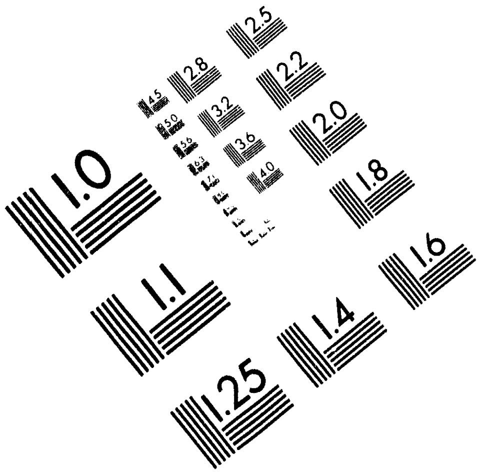

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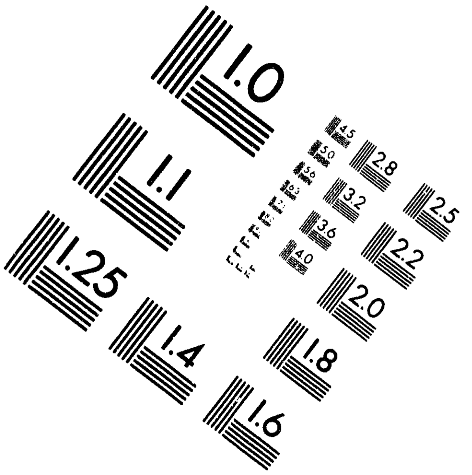

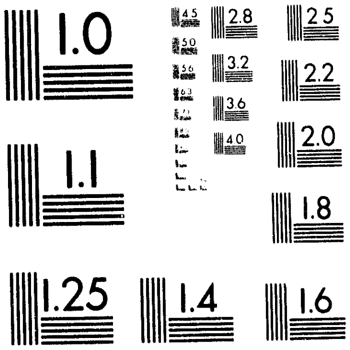

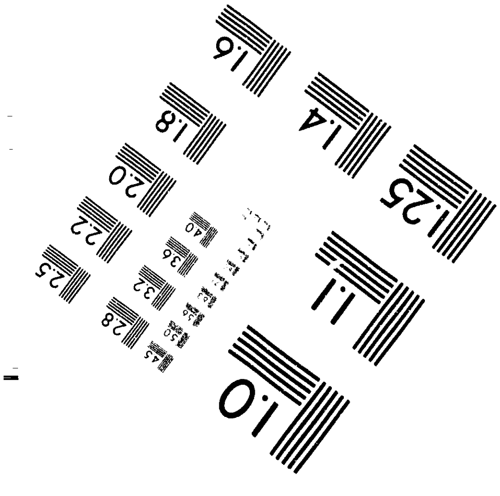

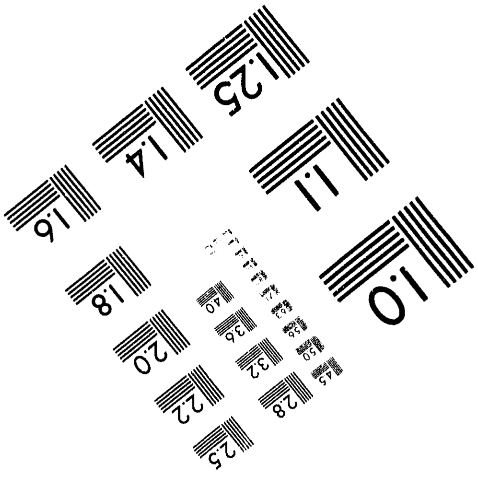

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SCALING FLUID CONTENT-PRESSURE RELATIONS OF DIFFERENT FLUID SYSTEMS IN POROUS MEDIA

R. J. Lenhard

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Pacific Northwest Laboratory
Richland, Washington 99352

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SCALING FLUID CONTENT-PRESSURE RELATIONS OF DIFFERENT FLUID SYSTEMS IN POROUS MEDIA

