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On the Inclusion of the Interfacial Area Between Phases in the Physical and Mathematical Description of Subsurface Multiphase Flow

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Research Objective

Improved capabilities for modeling multiphase flow in the subsurface requires that several aspects of the system which impact the flow and transport processes be more properly accounted for. A distinguishing feature of multiphase flow in comparison to single phase flow is the existence of interfaces between fluids. At the microscopic (pore) scale, these interfaces are known to influence system behavior by supporting non-zero stresses such that the pressures in adjacent phases are not equal. In problems of interphase transport at the macroscopic (core) scale, knowledge of the total amount of interfacial area in the system provides a clue to the effectiveness of the communication between phases. Although interfacial processes are central to multiphase flow physics, their treatment in traditional porous-media theories has been implicit rather than explicit; and no attempts have been made to systematically account for the evolution of the interfacial area in dynamic systems or to include the dependence of constitutive functions, such as capillary pressure, on the interfacial area.

This project implements a three-pronged approach to assessing the importance of various features of multiphase flow to its description. The research contributes to the improved understanding and precise physical description of multiphase subsurface flow by combining: 1) theoretical derivation of equations, 2) lattice Boltzmann modeling of hydrodynamics to identify characteristics and parameters, and 3) solution of the field-scale equations using a discrete numerical method to assess the advantages and disadvantages of the complete theory. This approach includes both fundamental scientific inquiry and a path for inclusion of the scientific results obtained in a technical tool that will improve assessment capabilities for multiphase flow situations that have arisen due to the introduction of organic materials in the natural environment.

Research Progress and Implications

This report summarizes work after 1.5 years of a 3-year project. The simulation aspects of the work rely on the availability of a continuum model for multiphase flow that incorporates processes of interest. Such a model serves to identify the data that must be extracted from the lattice Boltzmann model and provides guidance for the development of a model of field scale equations appropriate for a system of interest. Because the equation development is a precursor to the other aspects of this study, and because of logistical issues in securing the funding for the national laboratory components of the work, most of the effort has been directed to equation development and quantitative assessment based on the lattice Boltzmann simulator.

The theoretical analysis is based on the premise that physical description of multiphase flow in porous media ideally should be based on conservation principles. In practice, however, Darcy’s law is typically employed as the foundation of multiphase flow studies. Darcy’s law is an empirical surrogate for momentum conservation based on data obtained from experimental study of one-dimensional single phase flow. In its original form, Darcy’s law contained a single, constant coefficient that depended on the properties of the medium. Since 1856, Darcy’s relation has been heuristically and progressively altered by allowing this coefficient to be a spatially dependent, non-linear function of fluid and solid phase properties, particularly of the quantities of these phases within the flow system. The shortcoming of this approach is that the governing flow equation is obtained by enhancing a simple empirical coefficient with complex functional dependences rather than by simplifying general conservation principles. As a result, some of the important physical phenomena may not be properly accounted for. Also, some assumptions intrinsic to the equations are overlooked, making accurate simulation more of an art than an entirely scientific exercise. A more general approach employs a mathematical procedure for deriving conservation principles at the length scale of interest, followed by imposition of thermodynamic constraints to restrict the generality of these expressions. This approach provides a framework in which the assumptions inherent in a hypothesized model of multiphase flow are clearly stated. Requirements for more comprehensive and physically complete models can then be specified.

The contributions to this area of research under the current project is in four areas. First, a manuscript [1] has been prepared which discusses the shortcomings of heuristic extensions of Darcy's observations to more general problems of single and multi-phase flow. This paper also argues for the importance of consistent and integrated theoretical, computational, and experimental work for progress in understanding multiphase flow. Second, the complete framework for the derivation of conservation equations for phases, interfaces, common lines, and common points has been presented [2]. Third, a comprehensive thermodynamic approach to macroscale system behavior has been implemented [3] which must also be supplemented by mechanical equilibrium constraints for the subscale geometric descriptors of the system [4].

Although not reported in the publications, additional work has been initiated to develop a reduced set of the balance equations for a simplified core-scale physical system. These will be used for the initial development of the continuum scale model and for the identification of constitutive parameters from the lattice model simulations. In light of the constitutive forms that arise in the analysis, several issues relating to the design of the lattice model simulations, as well as the extraction of sufficient and appropriate data from them, have been identified; and some success has been achieved in calculation of the needed information [5].

1. Muccino, J.C., W.G. Gray, and L.A. Ferrand, "Toward an Improved Understanding of Multiphase Flow in Porous Media," Reviews of Geophysics (in press, 1998).
2. Gray, W.G., and S.M. Hassanizadeh, "Macroscale Continuum Mechanics for Multiphase Porous-media Flow Including Phases, Interfaces, Common Lines, and Common Points," Advances in Water Resources, Vol. 21, No. 4 (July, 1998) pp. 261-281.
3. Gray, W.G., "Thermodynamics and Constitutive Theory for Multiphase Porous-media Flow Considering Internal Geometric Constraints," Advances in Water Resources (in press, 1998).
4. Gray, W.G., "Macroscale Equilibrium Conditions for Two-phase Flow in Porous Media" (in review, 1998).
5. Soll, W.E., W.G. Gray, and A.F.B. Tompson, "Influence of Wettability on Constitutive Relations and Its Role in Upscaling," Proceedings of the XII International Conference on Computational Methods in Water Resources (in press, 1998).

Planned Activities

Over the next 1.5 years, activities are planned in all three areas of the research project. The theoretical study will incorporate chemical species transport into the full set of equations (6 mos.), extend the mechanical analysis to include four phase systems (1 yr.), and assess the ability of the theoretical approach to account for disjoining pressure in macroscale analysis (1.5 yr.). The lattice Boltzmann work will be re-implemented on current architecture for large scale high performance computing. (6 mos.). Additionally, a variable grid lattice method that has been developed will be tested. This will allow for more efficient simulation at the pore scale and enhanced ability to extract data (1 yr.). Based on lattice simulations, data analysis will be performed to obtain, as a primary constitutive function, the dependence of capillary pressure on interfacial areas as well as saturation. Dynamic relations among geometric parameters obtained from the theoretical analysis will be tested in the lattice Boltzmann framework (1.5 yr.). As improved equations and the data to support them are developed, the results will be tested in the numerical simulator of the equations (1.5 yr.).