quad [6-1]$$

and

$$B = 1 - \frac{\rho_n}{\rho_w} \quad [6-2]$$

Equation [6] gives the accurate distribution of the capillary pressure head with elevation in the pressure cell. In the standard computational procedure, the variation of capillary pressure

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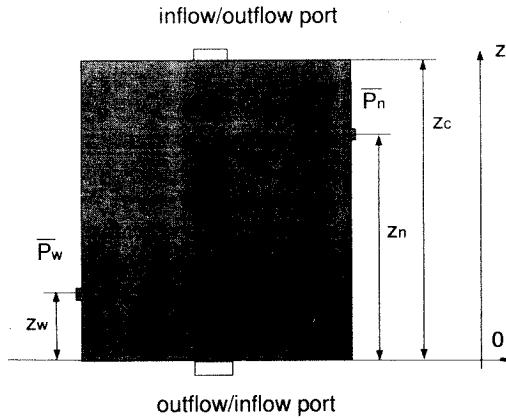


Fig. 1. Diagram representing a pressure cell with height z_c ; z_n and z_w are the elevations at which the nonwetting fluid pressure (P_n) and the wetting fluid pressure (P_w), respectively, are known.

head in the vertical direction is ignored, which is reasonable only if \bar{h}_c is much larger than the sum of the other two terms on the right-hand side of Eq. [6].

The distribution of the local volumetric content of the wetting fluid, θ_w ($L^3 L^{-3}$), can be represented by an empirical relation between h_c and θ_w . In this study, we use the Brooks-Corey relation (Brooks and Corey, 1964):

$$S_e = \frac{S - S_r}{1 - S_r} = \left(\frac{P_d}{P_c} \right)^\lambda \quad \text{for } P_c > P_d \quad [7-1]$$

$$S_e = 1 \quad \text{for } P_c \leq P_d \quad [7-2]$$

where S_e and S_r are the effective and residual local wetting fluid saturations, respectively, and P_d ($M L^{-1} T^{-2}$) is the displacement pressure. The Brooks-Corey relation can be rewritten in terms of h_c and θ_w as:

$$\theta_w = \theta_{wr} + (\theta_{ws} - \theta_{wr}) \left(\frac{h_d}{h_c} \right)^\lambda \quad \text{for } h_c \geq h_d \quad [8-1]$$

$$\theta_w = \theta_{ws} \quad \text{for } h_c < h_d \quad [8-2]$$

where θ_{wr} and θ_{ws} are the residual and saturated volumetric wetting fluid contents, respectively, and $h_d = P_d/(\rho_w g)$ is the displacement capillary pressure head (L). Since use of the pressure cell results in \bar{h}_c and $\bar{\theta}_w$, we need to find a relation between $\bar{h}_c(\bar{\theta}_w)$ and $h_c(\theta_w)$ at a given elevation within the sample, assuming the latter to be correctly represented by Eq. [8]. Based on the assumption that the porous medium is perfectly homogeneous, the basic relation between $\bar{\theta}_w$ and θ_w can be expressed as

$$\bar{\theta}_w = \frac{1}{z_c} \int_0^{z_c} \theta_w(h_c) dz \quad [9]$$

Before detailed expressions for $\bar{\theta}_w$ can be developed, we need to find the location ($z = z_{cr}$) of the boundary between the saturated and unsaturated zones of the wetting fluid in the pressure cell, which is defined by $h_c = h_d$. From Eq. [6], the critical position z_{cr} (L), corresponding to $h_c = h_d$, is given by:

$$z_{cr} = - \frac{(A - h_d + \bar{h}_c)}{B} \quad [10]$$

It is useful to note that z_{cr} is a function of \bar{h}_c , and therefore has different values for different data points measured with a pressure cell. Since values of $z_{cr} < 0$ and $z_{cr} > z_c$ have no physical meaning for the system under consideration, an alternative

variable, z^* , is defined by

$$z^* = 0 \quad \text{for } z_{cr} \leq 0 \quad [11-1]$$

$$z^* = \min[z_c, z_{cr}] \quad \text{for } z_{cr} > 0 \quad [11-2]$$

With the variable z^* , the saturated zone of the wetting fluid in a pressure cell can be defined in a general manner, i.e., $z^* \leq z \leq z_c$ for $\rho_w < \rho_n$ and $0 \leq z \leq z^*$ for $\rho_w > \rho_n$. Expressions for $\bar{\theta}_w$ are obtained for three cases.