R. J. Lenhard[1]

ABSTRACT

Two-fluid-phase relations among fluid saturations (S) and pressures (P) have historically been used to predict S-P relations for three-fluid-phase systems consisting of a gas, nonaqueous phase liquid (NAPL), and water, because measurements of three-phase S-P relations are complex. Two-phase S-P relations of air-NAPL systems are generally used to predict the behavior between total-liquid saturations of three-phase systems and air-NAPL capillary pressures. Two-phase S-P relations of NAPL-water systems are generally used to predict the behavior between water saturations of three-phase systems and NAPL-water capillary pressures. Because S-P measurements are very time-consuming, investigators have attempted to scale S-P relations so that fewer measurements would be required. A S-P scaling technique is discussed in this paper, and methods to predict the scaling factors are evaluated.

INTRODUCTION

Relationships between fluid saturations (S) and pressures (P) are needed to predict the transient flow behavior of multiple fluids in porous media. Typically, these relations are measured in the laboratory using relatively small-volume samples, disturbed or undisturbed. However, some researchers have found limited success in predicting S-P relations of sandy porous media from their grain-size distributions [Arya and Paris, 1981; Mishra et al., 1989]. Because measurements of S-P relations can be very time-consuming,

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[1] P.O. Box 999, Pacific Northwest Laboratory, Richland, WA 99352

investigators have attempted to predict these relations from properties that can be measured more easily.

For two-fluid-phase systems (e.g., gas-liquid or liquid-liquid) in porous media, the measurement of S-P relations is relatively straightforward. Usually in the laboratory, a pressure difference between the fluid phases is imposed, and the fluid contents are allowed to adjust to this differential [Klute, 1986]. Measurement techniques commonly employ pressure cells or centrifuges to control fluid pressures and capillary barriers to control fluids exiting or entering the test samples. The fluid-phase pressure differential acting across the interfaces between immiscible fluids is called the capillary pressure of the fluid pair.

For three-fluid-phase systems (e.g., gas-liquid-liquid), the measurement of S-P relations is more complex. Three-phase S-P measurements have generally been conducted only for conditions where at least one fluid phase was assumed to be immobile. However, Lenhard and Parker [1988a] have measured S-P relations for a fluid system consisting of gas, nonaqueous phase liquid (NAPL), and water, using specially treated porous ceramics, for arbitrary conditions. Ferrand et al. [1990] and Dane et al. [1992] also measured S-P relations of air-NAPL-water systems, but they used dual-energy, gamma-radiation attenuation apparatuses.

Because of the difficulty in measuring S-P relations of gas-NAPL-water fluid systems, modelers have commonly employed two-fluid-phase S-P relations to predict three-fluid-phase behavior. However, very little experimental research has been conducted to evaluate the assumptions implicit in extending two-phase S-P measurements to predict fluid behavior in air-NAPL-water systems. The S-P relations of air-NAPL systems are typically used to predict S-P relations between total-liquid saturations and air-NAPL capillary pressures in air-NAPL-water systems, where total-liquid saturations are defined as the sum of the NAPL and water saturations. The S-P relations of NAPL-water systems are typically used to predict S-P relations between water saturations and NAPL-water capillary pressures in air-NAPL-water systems. For these predictions to be valid, the same NAPL must be used in both the two- and the three-phase measurements because the fluid properties need to be the same among all systems.

Therefore, S-P measurements for air-NAPL and NAPL-water systems are needed to predict fluid flow of air-NAPL-water systems in porous media, as would occur following a NAPL-contamination event. If one is also interested in modeling fluid flow prior to NAPL contamination or in regions of the subsurface not contaminated by NAPL, then S-P measurements of an air-water system are required as well. Thus, three sets of time-consuming S-P measurements are needed to model the movements of an NAPL through the subsurface as a result of a spill or leak in a storage facility.

