Multiphase flow in complex fracture apertures under a wide range of flow conditions. EMSP Project 86977:

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FY 2005 Report

Research Objectives

The primary purpose of this project is to use a combination of computer modeling and laboratory experiments to obtain a better understanding of multiphase flow in geometrically complex fracture apertures under a wide range of flow conditions. Because most traditional grid-based numeral methods perform poorly for multiphase flows with complex dynamic interfaces due to problems such as artificial interface broadening, grid entanglement, loss or gain of mass and their inability to handle fluid-fluid-solid contact line dynamics, the modeling component of the program relies primarily on particle based methods. In particle based models, the fluid-fluid interfaces move as the particles representing the fluids move - there is no need for explicit interface tracking, and no artificial front broadening. In addition, the fluid-fluid-solid contact line dynamics is also handled automatically by adjusting the interactions between the fluid particles and the particles used to represent solid boundaries. However, it can be difficult to select fluid-particle/solid-particle interactions that reproduce the wetting behaviors observed in experimental or natural systems.

Because, different model approaches have characteristic strengths and weaknesses, three different classes of particle-based models (lattice Boltzmann, dissipative particle dynamics and smoothed particle hydrodynamics) are being employed in this program. This will allow us to achieve our objective of simulating multiphase flow under a wide range of flow conditions for a wide range of fluid properties.

In the second year of the program, we investigated the possibility of developing grid-based (finite difference) methods coupled with level-set methods for capturing fluid-fluid interfaces. The advantage of this approach is the greater numerical efficiency of grid-based methods. However, this method does not rigorously conserve mass, and code development is substantially more difficult. In the third year of the project, we investigated the application of the volume-of-fluid interface tracking method to the simulation of multiphase fluid flow in fracture apertures, fracture junctions and simple fracture networks. Our Navier-Stokes solver/volume-of-fluid (volume-of-fluid hereafter) simulations were based on the two-dimensional ‘RIPPLE’ volume-of-fluid code developed at the Los Alamos National Laboratory. Two important modifications were made: 1. We replaced the algorithm used to reconstruct fluid-fluid interfaces from the fluid phase volume fractions in each grid cell, which restricts the orientation of the interface within a grid cell to two directions aligned with the grid axes, by an improved interface reconstruction algorithm which allows the interface within a grid cell to be oriented in any direction; and 2. We replaced the single contact angle model used in RIPPLE with a model that includes three contact angles (advancing, receding and near-equilibrium).

One of the most important objectives of the program is to use the results of the computer modeling and experimental studies to develop improved conceptual models for fluid flow in fractured systems. This will be the main link between our basic investigation of fluid flow on short length scales and application to practical problems on the field scale.

Another objective of the research is to shorten the delay between the development of innovative computer modeling methods by the physics community and their application to subsurface science (which has been a quarter of a century in the case of smoothed particle hydrodynamics). We also hope to contribute to the development of the basic numerical methods.

Research Progress and Implications

This report summarizes progress during the third year of a three-year project.

Grid-based methods

Although it is difficult to apply grid-based methods to systems with complex dynamic fluid-fluid interfaces and/or systems in which contact-line dynamics plays an important role, we have placed increased emphasis on this approach because of greater computational efficiency of grid-based methods.

<u>Volume of fluid simulations (Hai Huang)</u>

Figure 1 illustrates the application of a grid-based Navier-Stokes equation solver coupled with volume-of-fluid interface tracking to the simulation of multiphase fluid flow in a fracture network.

