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6815

Application of Graph Theory to the Simulation of Percolation and Unsaturated Flows in Reservoir Rocks and Heterogeneous Vadose Zones

G. Yang, N. G. W. Cook, and L. R. Myer

The underground migration of contaminants is determined directly by the porosity and permeability of rock matrix to water and air. In principle, the necessary constitutive relationships can be obtained from laboratory measurements of capillary pressure and relative permeability data, both as a function of saturation, for each lithologic unit. Such an empirical approach is impracticable and uneconomic. Furthermore, such constitutive relationships are, in fact, only averages of these properties at the scale of the measurements. Heterogeneity, at all scales from pores to aquifers, frequently renders calculations based on homogeneous average properties inexact and inadequate. An understanding of the relationships between these properties and the microgeometry and topology at the pore level would go far toward alleviating these problems.

A variety of conceptual models ranging from bundles of capillary tubes to percolation theory, have been invoked to analyze and understand these complex relationships. Although the contributions of these models cannot be overemphasized, their weaknesses should not be ignored. We have recently conducted one-dimensional, nonwetting-phase invasion experiments on cores of Berea sandstone using Wood's metal. These experiments revealed the surprising result that "preferred paths" of best-interconnected pores and throats dominate breakthrough, relative permeability, and electrical resistivity. The concept of "preferred paths" on a different scale has become topical in hydrology of vadose zone, which is the major concerning zone in groundwater pollution.

The objectives of this study are to obtain a much better understanding than currently existing micronetwork models provide of unsaturated flow through heterogeneous porous materials and of the relationship between the material properties and the geometry or topology of the pore space. These objectives can be attained through numerical experiments on irregular networks, with different stochastic and spatially correlated properties, representing the geometry and interconnectedness of the pore space using the techniques of network analysis and graph theory. We expect that this will lead to a fundamentally different and more useful understanding of two-phase flow in porous media. Such an understanding is needed to improve our ability to determine those characteristics of such media important to contaminant migrations from a variety of different measurements. These concepts can also enable us to provide more realistic models for the analysis of two-phase flow; i.e., models that recognize the intrinsically heterogeneous and stochastic nature of the pore space.

To analyze the "preferred path" phenomenon and its relationship to pore geometry and interconnectedness, we have developed a numerical simulation program based on an irregular, two-dimensional, stochastic, and spatially correlated network. We analyze the behavior of this network using network techniques and graph theories. The analyses have revealed (1) the effects of stochastic and spatially correlated properties of the pore space on wetting or nonwetting-phase breakthrough, invasion, imbibition, draining, and trapping and (2) the influence of viscous, capillary, and gravity forces and micropermeability. A hierarchical method is used to find the path with largest minimum throat diameter or largest "bottleneck." Individual elements are placed into the network in decreasing order of throat diameter until a percolating path is formed. This is the critical path along which the first breakthrough takes place with the minimum capillary pressure. Although it is highly conductive, it is not necessarily the most conductive path. To find the preferred path of greatest conductance, several "priority first search" (Sedgewick, 1990) techniques have been used. To simulate the imbibition and drainage process, we used a priority queue structure according to which all connected neighbors are queued in the order of their diameters. The searching methods are employed to identify preferred paths for irregular networks with both near-uniform and highly skewed distributions of throat diameters, with or without spatial correlation. The results show that preferred paths become increasingly dominant as the throat diameters become more spatially correlated.

We compared the strongly spatially correlated networks with homogeneous ones in various probabilistic distributions. The simulation results show that the preferential pattern is the dominating feature in the spatially correlated network (Figure 1). For the homogeneous network, the patterns of preferred path might be seen if the throat diameters are distributed over a wide range. If the diameter distribution is narrowed down to a small range, the invasion will have basically a uniform front. For the invasion simulation, it can be seen that the computer results resemble the basic features of the lab experiment by Agrawal et al. (1991). For the imbibition and drainage simulation, the results can also be verified by Schlueter's experiments using wax as wetting fluid (Schlueter et al., 1992). Schlueter discovered that, under a microscope, most of the small voids are seen to be filled with wax, but some large voids are coated with wax. It is evident that the wax flows through the large diameters as preferred paths but is sucked into smaller diameters because smaller throats have larger