Case 1. $\rho_n = \rho_w$ or $B = 0$

As shown by Eq. [6], both h_c and θ_w are constant with elevation at hydraulic equilibrium. Substituting Eq. [6] and [8] into Eq. [9] yields:

$$\bar{\theta}_w = \theta_{wr} + \frac{\theta_{ws} - \theta_{wr}}{\left(\frac{\bar{h}_c - z_w + z_n}{h_d} \right)^\lambda} \quad \text{for } \bar{h}_c \geq z_w - z_n + h_d \quad [12-1]$$

$$\bar{\theta}_w = \theta_{ws} \quad \text{for } \bar{h}_c < z_w - z_n + h_d \quad [12-2]$$

Case 2. $\rho_n < \rho_w$ or $B > 0$

As shown by Eq. [6], h_c increases and θ_w decreases (for $h_c \geq h_d$) with z . Based on Eq. [6], [11], and [8], the distribution of θ_w in the pressure cell can be described by

$$\theta_w = \theta_{wr} + (\theta_{ws} - \theta_{wr}) \left(\frac{h_d}{h_c} \right)^\lambda \quad \text{for } z^* \leq z \leq z_c \quad [13-1]$$

$$\theta_w = \theta_{ws} \quad \text{for } z < z^* \quad [13-2]$$

Substituting Eq. [13] and [6] into Eq. [9], and performing the integration in two steps, i.e., from zero to z^* and from z^* to z_c , yields

$$\bar{\theta}_w = \frac{z^*}{z_c} \theta_{ws} + \frac{z_c - z^*}{z_c} \theta_{wr} + \frac{\theta_{ws} - \theta_{wr}}{(h_d)^{-\lambda} z_c B} I_1 \quad [14]$$

where

$$I_1 = \ln \frac{A + Bz_c + \bar{h}_c}{A + Bz^* + \bar{h}_c} \quad \text{for } \lambda = 1$$

$$I_1 = \frac{1}{1 - \lambda} [(A + Bz_c + \bar{h}_c)^{1-\lambda} - (A + Bz^* + \bar{h}_c)^{1-\lambda}] \quad \text{for } \lambda \neq 1$$

Case 3. $\rho_n > \rho_w$ or $B < 0$

In this case, h_c decreases and θ_w increases with z and the distribution of the wetting fluid content is given by

$$\theta_w = \theta_{wr} + (\theta_{ws} - \theta_{wr}) \left(\frac{h_d}{h_c} \right)^\lambda \quad \text{for } 0 \leq z \leq z^* \quad [15-1]$$

$$\theta_w = \theta_{ws} \quad \text{for } z > z^* \quad [15-2]$$

Substituting Eq. [15] and [6] into Eq. [9] yields:

$$\bar{\theta}_w = \frac{z^*}{z_c} \theta_{wr} + \frac{z_c - z^*}{z_c} \theta_{ws} + \frac{\theta_{ws} - \theta_{wr}}{(h_d)^{-\lambda} z_c B} I_2 \quad [16]$$

where

$$I_2 = \ln \frac{A + Bz^* + \bar{h}_c}{A + \bar{h}_c} \quad \text{for } \lambda = 1$$

$$I_2 = \frac{1}{1-\lambda} [(A + Bz^* + \bar{h}_c)^{1-\lambda} - (A + \bar{h}_c)^{1-\lambda}] \quad \text{for } \lambda \neq 1$$

It should be emphasized that the derived $\bar{\theta}_w(\bar{h}_c)$ expressions are related to the local $\theta_w(h_c)$ relation (Eq. [8]) through h_d , λ , θ_{ws} and θ_{wr} . A curve-fitting procedure, similar to the one of van Genuchten (1980), for example, can thus be used to determine the parameters describing $\theta_w(h_c)$ based on data for $\theta_w(\bar{h}_c)$. Although we used the Brooks-Corey equation to describe $\theta_w(h_c)$, other empirical relations between θ_w and h_c , such as the van Genuchten (1980) equation, can also be used to develop the $\bar{\theta}_w(\bar{h}_c)$ expressions.