Parker et al. [1987] recognized the need to reduce the effort to acquire the necessary S-P relations and the need to simplify parametrization of numerical multiphase flow codes and, therefore, proposed an empirical method to scale S-P relations of arbitrary fluid systems. In their technique, the product of a fluid-system-dependent scaling factor and the appropriate capillary pressure is used to predict fluid contents. The scaling format for two-fluid systems consisting of nonwetting fluid (i) and wetting fluid (j) is

$$\mathbf{S}_j(\beta_{ij} h_{ij}) = \mathbf{S}^*(h^*) \qquad (1)$$

in which $\mathbf{S}_j = (S_j - S_m)/(1 - S_m)$ is the effective wetting-fluid phase saturation, S_j is the actual wetting-fluid phase saturation, S_m is a minimum (also termed an irreducible or residual) actual wetting-phase saturation, β_{ij} is the fluid-system-dependent scaling factor, h_{ij} is the capillary-pressure head between fluid phases i and j (i.e., $h_{ij} = h_i - h_j$), and $\mathbf{S}^*(h^*)$ are the scaled S-P relations for a porous medium. (Notice that the boldface S symbols refer to scaled saturations; the non-boldface S symbols refer to actual saturations.)

A reference fluid system is needed to define the parameters of $\mathbf{S}^*(h^*)$ to avoid problems of uniqueness. The choice of a reference system is arbitrary, but it is practical to use an air-water system as the reference because air-water S-P measurements are commonly conducted, and investigators need not to be subjected to hazardous chemicals. Therefore, Parker et al. [1987] defined β_{aw} as 1, and all other fluid systems are scaled to S-P relations of a two-phase air-water system. (The subscripts a and w refer to air and water, respectively.)

Using this scaling approach, which is only applicable to fluid-porous medium systems in which the fluids do not affect the pore sizes, the number of parameters required to define air-water, air-NAPL, and NAPL-water S-P relations is significantly reduced. For example, using two-parameter S-P functions, such as the van Genuchten [1980] or Brooks and Corey [1964] retention functions, six parameters would be needed to define the set of three two-phase S-P relations. If the above scaling format is used, only four parameters are required, i.e., the two retention parameters and two scaling factors, β_{ao} and β_{ow}. (The subscript o refers to NAPL.)

Air-NAPL-water S-P relations can be predicted via (1), by extending the two-phase S-P relations. Assuming that the water saturation in a three-phase system is a function of the NAPL-water capillary-pressure head, and that the total-liquid saturation is a function of the air-NAPL capillary-pressure head, three-phase S-P relations can be predicted from

$$S_w(\beta_{ow} h_{ow}) = S^*(h^*) \tag{2}$$

$$S_{tl}(\beta_{ao} h_{ao}) = S^*(h^*) \tag{3}$$

in which S_w and S_{tl} are effective water and total-liquid saturations defined analogously to those in (1). The NAPL-water and air-NAPL scaling factors (i.e., β_{ow} and β_{ao}, respectively) are the same as those defined for two-phase systems. They were initially intended by Parker et al. [1987] to be empirical; however, Lenhard and Parker [1987] later suggested that they can be estimated from ratios of interfacial tensions according to

$$\beta_{ij} = \sigma^* / \sigma_{ij} \tag{4}$$

in which σ^* is the interfacial tension of the reference fluid system and σ_{ij} is the interfacial tension of the fluid system being scaled. Using this approach, Lenhard and Parker [1987] found good agreement between scaling factors estimated from measured interfacial tensions and those determined via regression analyses of S-P relations. Scaling two-phase S-P relations by a ratio of interfacial tensions has also been employed in petroleum reservoir engineering [Amyx et al., 1960]. Research by other petroleum engineers using sandstone and limestone cores has suggested that S-P scaling factors depend on porous-medium properties as well as fluid properties.

The focus of this paper is to discuss methods for determining the scaling factors, β_{ao} and β_{ow}. This will be accomplished by considering relations that must be obeyed to predict a smooth transition in fluid contents as a two-phase air-water system becomes a three-phase air-NAPL-water system. Data from two-phase air-water, air-NAPL, and NAPL-water S-P measurements will be scaled to determine best-fit scaling factors via a least-squares regression algorithm. The best-fit β_{ao} and β_{ow} will be compared to those from the prediction methodologies to investigate the best approach to predict the scaling factors.

