Incorporating Low Hydraulic Conductivity in a Numerical Model for Predicting Air−Water Interfacial Area in Wet Unsaturated Particulate Porous Media

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A numerical model to calculate the air−water interfacial area in wet unsaturated particulate systems is modified to take account of the low hydraulic conductivity experienced by real systems at low relative water saturations. The original model is based on simulated annealing and random swapping of air and water elements in the system to achieve a global energy minimum. In the modified model a limitation is placed on the separation distance between swapped elements. The modified model represents real systems well at low water saturations but is actually inferior to the original model at high water saturations. This fact suggests a transition in system behavior at intermediate saturations that is not accounted for by the calculated hydraulic conductivities. The role of hydraulic conductivity in achieving system equilibrium is discussed.

Introduction

The quantity of air−water interfacial area present in wet unsaturated porous media is important in that it determines how the particle assembly is held together, as well as two-phase mass transfer and fluid flow properties that exist within the system. Because of this importance, beginning in 1940 various researchers[1−5] have developed models from which this area could be calculated. However, because no experimental method for measuring interfacial area in such systems was available, model predictions could not be tested. This situation changed in 1996 when Karkare and Fort[6] published the first experimental means for determining air−water interfacial areas in wet unsaturated porous media. A second, complementary technique has subsequently been published.[7]

Availability of a means of measuring air−water interfacial areas made it possible to evaluate model predictions. In a prior manuscript[8] we report results of tests in which areas calculated from models are compared with experimental determinations made on real systems. Most of the models make reasonable predictions of air−water interfacial areas at high water saturations. However, they do not simulate real systems well at low water saturations. Experimental data yield higher areas in this saturation range than the models predict. This fact led us to develop a new numerical model[8] which, we hoped, would better represent real system behavior. The simulations involved rearranging air and water elements in the system to minimize the total interfacial energy[9] through an optimization technique called simulated annealing.[10,11] Unfortunately, our new model also yielded inaccurate interfacial areas at low water saturations.

This result implies that there is a difference in the way the systems behave at high water saturations and at low water saturations. Models based on fundamental thermodynamics should work at all water saturations if it were always possible for the system to reach a global minimum energy. The fact that they do not implies that global energy minimization does not occur at low system saturations. This means that at these conditions the driving force for water movement must be less than the energy barrier to achieve this movement. Such an energy barrier could explain the reduced hydraulic conductivity observed in low water saturation real systems, and also, the observation that the areas predicted by thermodynamic models at low water contents are lower than the areas determined from experiments on real systems.

In this paper, we modify our numerical model[8] to represent the effects of reduced hydraulic conductivity on air−water interfacial areas in these systems. The modifications are made by translating physical and theoretical considerations into terms that may be approximated by the model system. At no point are the values of parameters fed to the model altered to make model predictions fit experimental data.

Modifications to Algorithm for Modeling Drainage

The model was modified by restricting the distance over which an annealing swap may be made. Then, instead of water and air elements, freely swapping across any distance, swaps are restricted to elements within a fixed distance from one another. To accomplish such a swap, the water element in the swap is selected first. Then, a randomly chosen distance less than or equal to the maximum move distance is selected for each of the possible

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directions of movement (2 in two dimensions and 3 in three dimensions). A move direction is chosen. The element in the position indicated by these random parameters is checked to see if it contains air. If it does, the move is evaluated as done in previous versions of the model. If it does not, another move is selected for the same water element. If no acceptable move can be found after some fixed number of attempts, another water element is selected as a candidate for swapping.

If a model limits the water movement, the "history" of the fluid and hysteresis effects become important. Previously, the saturation of the system was established by randomly converting a fixed number of air elements to water elements. A combination of an unrestricted swap distance with random movement at high annealing temperatures ensured that the distribution of water within the system was near the global energy minimum. However, if move distance is restricted, the initial placement of water becomes important because it is possible that water will not move a significant distance from its initial position. Because we know real systems experience hysteresis, this side effect contributes to the realism of the model simulation.

In this work, a reproducible initial condition is established by completely saturating the system initially and then removing or draining water until the desired final saturation of the system is achieved. To simulate drainage in the model, the bottom edge of the model space is treated as "free water" or as an exit plane. When the fluid content is above the desired saturation, any proposed air−water swaps that would take a water element out of the model space result in that water element being removed from the system. This approach results in some hysteresis because the path followed in draining the system plays a significant role in determining final fluid configuration. The target saturation of the system is reached before the first iteration is allowed to complete. The simulation continues until no change in the system configuration occurrs.