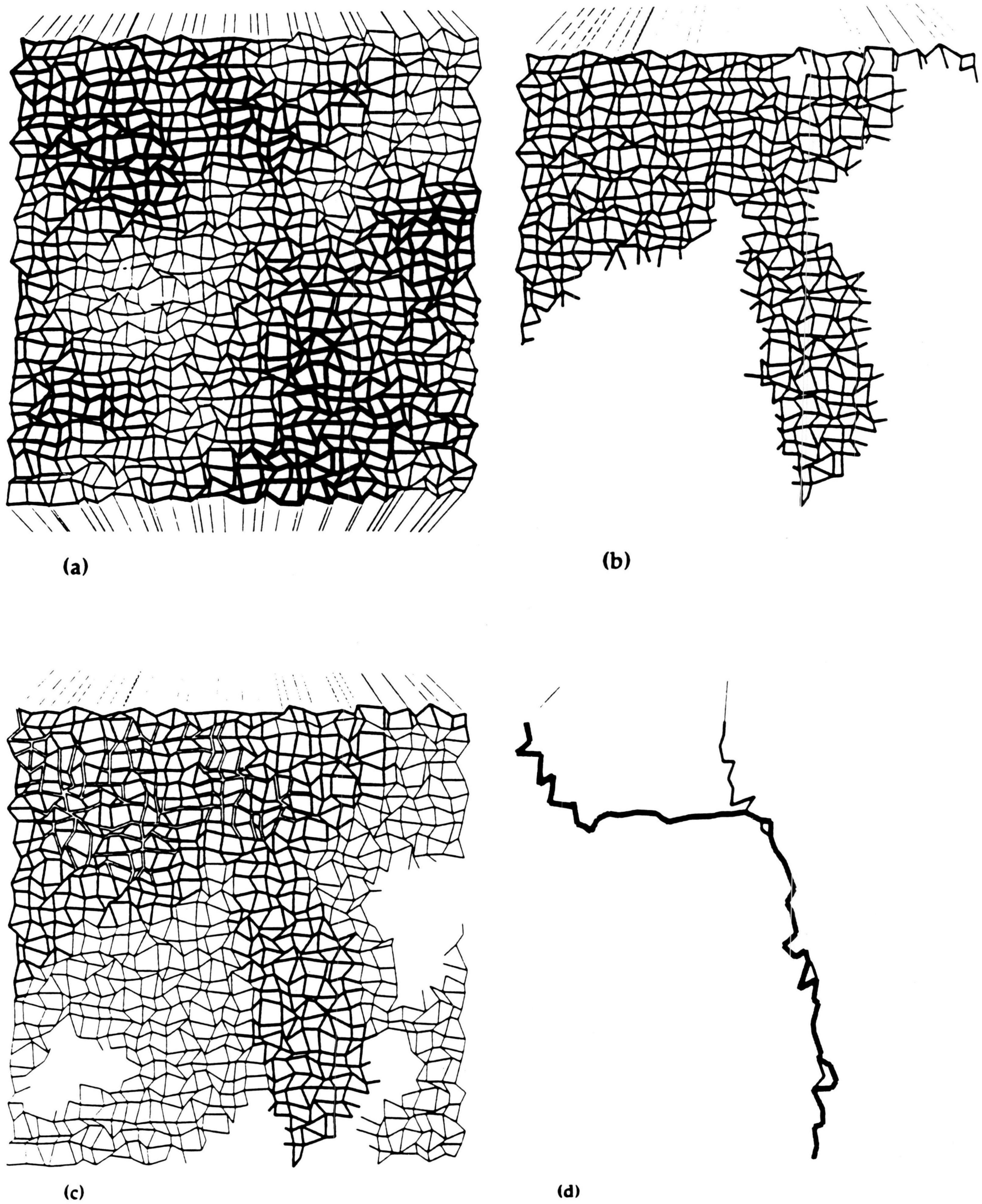

Figure 1. **(a)** Randomly generated network. **(b)** The invasion process. **(c)** The imbibition and drainage process. **(d)** Critical path (heavy line) and preferred path (light line) for spatially correlated distribution. [XBL 934-503]

capillary force. The simulation results show that the preferential trend of a medium is a strong function of spatial correlation, whether the fluid is wetting or nonwetting. For the random distributions without spatial correlation, the preferential trend is not very clear. Especially when the range of the distribution is narrow and uniform, the medium shows little possibility of forming any preferred path. The explanation for this is that connectivity rather than conductivity is the major factor in a heterogeneous flow field; high conductivity at local sites may contribute little to the global flow. Spatial correlation makes it possible for clusters of highly conductive elements to form bundles of channels that become the major contributors to the global flow.

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