DISCUSSION

The estimation of β_{ao} and β_{ow} is more complicated than originally suggested by Lenhard and Parker [1987], particularly if the factors are to be used in multiphase flow codes to predict NAPL migration through the subsurface. Originally, Lenhard and Parker [1987] suggested that the scaling factors should be estimated in accordance with (4), where σ^* is the uncontaminated, air-water interfacial tension (i.e., $\sigma_{aw} = 0.072$ N m^{-1}). When they evaluated this estimation approach, they noted that closer agreement with the scaling factors determined via regression analyses of the S-P data was obtained when they employed measured interfacial tensions rather than handbook values for pure fluids and when σ^* was assumed to be the measured air-water interfacial tension after the aqueous phase was brought in contact with the NAPL. In a later amendment [Lenhard and Parker, 1988b], they concluded that σ^* should be the uncontaminated air-water interfacial tension (σ_{aw}) and not a contaminated air-water interfacial tension such as occurs when the aqueous phase has dissolved organic chemicals on its interface with the gaseous phase. They defined the contaminated air-water interface as σ'_{aw}. They noted, however, that at local phase equilibrium in air-NAPL-water systems, water and air will be saturated with organic components, and scaling factors will be related by

$$\frac{1}{\beta_{ao}} + \frac{1}{\beta_{ow}} = \frac{1}{\beta'_{aw}} \qquad (5)$$

in which $\beta'_{aw} = \sigma_{aw}/\sigma'_{aw}$. From scaling factor definitions given by (4) and from (5), the relationship among the interfacial tensions can be derived as

$$\sigma_{ao} + \sigma_{ow} = \sigma'_{aw} \qquad (6)$$

When the scaling factors are estimated according to (4), and (6) holds as well, there will be no point where three-phase S-P relations and two-phase air-water relations coincide. Therefore, there will be a discontinuity in water contents as the fluid system changes from a two- to a three-phase system. This behavior is shown in Figure 1, where two-phase water contents and three-phase water and total-liquid contents are plotted as a function of elevation above a NAPL-water interface in a monitoring well using theory and equations reported by Lenhard and Parker [1990]. In Figure 1, a three-phase fluid system is predicted to extend to approximately 40 cm above the NAPL-water interface in the monitoring well. Therefore, above this elevation, S-P relations for an air-water system are shown as the thick solid line; below this elevation, S-P relations for an air-NAPL-water system are also shown as thick solid lines. Notice the discontinuity in predicted fluid contents at the elevation where the fluid system changes from a two- to a three-phase system.

When the relationships among the scaling factors are such that

$$\frac{1}{\beta_{ao}} + \frac{1}{\beta_{ow}} = \frac{1}{\beta_{aw}} \qquad (7)$$

where $\beta_{aw} = 1$, the predicted fluid contents corresponding to the same conditions in Figure 1 are shown in Figure 2. In this figure, there is a point where three-phase S-P relations and two-phase air-water relations coincide. Hence, there is no discontinuity in water or total-liquid contents with elevation or capillary-pressure heads.

Figure 1. Predicted water contents ($S_W{}^{aw}$) of an air-water fluid system and predicted water (S_W) and total-liquid (S_{tl}) contents of an air-NAPL-water system as a function of elevation above the NAPL-water interface measured in a monitoring well using theory reported by Lenhard and Parker [1990] when the scaling factors conform to equation (5).

This smooth behavior in predicted fluid contents as the fluid system changes from a two- to a three-phase system is important when predicting transient multiphase flow with numerical codes. If there is a discontinuity in fluid contents with pressure, as is shown in Figure 1, then convergence may be difficult to achieve for nodes that are changing from an air-water to an air-NAPL-water system. Therefore, the scaling factors that are used in numerical codes should predict the phase behavior shown in Figure 2, i.e., a smooth transition of fluid contents as the fluid system changes from a two- to a three-phase system and vice versa. A methodology must be developed that estimates the scaling factors from properties that are more readily measured than S-P relations, but that does not yield discontinuities in fluid contents when fluid systems change.

