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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

The mathematical description of multiphase flow and transport in the subsurface should be based on conservation principles. In practice, however, equations used for modeling multiphase flow are actually obtained by starting with the single fluid equation and then enhancing the simple empirical coefficients that arise with complex functional dependences. These manipulations are also supplemented by equilibrium expressions for capillary pressure as a function of saturation that is equal to the pressure difference between adjacent phases. The shortcoming of this approach is that the governing flow equations do not account for some of the important physical phenomena. Therefore accurate simulation is more of an art than a scientific exercise. Experimental and field programs designed to measure data in support of these equations may actually be seeking curve fitting coefficients rather than information characteristic of physical phenomena. A more general approach to the description of multiphase flow physics has been evolving over the last thirty years. This approach relies on a series of mathematical procedures that allow for derivation of conservation principles at a length scale on the order of tens to hundreds or more of pore diameters. The components of this procedure are: 1) derivation of conservation equations for phases, interfaces between phases, and common lines where interfaces intersect; 2) use of thermodynamic considerations to obtain the functional dependence of energy; 3) followed by imposition of thermodynamic constraints to restrict the generality of these expressions. The product of this approach is a set of balance equations which provides a framework in which the assumptions inherent in a hypothesized model of multiphase flow are clearly stated. However, support for the coefficients in these models is still required.

This basic research project implements a three-pronged approach to assessing and implementing the extended description of system physics. Aspects of the research include: i) derivation of conservation equations and thermodynamic description of phases, interfaces and common lines; ii) lattice Boltzmann modeling of hydrodynamics at the pore scale to identify characteristics and parameters at the macroscale, and iii) solution of the field-scale equations using a discrete numerical method to assess the advantages and disadvantages of the complete theory. This approach relies on fundamental scientific inquiry to develop a tool for improved assessment capabilities of multiphase flow situation. This work will impact both the study of flow of organic phases introduced into the natural environment and the study of natural multiphase systems such as petroleum and geothermal reservoirs.

RESEARCH PROGRESS AND IMPLICATIONS

This report summarizes work after 2.5 years of a 3-year project that will be extended, at no cost, to a fourth year. As its underpinning, this research requires a set of macroscale continuum equations. These equations have been derived and are contained in reference [2]. The availability of these equations then leads to important questions such as: 1) What is the proper way to develop the thermodynamics at the macroscale? 2) Which of the many parameters that arise are of importance? 3) What is a minimal description that can be used to describe multiphase flow? 4) How can a deficit in the number of equations that arises at the macroscale (due to the introduction of geometric parameters such as porosity, saturation, interfacial area per volume, and common line length per volume) be overcome? 5) How can the model parameters be obtained from a lattice Boltzmann simulation? 6) What advantage does implementation of the new equation set have over the standard formulation? and 7) Can the complex mathematical analysis be made accessible to a wider audience by physical interpretation of the results? Our efforts have been directed toward answering these questions, and progress will be discussed here.

The proper and complete postulation of the thermodynamic dependence of energy on independent variables is essential to the task of developing the system description. Reference [3] provides the postulation of the thermodynamics of macroscale phases, interfaces, and common lines so that the geometric parameters are included as independent variables. Here, the averaging theorems are used to assist in developing geometric constraints that serve to supplement the conservation equations and overcome the equation deficit. Reference [4] makes use of variational analysis to obtain the correct macroscale equilibrium constraints. These results may then be used to improve the auxiliary conditions for the conservation equations. The completion of these tasks results in equations that contain a large number of parameters. The investigators have met to pare down the parameters to their essential set for system description. We have also discussed how disjoining pressure influences

the results. We have obtained equations that describe the evolution to an equilibrium form of capillary pressure and spreading pressure. We are thus able to describe all dynamic aspects of a system. But we need to continue to work on parameterization and validation of our reduction to a minimal set. The lattice Boltzmann model is being used to provide data at the macroscale [5]. Issues that have arisen include the identification of both the position and the magnitude of interfacial area between phases from the digitized results of the small scale simulation. During the coming year we will develop a data set that can provide additional insights. The very small scale results obtained can be used to provide macroscale quantities, such as velocity and saturation, and also values of the parameters that appear in our dynamic equations. This work will lead to additional information concerning the importance of various terms that appear in the expanded equations. Our results already indicate that modeling of the interfacial area between phases is very important to a physically based description of multiphase flows. We are working on simple models that demonstrate this fact and the validity of our equations as well as on simulations based on our expanded system description.

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].

PLANNED ACTIVITIES

Over the next 1.5 years, we are planning to complete several aspects of our study and will also identify questions that require additional attention. We will be reporting our findings in several publications. Estimated time to completion is indicated in parentheses. The articles include an invited survey manuscript on closure of multiphase flow equations (6 mos); chemical species transport equations (6 mos). demonstration of constitutive theory with simple examples (8 mos.); exposition of the fundamental ideas for a wider audience (12 mos.); lattice Boltzmann measurement of simple parameters (12 mos.); one-dimensional simulations (14 mos.).

INFORMATION ACCESS

1. Muccino, J. C., W. G. Gray, and L. A. Ferrand, Toward an improved understanding of multiphase flow in porous media, *Reviews of Geophysics*, Vol. 36, No. 3 (August, 1998) pp. 401-422.
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*, Vol. 22, No. 5 (January, 1999) pp. 521-547.
4. Gray, W. G., Macroscale equilibrium conditions for two-phase flow in porous media, *International Journal of Multiphase Flow* (in press, 1999).
5. Soll, W. E., W. G. Gray, and A. F. B. Tompson, Influence of wettability on constitutive relations and its role in upscaling, in *Computational Methods in Water Resources XII*, Vol. 1 (edited by V. N. Burganos, G. P. Karatzas, A. C. Payatakes, C. A. Brebbia, W. G. Gray, and G. F. Pinder), Computational Mechanics Publications, Southampton (1998), pp. 413-420.