The expressions for $\bar{\theta}_w$ (Eq. [12], [14], and [16]) clearly show that the average relation $\bar{\theta}_w(\bar{h}_c)$, measured with the pressure cell method, depends on the pressure cell geometry, the fluid properties, and the porous medium properties. Some of these factors can give rise to considerable errors in the determination of capillary pressure head-volumetric fluid content relations for coarse porous media containing fluids with small interfacial tensions (Dane et al., 1992). As indicated above, the local relation is considered to be accurate. In the method of Dane et al. (1992), this local relation can be directly determined from known fluid pressure distributions and measurements of volumetric fluid contents at a given point with a gamma radiation system. In this study, we propose a simple curve-fitting approach to determine the local (point) relation from pressure cell data. For a given pressure cell geometry (z_c , z_n , and z_w) and fluid densities, the unknown parameters in the expressions for $\bar{\theta}_w(\bar{h}_c)$ (Eq. [12], [14], and [16]) are h_d , λ , θ_{ws} and θ_{wr} . By fitting the parametric expressions for $\bar{\theta}_w(\bar{h}_c)$ through the pressure cell data, the best estimations of these parameters can be obtained. Subsequently, the local relation in terms of these parameters (Eq. [8]) is then completely determined (a Fortran code to perform the proposed curve-fitting procedure is available from the authors). Traditionally, the pressure cell data are fitted by an empirical local relation, such as the Brooks-Corey relation, before they are used to model fluid flow. In other words, the pressure cell is considered to be a point. The main contribution of the proposed method, therefore, is that local relations are derived from average relations measured with a pressure cell. The traditional method uses the average relations as such. Due to the consideration of the detailed nonuniform distributions of the capillary pressure head and the volumetric fluid contents in the pressure cell, the proposed method should be more accurate. Finally, it should be indicated that the capillary pressure head-volumetric nonwetting fluid content relation can be obtained by the relation between wetting and nonwetting fluid contents, i.e., $\theta_n = \theta_t - \theta_w(h_c)$, where θ_n ($L^3 L^{-3}$) is the local volumetric nonwetting fluid content and θ_t ($L^3 L^{-3}$) is the total volumetric fluid content.

SENSITIVITY ANALYSIS

To evaluate the inaccuracy of the standard procedure using pressure cells and to show the usefulness of the proposed procedure, a sensitivity analysis was performed. A reference (local) capillary pressure head-volumetric fluid content curve was obtained by fitting the Brooks-Corey expression through the local experimental data obtained during the displacement of water by trichloroethylene (Dane et al., 1992). The fitted Brooks-Corey parameters are $\lambda = 5.01$, $h_d = 10.0$ cm, $\theta_{wr} = 0.033$, and $\theta_{ws} = 0.270$. The ratio of the density of trichloroethylene (nonwetting fluid) to that of water (wetting fluid) is 1.456.

Dimensionless capillary pressure heads $H_c = h_c/h_d$ and $H_{av} = \bar{h}_c/h_d$ will be used in our analysis, because the use of dimensionless variables renders the analysis independent of the values of the displacement pressure head and height of the pressure cell. We will also limit our analysis to cases for $B < 0$ ($\rho_w < \rho_n$), because nonaqueous contaminants denser than groundwater play a much more important role in groundwater pollution than those lighter than groundwater (Domenico and Schwartz, 1990).

For $B = -0.5$ and $z_n = z_w = 0.5z_c$, the effects of the dimensionless height ($Z = z_c/h_d$) of the pressure cell on "measured" results by the standard procedure, calculated from Eq. [16], are shown in Fig. 2. As expected, the larger the value of Z , the bigger the disagreement between the "measured" curve and the local curve. For a given porous medium, the value of the displacement capillary pressure head is a measure of the interfacial tension between the fluids. The larger the radii of the biggest pores and the smaller the interfacial tension between the fluids, the smaller will be the displacement capillary pressure head, and subsequently the larger will be the values for the dimensionless height. This, in turn, will result in a greater error in the capillary pressure head-volumetric fluid content relation when the standard procedure is used.