Figure 2. Predicted water contents ($S_w{}^{aw}$) of an air-water fluid system and predicted water (S_w) and total-liquid (S_{tl}) contents of an air-NAPL-water system as a function of elevation above the NAPL-water interface measured in a monitoring well using theory reported by Lenhard and Parker [1990] when the scaling factors conform to equation (7).

To investigate a methodology for estimating the scaling factors, two-phase air-water, air-NAPL, and NAPL-water and three-phase S-P relations will be examined. In Figure 3, measured S-P relations are shown for two-phase air-water, air-NAPL, and NAPL-water systems, using the same sandy porous medium packed to an identical bulk density for the different fluid-system measurements. The NAPL is

Soltrol 220®, which is a mixture of branched alkanes having low solubility in water and a liquid density of 0.80 Mg m^{-3}; the aqueous phase is distilled water. The air-NAPL and NAPL-water interfacial tensions are 0.026 and 0.036 N m^{-1}, respectively, and reflect prolonged contact between the NAPL and aqueous phases. The symbols in Figure 3 are measured data, and the solid lines connect successive measurements. In Figure 4, scaled S-P relations are shown, where the scaling factors were determined via regression analyses using (1). The best-fit β_{ao} was 2.48, and the best-fit β_{ow} was 1.82. The solid line represents $S^*(h^*)$ using the van Genuchten [1980] retention function.

Figure 3. S-P relations of air-water, air-NAPL, and NAPL-water systems as a function of air-water, air-NAPL, and NAPL-water capillary-pressure heads, respectively, in a sandy porous medium.

Figure 4. Two-phase air-water, air-NAPL, and NAPL-water S-P relations of the data shown in Figure 3 that are scaled by using equation (1).

One approach to predicting the scaling factors, Method 1, is to use (4) where $\sigma^* = 0.072$ N m^{-1} (i.e., the uncontaminated handbook value for the air-water iterfacial tension). The resulting β_{ao} and β_{ow} are 2.77 and 2.00, respectively. Using these values to predict three-phase water and total-liquid contents would yield a discontinuity in fluid contents as the fluid system changes from a two- to a three-phase system, similar to that shown in Figure 1, because (7) is not obeyed. Although the predicted values could be considered to approximate the best-fit values, using them in numerical fluid flow codes may be problematic. Another approach, Method 2, is to use (4) to estimate the scaling factors, but assume that $\sigma^* = \sigma_{ao} + \sigma_{ow}$. The resulting β_{ao} and β_{ow} for Method 2 are 2.38 and 1.72, respectively. Using these values to predict three-phase water and total-liquid contents would yield a smooth transition as fluid systems changed from a two- to a three-phase system because (7) is obeyed.

In a recent investigation, White and Lenhard [1993] used Method 2 to predict three-phase S-P relations from knowledge of air-water S-P relations and measurements of air-NAPL and NAPL-water interfacial tensions. The predicted scaling factors were used in a numerical simulation of a fluctuating water-table experiment involving a NAPL. The agreement between the measured water and NAPL contents and those predicted was close, giving credibility to the Method 2 approach.

Further research is needed to assess how interfacial tensions and, hence, scaling factors change as a two-phase air-water system becomes a three-phase system and vice versa. It is unlikely that there should be a discontinuity in fluid contents when fluid systems change. It is more likely that a thin film of NAPL may form on water surfaces before pores spaces become filled with NAPL, particularly for spreading NAPLs. Hence, the definition of a three-phase system may be somewhat arbitrary. Furthermore, it is expected that as film thicknesses increase, the air-water interfacial tension will be affected. Quantifying these changes will be a challenging research endeavor. In future modeling efforts, it may be necessary to modify the air-water interfacial tension for nearest-neighbor nodes of a three-phase system to provide for a smoother transition from an air-water system to a three-phase system. Additional research is also needed to assess S-P relations likely to result after the NAPL content becomes negligible, i.e., as a three-phase system transitions to a two-phase air-water system.