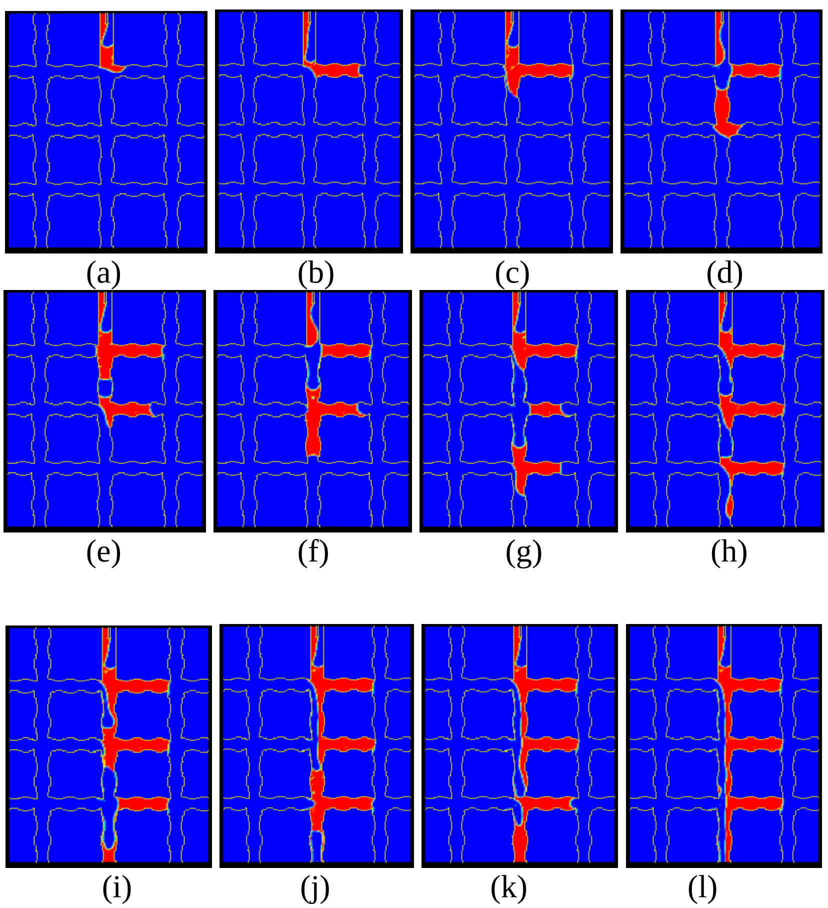


Figure 1: Twelve stages in a two-dimensional volume of fluid simulation of two-phase fluid flow in a small fracture network.

Like many laboratory experiments, our simulation results reveal that fluid motion in unsaturated fractures is complex, even for very simple fracture geometries and under constant liquid injection conditions. Different flow behaviors within unsaturated fractures, including continuous film flow, intermittent mixed film flow, stationary capillary droplet formation and snap-off/reconnection, can coexist, depending on the fracture geometry, wetting behavior, fluid properties, inflow conditions and so on.

Particle-based methods

Our primary research focus has been on smoothed particle hydrodynamics, dissipative particle dynamics and lattice Boltzmann methods. All three of these methods rigorously conserve mass, there is no need for interface tracking and the interactions between the fluids and geometrically complex boundaries can be simulated quite easily using interactions between fluid particles and boundary particles.

<u>Lattice Boltzmann simulations (Hakan Basagaoglu)</u>

Figure 2 shows a three-dimensional lattice Boltzmann of fluid behavior in a fractured system. The fractures are filled with two immiscible fluids that have different wetting properties.