For $B = -0.5$, $Z = 0.5$, and $z_n = 0.5z_c$, the effects of the difference between z_w and z_n on "measured" curves by the standard procedure, calculated from Eq. [16], are presented in Fig. 3. It is interesting to note that this difference has a significant effect on the "measured" curves and that, as one might expect, the smallest error is obtained for $z_n = z_w$. To evaluate the influence of the values of z_n on "measured" curves for $Z = 1$ and $z_n =$

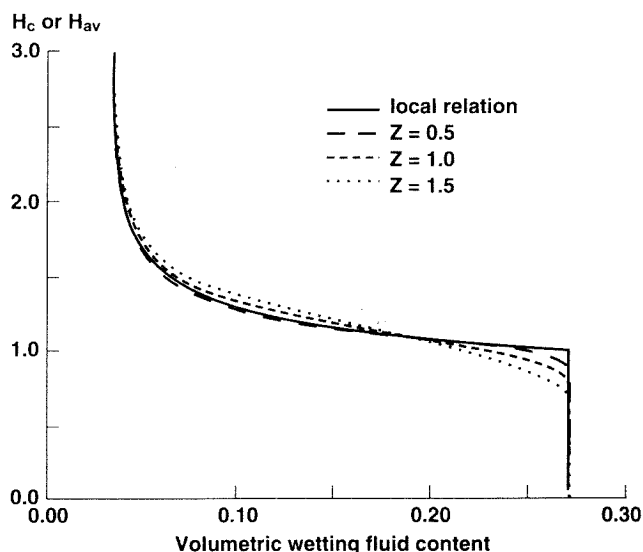


Fig. 2. Comparison between the local capillary pressure head-volumetric fluid content relation and "measured" relations for different values of relative pressure cell height $Z = z_c/h_d$. The "measured" values were calculated from Eq. [16] for a relative density difference of the fluids $B = -0.5$ and $z_w = z_n = 0.5z_c$, where z_w and z_n are the elevations at which the wetting and nonwetting fluid pressures, respectively, are measured; z_c is the height of the pressure cell; h_d is the displacement pressure head; and H_c and H_{av} are the relative local and "measured" capillary pressure heads, respectively.

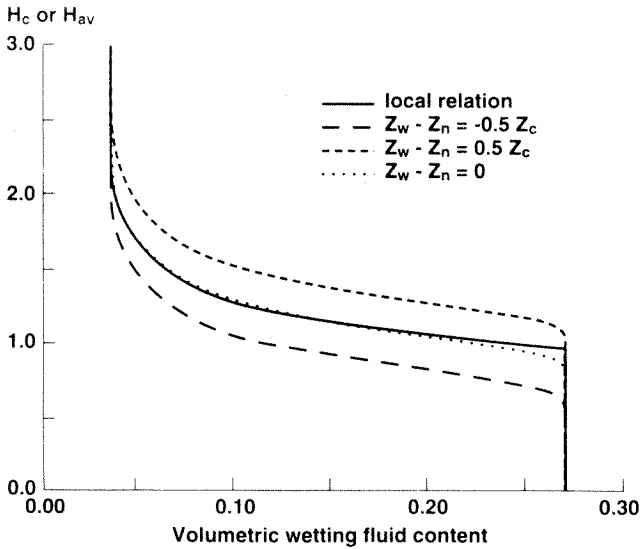


Fig. 3. Comparison between the local capillary pressure head-volumetric fluid content relation and the “measured” relations for different values of $z_w - z_n$. The “measured” values were calculated from Eq. [16] for a relative density difference $B = -0.5$, a relative pressure cell height $Z = 1$, and $z_n = 0.5z_c$, where z_w and z_n are the elevations at which the wetting and nonwetting fluid pressures, respectively, are measured and H_c and H_{av} are the relative local and “measured” capillary pressure heads, respectively.

z_w , three curves, calculated from Eq. [16] for different values of z_n , are plotted together with the local curve in Fig. 4. It is obvious that the best results are obtained for $z_n = 0.5z_c$. We, therefore, suggest that the capillary pressure head, determined in the middle of the pressure cell, be used for determining the capillary pressure head-volumetric fluid content relation if the standard procedure is used.