CONCLUSIONS

A methodology is needed to predict S-P relations of air-NAPL-water systems from S-P relations of air-water systems and easily measured fluid properties. The predicted relations should allow for smooth transitions in fluid contents as a two-phase air-water system becomes a three-phase air-NAPL-water system and vice versa. A methodology is proposed in which the scaling factors can be used to predict water and total-liquid contents of three-phase systems. The approach assumes that the reference interfacial tension, which is used in determining the scaling factors, is set equal to the sum of the air-NAPL and NAPL-water interfacial tensions. This approach provides for a smooth transition in fluid contents as a two-phase air-water system becomes a three-phase air-NAPL-water system, so that numerical convergence problems can be minimized when simulating the migration of NAPL through porous media. It is likely that further refinement will be needed as additional S-P studies are completed; the physical and chemical processes occurring when NAPLs imbibe in porous media are not well understood.

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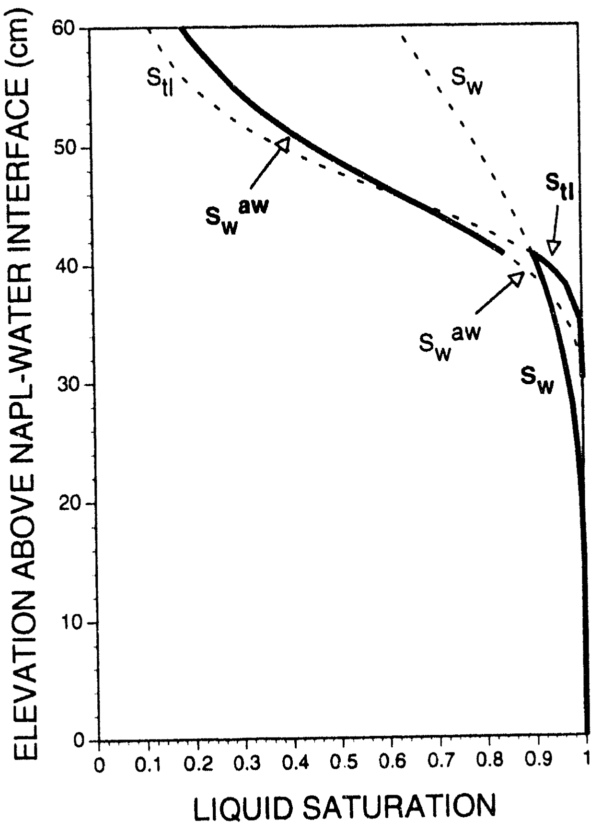
ELEVATION ABOVE NAPL-WATER INTERFACE (cm)
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LIQUID SATURATION
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Fig 1

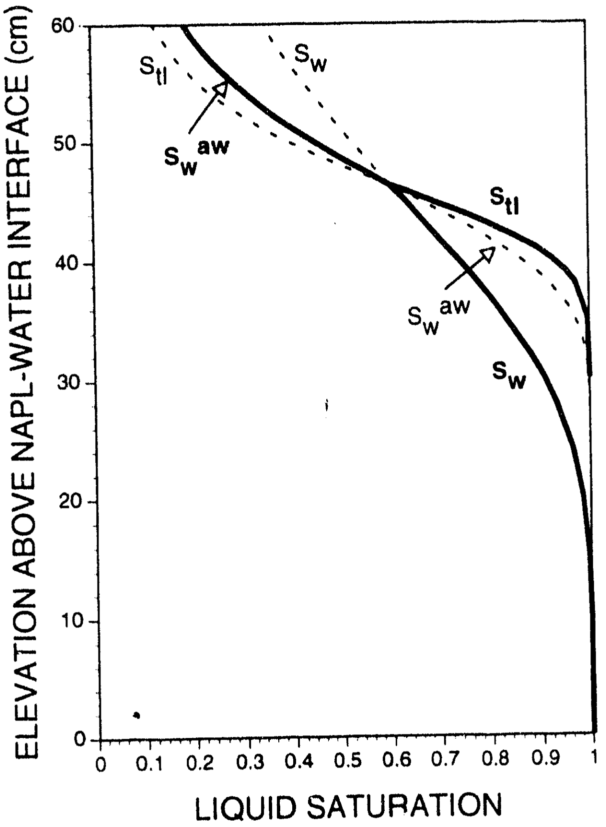
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Fig 2

