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INTRODUCTION

This research is part of a joint project with Dr. Andrew F. B. Tompson of Lawrence Livermore National Laboratory and Dr. Wendy E. Soll of Los Alamos National Laboratory. The work is designed to integrate a continuum theory approach to multiphase flow modeling (Gray) with lattice Doltzmann studies (Soll) and study of the model in the context of a field simulation (Tompson). Because of some difficulties with the funding procedure, the support for Drs. Tompson and Soll was delayed such that it begins with the second year during with I will be supported. Because of this fact, the efforts to integrate the theory with the modeling efforts has been delayed but will be able to be approached with particular vigor during this coming year. I have met with Drs. Soll and Tompson and plan to meet with them again next month to ensure that our efforts are coordinated. During this first year, my funding has been used to advance the theory and develop a basic understanding that will assist in development of the simulation models. It should be noted that in addition to this grant. I am supported by a subcontract of part of a DOE grant to Cornell (PI Carlo Montemagno) under this same funding program. Both grants require development of theory and are thus related. However, the interactions and ultimate goals of the two studies are different. Simplistically, one might differentiate between the two projects in that the DOE-Cornell grant is concerned with the equilibrium states of the system and the parameters needed to describe those states while the present grant is concerned with dynamic processes and the parameters needed for their description. It is not possible to definitively compartmentalize the findings made in my studies of multiphase flow as belonging exclusively to one grant or the other.

APPROACH AND RESULTS

To model multiphase flow in porous media, it is necessary to develop equations at a "macroscale" a scale that characterizes a region of the study system encompassing all the phases and interfaces present. The macroscale equations contain parameters that characterize the system but which are in some sense related to processes occurring at the microscale. The lattice Boltzmann and field simulation studies deal with dynamic systems. On the one hand the lattice Boltzmann model provides the system dynamics at a small scale and can be used to simulate flow and transport in the pores a core sample. The field model, on the other hand attempts to model a system by characterizing its heterogeneities and dynamics in terms of macroscale differential equations discretized over the entire region. The continuum macroscale model makes use of lattice Boltzmann results to obtain parameters that can be incorporated into the field model. This is an ambitious effort, but a necessary one if understanding of the multiphase flow processes is to be better under stood. The goals of the research are to provide linkages among the lattice Boltzmann model. the continuum model, and the field model. Because of funding delays relating to the work being done at the national laboratories on the simulation models, efforts to establish linkages are behind what was initially envisioned. However, the continuum model has developed beyond what was initially proposed and appears to be in a good position to support the modeling studies that are commencing in the second year.

The following have been accomplished during the first year:

- First, the procedure for development of the macroscale equations has been made more systematic. The most important contribution in this area has been the development of a consistent procedure for postulating the thermodynamic dependence of energy on independent variables. Because of this consistency, it is easier to relate macroscale processes to microscale counterparts.
- Second. a manuscript has been prepared highlighting the necessity for an expanded theory of multiphase flow if it is to be modeled properly. This manuscript is intended to provide the motivation of the development of a continuum model in a style that is accessible to the non-specialist. We hope that this will improve the receptivity of the scientific community to our approach and encourage others to consider some of the shortcomings of currently employed models. This manuscript has been submitted to a peer-reviewed journal.
- Third, a technical manuscript has been prepared that provides the complete: framework for development of the conservation equations for phases, interfaces. and common lines. This manuscript provides a new approach to obtaining the macroscale equations provides the macroscale equation for a common line (a curve formed as the locus where interfaces between phases intersect) for the first time, provides the modification needed it the interfaces and common lines are massless, and develop; the general entropy inequality of the system that can be used with the constitutive theory. This manuscript has been accepted by *Advances in Water Resources* and is in the last stages of incorporation into a forthcoming issue of the journal.
- Fourth a manuscript is in preparation that explains the exploration of the entropy inequality to obtain the governing equations. This work is important as it indicates the parameters that need to be obtained from the lattice Boltzmann model and their dependence. This work makes use of a new systematic procedure for hypothesizing the thermodynamics at the macroscale. Additional work on the use of geometric relations to gain insight into the parameters that arise in the equations will contribute to a subsequent manuscript. As a part of the study leading to this manuscript, film flow has been considered, including the spreading of a wetting fluid over a solid.
- Work has been done on the incorporation of multiple specics into the model. This work has importance for mass transfer between phases and when chemical reac tions occur. Heretofore, the development of appropriate equations has relied on momentum and energy equations for each species. Thus, the theoretical development was extremely cumbersome, if not intractable. A new approach has been

developed which allows for the study of transport problems within a manageable framework Further development of these equations will occur during the coming year.

Conclusion

The development of the theoretical model for multiphase flow has proceeded well during this past year. A number of initiatives have been undertaken designed to make the work accessible, rigorous, and tractable. Equations that have been derived need to he related to lattice Boltzmann and field models. Efforts to accomplish this will be the main thrust of the coming year of work.