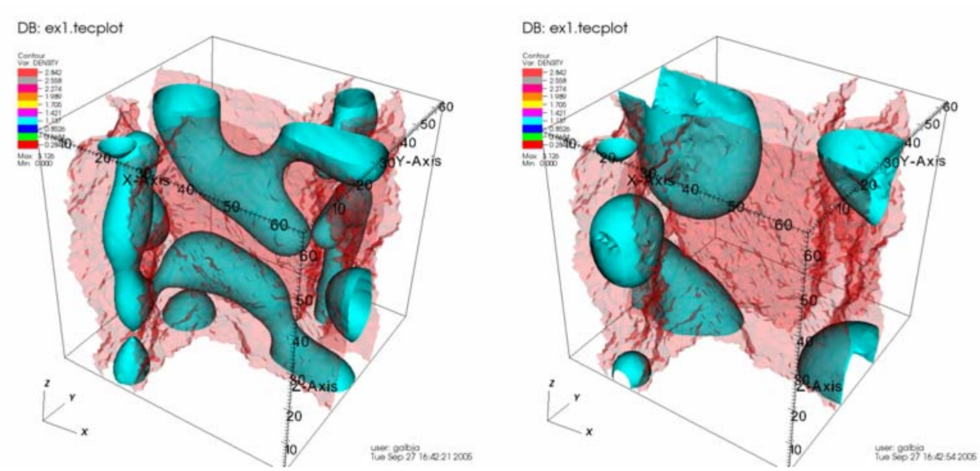
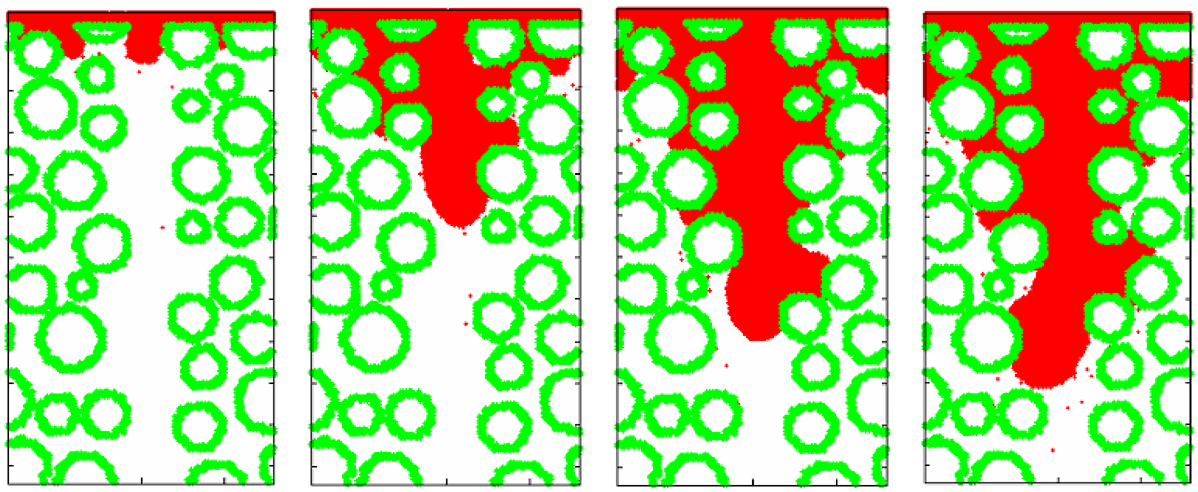


Figure 2: A three-dimensional simulation of fluid behavior in fracture junctions. The figure on the left-hand side shows the initial fluid distribution, which redistributes itself to the distribution shown on the right-hand-side under the influence of gravity, surface tension and wetting characteristics. The rough surfaces of the fracture aperture are shown in red, the non-wetting fluid is shown in blue, and the wetting fluid is not shown.

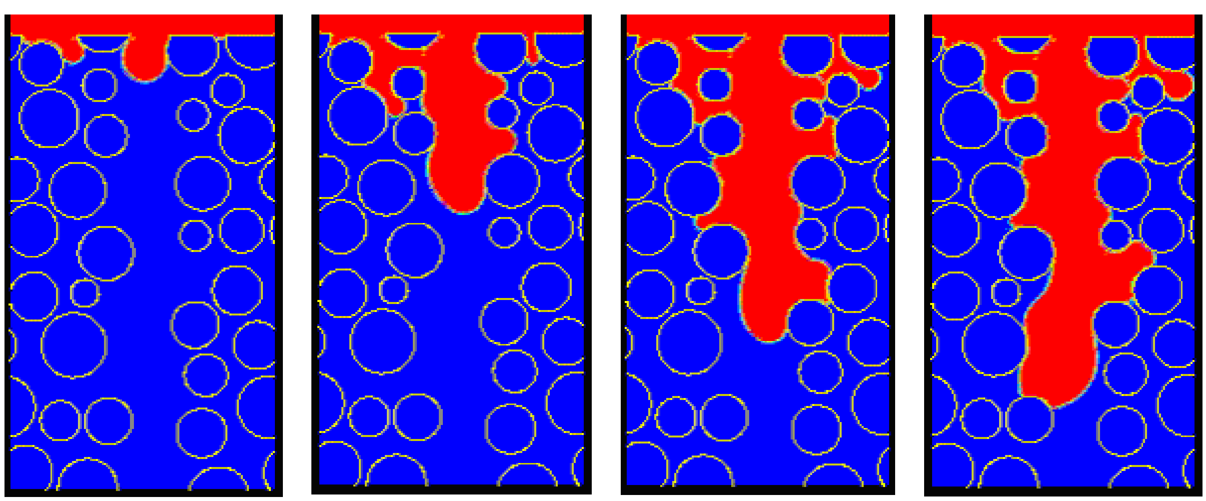
<u>Dissipative particle dynamics (Moubin Liu)</u>