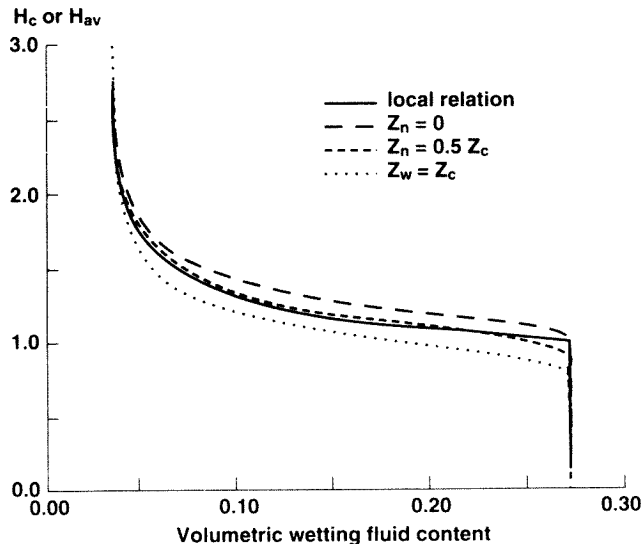


Fig. 4. Comparison between the local capillary pressure head-volumetric fluid content relation and the “measured” relations for different values of z_n . The “measured” values were calculated from Eq. [16] for a relative density difference $B = -0.5$, a relative pressure cell height $Z = 0.5$, and $z_w = z_n$, where z_w and z_n are the elevations at which the wetting and nonwetting fluid pressures, respectively, are measured and H_c and H_{av} are the relative local and “measured” capillary pressure heads, respectively.

For $z_w = z_n = 0.5z_c$ and $Z = 1$, the influence of B , representing the relative density difference of wetting and nonwetting fluids, on “measured” results is given in Fig. 5. As expected, smaller (more negative) B values result in larger “measuring” errors. On the other hand, when B is near zero, the “measured” curve is very close to the local one. In fact, if $B = 0$ and $z_n = z_w$, $A = 0$ and the “measured” curve is the same as the local one as shown by Eq. [6] and [12]. In other words, the standard procedure gives accurate capillary pressure head-volumetric fluid content relations only if $B = 0$ and $z_n = z_w$.

In summary, a number of factors, such as the pressure cell height, positions of the pressure measuring devices, which can coincide with the in- and outflow ports, and the relative density difference of the fluids, can give rise to considerable errors in the determination of capillary pressure head-volumetric fluid content relations by the standard procedure using pressure cells. Although possible errors can be minimized by using capillary pressure head values, determined at the middle of the pressure cell from Eq. [6], the application of Eq. [12], [14], or [16] should give superior results.

CONCLUSION

An improved computational method to determine capillary pressure head-volumetric fluid content relations for multiphase fluids using pressure cells has been proposed. In the proposed method, nonuniform distributions of both capillary pressure head and wetting fluid content, which contribute to the inaccurate determination of the capillary pressure head-volumetric fluid content relation by the standard procedure using pressure cells, were considered. The proposed method should be especially

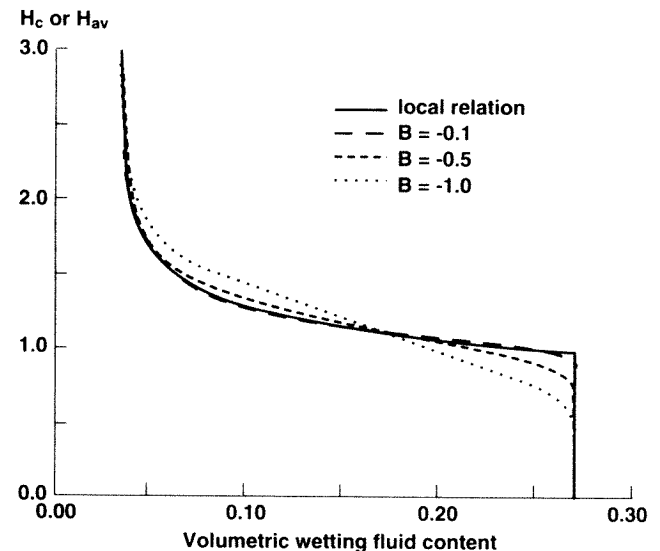


Fig. 5. Comparison between the local capillary pressure head-volumetric fluid content relation and “measured” relations for different values of B . The “measured” values were calculated from Eq. [16] for a relative pressure cell height $Z = 0.5$ and $z_w = z_n = 0.5z_c$, where z_w and z_n are the elevations at which the wetting and nonwetting fluid pressures, respectively, are measured and H_c and H_{av} are the relative local and “measured” capillary pressure heads, respectively.

useful for relatively coarse porous media containing fluids with relatively small interfacial tensions, because the nonuniformity of the fluid content distribution is more apparent in this case.

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