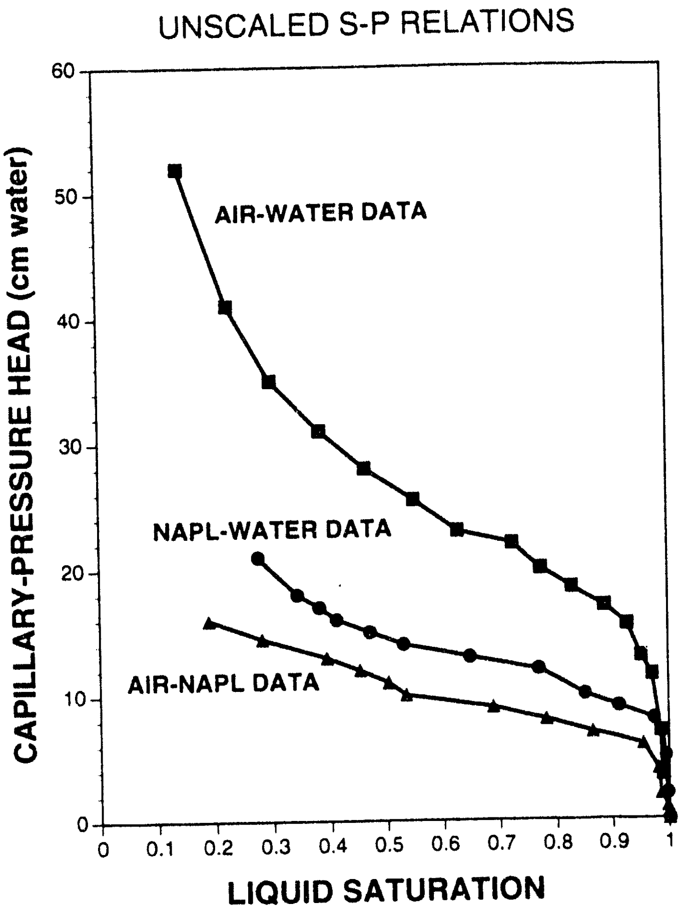
UNSCALED S-P RELATIONS
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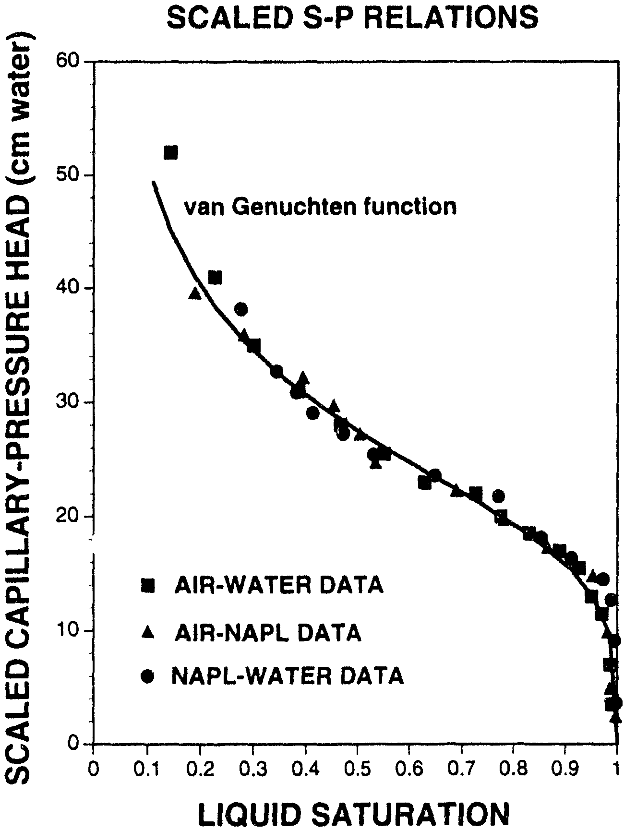
Fig 3


SCALED S-P RELATIONS
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LIQUID SATURATION
van Genuchten function
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▲ AIR-NAPL DATA
● NAPL-WATER DATA

Fig 4

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