In the third year of the program we compared different methods and compared simulation results with experiments to assess the validity of the various models, and to learn more about their relative strengths and weaknesses. For example, figure 3 shows a comparison between simulations carried out using dissipative particle dynamics and the volume-of-fluid method described above for the gravity-driven penetration of a non-wetting fluid into a small vertical fracture in a porous medium.



(a) (b) (c) (d)

Figure 3a: a DPD simulation of flow through a two-dimensional fractured porous media at 4 stages.



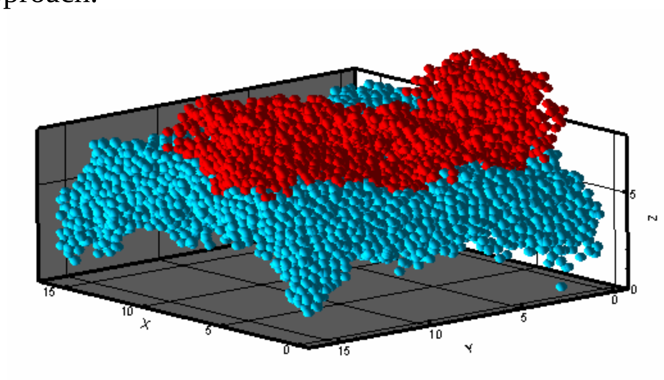
(a) (b) (c) (d)

Figure 3b: Volume-of-fluid simulation of flow through a two-dimensional fractured porous media at 4 stages equivalent to those shown Figure 1.

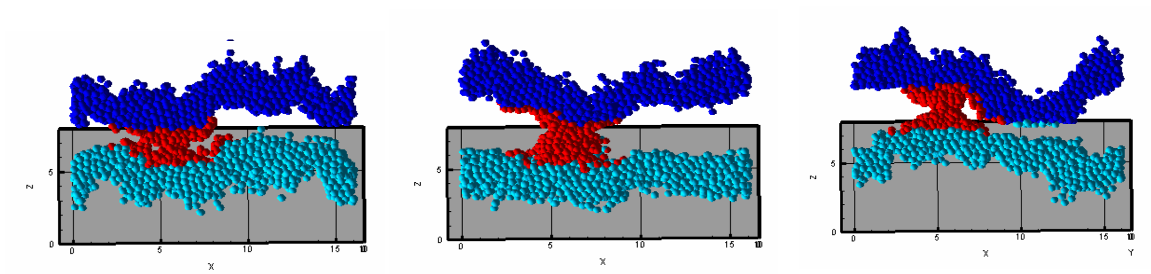
The good agreement between the two simulations enhances our confidence in the reliability of both methods. However, it is important to recognize the fundamental parameters in the volume-of-fluid simulations are the fluid density, fluid viscosity, surface tension and contact angles, gravitational acceleration while the fundamental parameters in the DPD simulations are particle-particle interactions and gravitational acceleration. To obtain the results shown in figure 3, the dissipative particle dynamics particle interaction parameters were tuned to match the dissipative particle dynamics simulations to the volume-of-fluid simulations.