Preliminary Simulations

The first obvious question is "what distance" is appropriate. As a preliminary step to determining the answer, a series of two-dimensional simulations were performed on a set of two-dimensional polydisperse randomly packed circles. This system had a total dimension of about 475−500 elements and an average particle diameter of 20 elements. Complete simulations were conducted with the distance of the move varying from 1 element to 15 elements. Air−water interfacial area (length) curves for each set of simulations are presented in Figure 1. An additional curve is presented in that figure to show the difference in areas (lengths) which result from saturating the system initially and using the original random distribution method. The number of swaps evaluated during the first iteration had to be extended in some cases to establish the correct target saturation. If the number of swaps was the same as normally considered in a single iteration, the saturation was only reduced to about 60% at best.

Figure 1 shows that restricting the move has the expected effect of increasing the area as the move distance decreases. The effect is more pronounced as saturation increases, which was unexpected. The reason will be explained shortly.

Because it is possible to adjust the predicted air−water interfacial area curve by restricting move distances, it would be easy to keep adjusting these distances to make

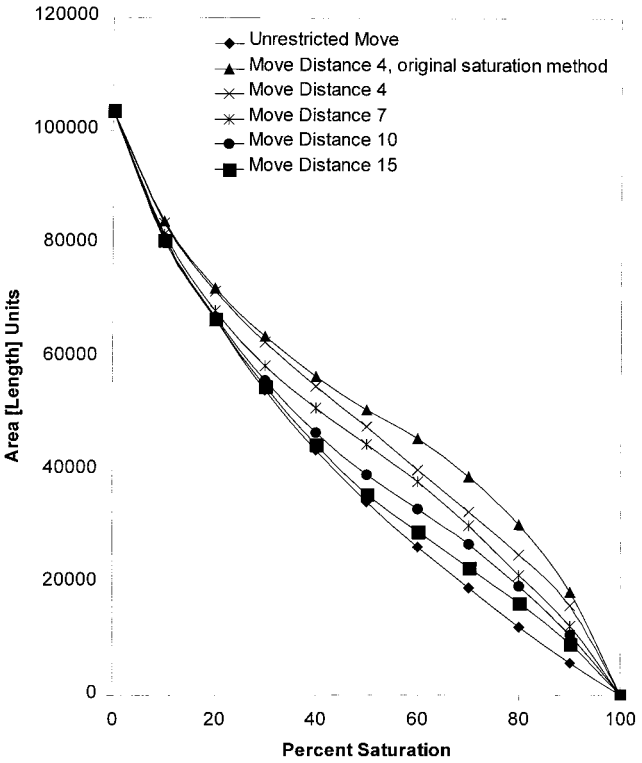

Figure 1. Plot of the effect of swapping distance on air−water interfacial area curves for a two-dimensional polydisperse randomly packed system.

the areas calculated from the model match experimental data at low water contents and to use the previous method at high water contents. However, doing so would not move us closer to our goal of providing a method to predict air−water interfacial areas using only readily measurable system parameters, such as particle size distribution or capillary pressure. To continue toward that goal, we reflect on the concepts upon which these model modifications are based.

The role of the restricted move distance is to more accurately represent the mobility of the water. When saturation is high, water mobility should be high. When saturation is low, water mobility should be low. Mobility changes as a function of saturation are not reflected if the move distance is fixed at all saturations as in Figure 1. Remember that only the elements within the move distance of an air element will swap. Hence, for example, two air pockets can exist where one would be preferred simply because a small move distance does not allow water which is clearly mobile to unite the air pockets. This is the cause of the increased effect of move distance at high saturations seen in Figure 1. So there are two problems that must be resolved using nonempirical methods: (1) the allowable distance of the restricted move must be determined and (2) the move must account for the mobility of the fluid as a function of total water content.

Both problems may be solved by application of a parameter calculated from the hydraulic conductivity of the system on which the model system is based. Clearly, it is undesirable to measure the hydraulic conductivity for every system of interest. There exist, however, methods of estimating hydraulic conductivity based on the capillary pressure of the system. Capillary pressure may easily be measured by automated methods and has been measured for every system for which we have measured interfacial areas.

In a near-saturated system, all of the water is interconnected and mobile. Every portion of the system can affect

every other. In a nearly dry system, mobility approaches zero. Activity in one section of the system will likely not affect any other. If the move distance in the simulated system at saturation is taken to be large enough so that any swap is possible, such as the characteristic length of the model system (the largest of the number of rows, columns, or layers in the system), the effect of high hydraulic conductivity is represented. Similarly, a minimal swap distance of 1 embodies the lack of hydraulic conductivity in the dry system. When hydraulic conductivity is used as a function of saturation obtained from capillary pressure data, the move distance can be varied as a function of saturation for a series of simulations. Such variation not only is a reasonable method for determining the restricted move distance but also reflects the differences in systems at different saturations.

Modeling Real Systems

To allow for meaningful comparison with the air−water interfacial area measurements and predictions reported earlier,[8] the three-dimensional system based on a collection of 20−106-μm glass beads was selected for a series of simulations. Computational constraints allowed for only one series to be completed a single time because the added calculations required significant additional time compared to that of previous simulations of the same system.

The method for calculating hydraulic conductivity from capillary pressure data of Jackson[12] was followed, using

$$K_i = K_s(S_{w_i})^c \sum_{j=i}^{m}[(2j + 1 - 2i)P_{c_j}^{-2}]/\sum_{1}^{m}[(2j - 1)P_{c_j}^{-2}]$$

The calculated values of conductivity were divided by the maximum calculated value of conductivity to determine the relative hydraulic conductivity as a function of water contents shown in Figure 2. The curve was then fit to a function of the form $y = ae^{bx}$, where a and b are constants. The simulation determined the maximum move distance as a function of the desired saturation by multiplying the characteristic length of the cubic array (in elements) by the relative hydraulic conductivity. The simulation initially saturated the system and then adjusted the saturation during the first iteration as described previously, using the maximum move distance for the target saturation.

The air−water interfacial areas predicted for this system by our original and modified models are compared with experimental areas in Figure 3. Areas calculated from the modified model check experimental areas at low and intermediate water contents well. This is the first modeling effort for air−water interfacial area that has achieved this result. The success of this simulation led to a series of simulations representing a set of 75−90-μm diameter glass beads modeled by a set of monodisperse randomly packed spheres. The air−water interfacial area curve for the system is presented in Figure 4. The shape of the curve again gives hope that this method will give accurate predictions of air−water interfacial area, though the model does miss the high water content points.

Discussion

The modified simulated annealing model appears to predict air−water interfacial areas for low water content systems better than any other method currently available. It does not do as well for high water content systems where its predictions are actually inferior to the original simulated annealing model. Figure 3 shows that areas at 30%, 40%, and 60% saturations are well-represented by the modified model while the area at 70% saturation is not. Figure 4 shows that the areas at 30% and 40% saturation are well-represented by the modified model while areas at 50%, 60%, and 70% saturation are not. These facts suggest a transition in the character of water redistribution somewhere between 60% and 70% saturation for the 20−106-μm diameter system and between 40% and 50% saturation for the 75−90-μm diameter system.

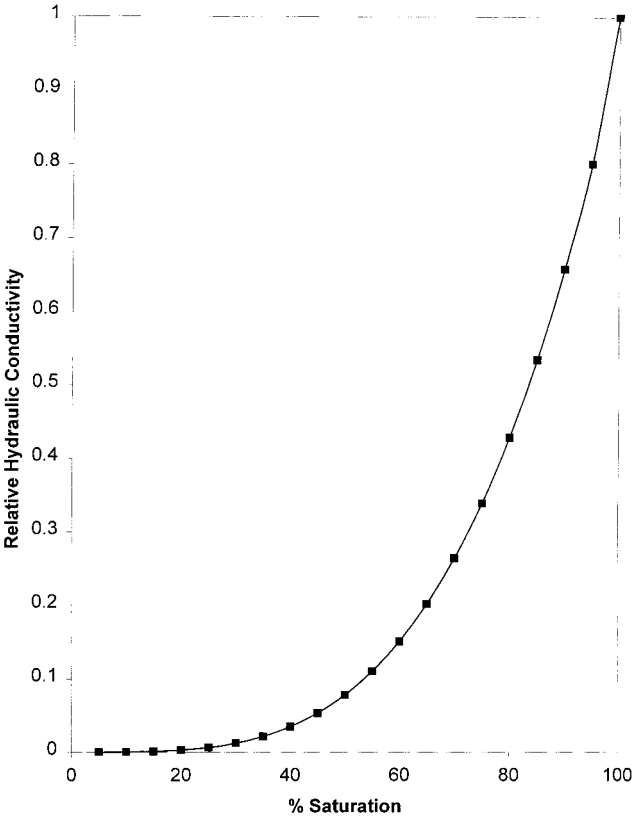

Figure 2. Relative hydraulic conductivity calculated by the method of Jackson[12] for a system of 20−106-μm micrometer diameter glass beads.

These results lead us to question the method we used to calculate the relative hydraulic conductivity of these systems. In particular, this method shows a smooth curve with ever-increasing slope when hydraulic conductivity is plotted vs percentage of saturation. No transitions, or hysteresis effects, are indicated. The method used to calculate hydraulic conductivities requires only porosities and capillary pressures as input variables. It is possible that these quantities are insufficient to calculate relative hydraulic conductivities for our systems. Others[13] have critiqued weaknesses of this calculation method. Additionally, the high porosities of the model systems used in these simulations, as noted in our previous paper,[8] may contribute to the failure of the modified model at high saturations.