Smoothed Particle Hydrodynamics (Alexandre Taratkovsky)

An important innovation that we introduced to smoothed particle hydrodynamics is the capability of simulating solute and chemical processes such as dissolution and precipitation. This allows us to investigate processes such as the dispersion of dissolved chemicals (salt or contaminants, for example) and changes in subsurface pore geometry and fracture geometry due to natural and controlled geochemical processes. We have also developed smoothed particle hydrodynamics models that can be used to simulate fluid-fluid systems with very large density and viscosity contrasts (such as water and air). This is an important deficiency of lattice Boltzmann models. Although we have developed lattice Boltzmann models to simulate fluid-fluid systems with density contrasts greater than 1000:1 (an concomitantly high viscosity contrasts) we have not yet fully evaluated this model or provided a firm theoretical foundation for it. Figure 4 illustrates our ability to simulate coupled fluid flow and reactive transport processes using a smoothed particle hydrodynamics approach.



a)



b) y = 4 *c*) y = 8 *d*) y = 12

Figure 4: Mineral precipitation in the 3D fracture with fractal wall geometries resulting from the reactive transport with Da' = 1.37 and Pe=19.43 at dimensionless time t = 520: a) three-dimensional view of the precipitated minerals (red particles) and lower fracture wall (green particles) b) –d) cross-sections in the direction parallel to the flow at $y = 4h$, $8h$ and $12h$. Red particles represent precipitated minerals and blue and green particles represent the upper and lower walls of the fracture.

Comparison with Experiments

Comparison between experiments and computer simulations is an important objective of this project. Figure 5 compares results from an experiment in which dyed water was infiltrated into a fabricated channel network with simulations carried out using volume-of-fluid, lattice Boltzmann and dissipative particle dynamics simulations.

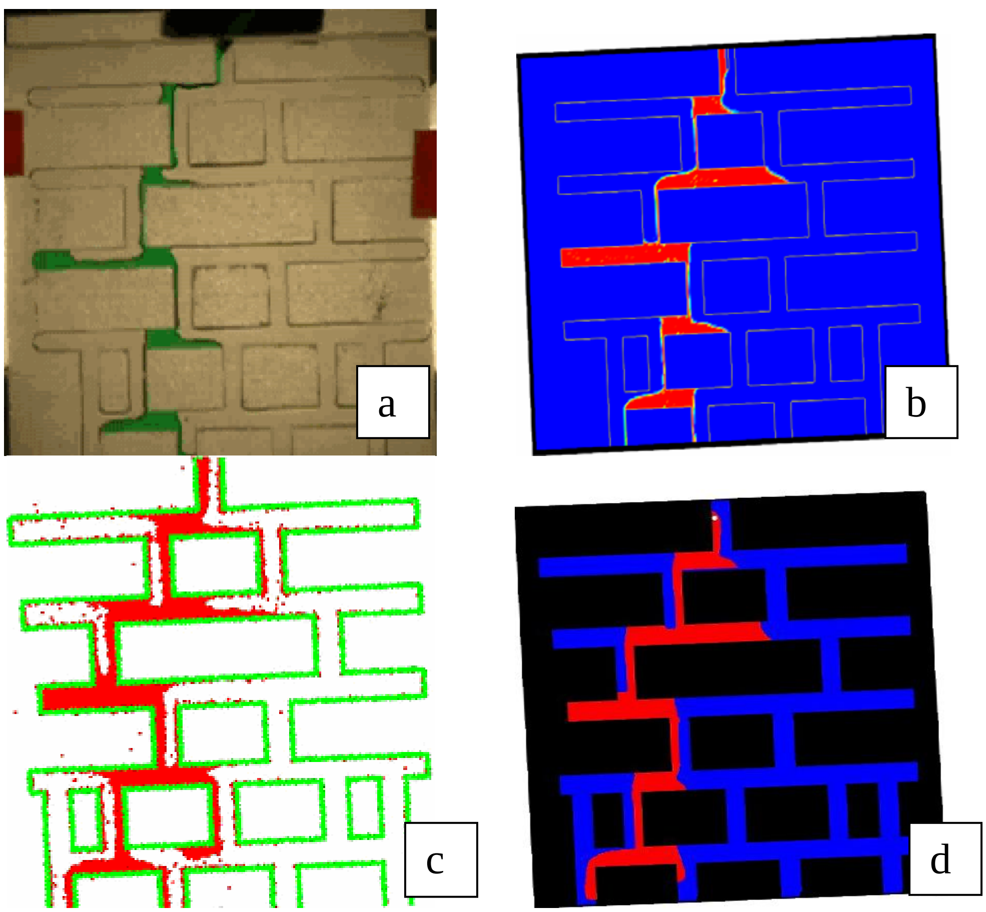


Figure 2:. Comparison of fracture flow experiment (a) with computer simulations: (b) Navier-Stokes-VOF simulation; (c) dissipative particle dynamics simulation; (d) lattice Boltzmann simulation.