Conclusions

Our previously published numerical simulated annealing model to calculate air−water interfacial areas in wet unsaturated systems has been modified to better simulate limited water movement in low-percentage saturation systems. The extent of movement limitation is determined

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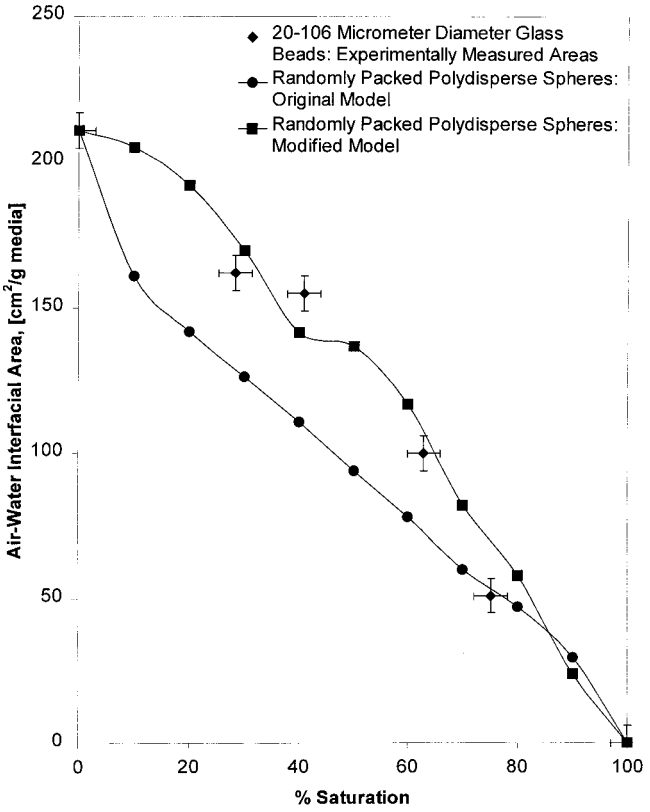

Figure 3. Predicted air−water interfacial areas for the original and modified annealing models and experimentally measured air−water interfacial areas for a system of 20−106-μm diameter glass beads. The model space used for the annealing model was a randomly packed array of spheres with a particle size distribution closely matching the distribution of the experimental system.

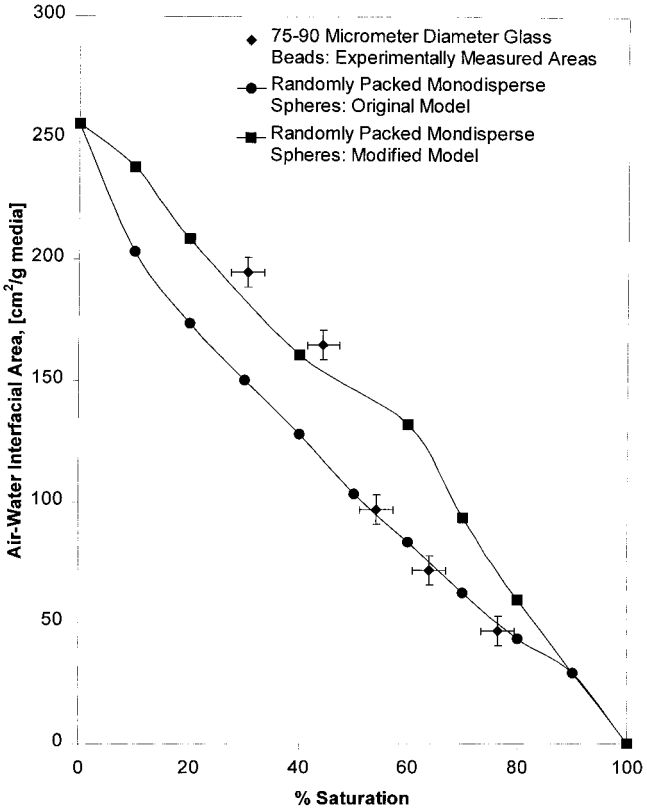

Figure 4. Predicted air−water interfacial areas for the original and modified annealing model and experimentally measured areas for a system of 75−90 μm diameter glass beads. The model space used for the annealing model was a randomly packed array of spheres of a single diameter.

from relative hydraulic conductivity, which is calculated from porosity and capillary pressure data. The modified model describes low water content systems well. It fails at high water contents where an unmodified simulated annealing model better represents the real system. A transition in behavior between high and low water contents is indicated. Future work will include obtaining experimental values for hydraulic conductivity for these systems to determine the applicability of the method by which conductivity was calculated and improving the model space representation of real systems by increasing packing density.

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