It is important to recognize that the experiments are fully three-dimensional while the simulations are two-dimensional. Nevertheless, the simulations do capture, in a qualitative manner, the behavior observed in the experiments.

Information Access:

Publications:

Published:

1. A. M. Tartakovsky and P. Meakin, Modeling of surface tensions and contact angles with smoothed particle hydrodynamics.' Physical Review **E72**: Article 026301 (2005)
2. A. M. Tartakovsky and P. Meakin, Simulation of unsaturated flow in complex fracture apertures., Vadose Zone Journal **4**: 848-855 (2005)
3. A. M. Tartakovsky and P. Meakin, A smoothed particle hydrodynamics model for miscible flow in three-dimensional fractures and the two-dimensional Rayleigh-Taylor instability., Journal of Computational Physics, **207:** 610-624 (2005)
4. G. E. Mc Creery and D. M. McEligot, Transition to Meandering Rivulet Flow in Vertical Parallel-Plate Channels. ASME Journal of Fluids Engineering, vol. **126**, 2004, pp. 498-499.

In Press:

1. H. Basagaoglu, P. Meakin P and S. Succi, Energy dissipation measures in three-dimensional disordered porous media., Physical Review E.
2. H. Basagaoglu, P. Meakin, C. T. Green and M. Mathew, Multiphase flow in geometrically simple facture intersections., Physica A.
3. H. Huang, P. Meakin and M. Liu, Computer simulation of two-phase immiscible fluid motion in unsaturated complex fractures using a volume of fluid method., Water Resources Research.
4. H. Huang, P. Meakin, M. Liu and G. Mc Creery, Modeling of multiphase fluid motion in fracture intersections and fracture networks., Geophysical Research Letters..

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1. M. Liu, P. Meakin and H. Huang, Dissipative Particle Dynamics Simulation of Fluid Motion Through An Unsaturated Fracture and Fracture Junction., Journal of Computational Physics (Under review).
2. M. Liu, P. Meakin and H. Huang, Dissipative particle dynamics with attractive and repulsive particle-particle interactions., Physics of Fluids (In revision).
3. A. M. Tartakovsky and P. Meakin, Pore-scale modeling of immiscible and miscible fluid flows using smoothed particle hydrodynamics., Advances in Water Research.
4. G. E. Mc Creery, P. Meakin and D. M. McEligot, 'Rivulet flow in vertical parallel-wall channels., The International Journal of Multiphase Flow.

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In Preparation

1. A. M. Tartakovsky, P. Meakin and T. Scheibe, Simulations of reactive transport and precipitation with smoothed particle hydrodynamics.
2. A. M. Tartakovsky, P. Meakin and T. Scheibe, A smoothed particle hydrodynamics model for reactive transport and mineral precipitation in porous and fractured porous media.
3. M.. Liu, P. Meakin and H. Huang, Dissipative Particle Dynamics Simulation of Pore-Scale Flow Through Porous Media.
4. H. Basagaoglu, P. Meakin, S. Succi S. and J. Welhan, Boundary effects on energy dissipation measures in porous domains.
5. H. Basagaoglu, P. Meakin, S. Succi, and G. Redden, Lattice-Boltzmann Simulation of Size Exclusion Effects in Colloidal Transport in Rough-walled Channels.
6. H. Basagaoglu, P. Meakin, S. Succi and D. Wildenschild, Multiphase Flow in Complex Fracture Geometries.
7. H. Basagaoglu, P. Meakin, S. Succi and R. Rossella, Density fluctuations in lattice Boltzmann simulations of multiphase fluids in porous and non-porous systems.

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