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

Paul Meakin (PI), Glenn E. McCreery and Donald McEligot. Idaho National Engineering and Environmental Laboratory.

In collaboration with:

Daniel H. Rothman. Department of Earth, Atmospheric and Planetary Sciences, Massachusetts Institute of Technology.

FY 2003 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 traditional grid-based numeral methods perform poorly for multiphase flows with complex dynamic interfaces due to problems such as artificial interface broadening and grid entanglement, the modeling component of the program relies 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. 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) will be 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.

The computer modeling will be closely integrated with experimental studies to enable to thoroughly test the computer models, use computer modeling under conditions that make experiments difficult and use experiments when computer modeling is impractical.

On 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 basis 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).

Research Progress and Implications

This report summarizes progress during the first 8 months of a three year project.

Basic computer models have been developed, based on all three particle-based methods (lattice Boltzmann, dissipative particle dynamics and smoothed particle hydrodynamics) for two-phase flow in realistically complex fracture apertures. The fracture models are based on the idea that the fracture of brittle materials generates rough surfaces with a self-affine fractal geometry. We have demonstrated that these models exhibit physically realistic behavior, but no quantitative results or detailed comparison with experiments have been carried out at this stage. Some of the simulations carried out using the dissipative particle dynamics model are shown in figures 1 and 2. Figure 1 shows two stages in the simulation of the displacement of a fluid by a more strongly wetting fluid in a complex fracture aperture.

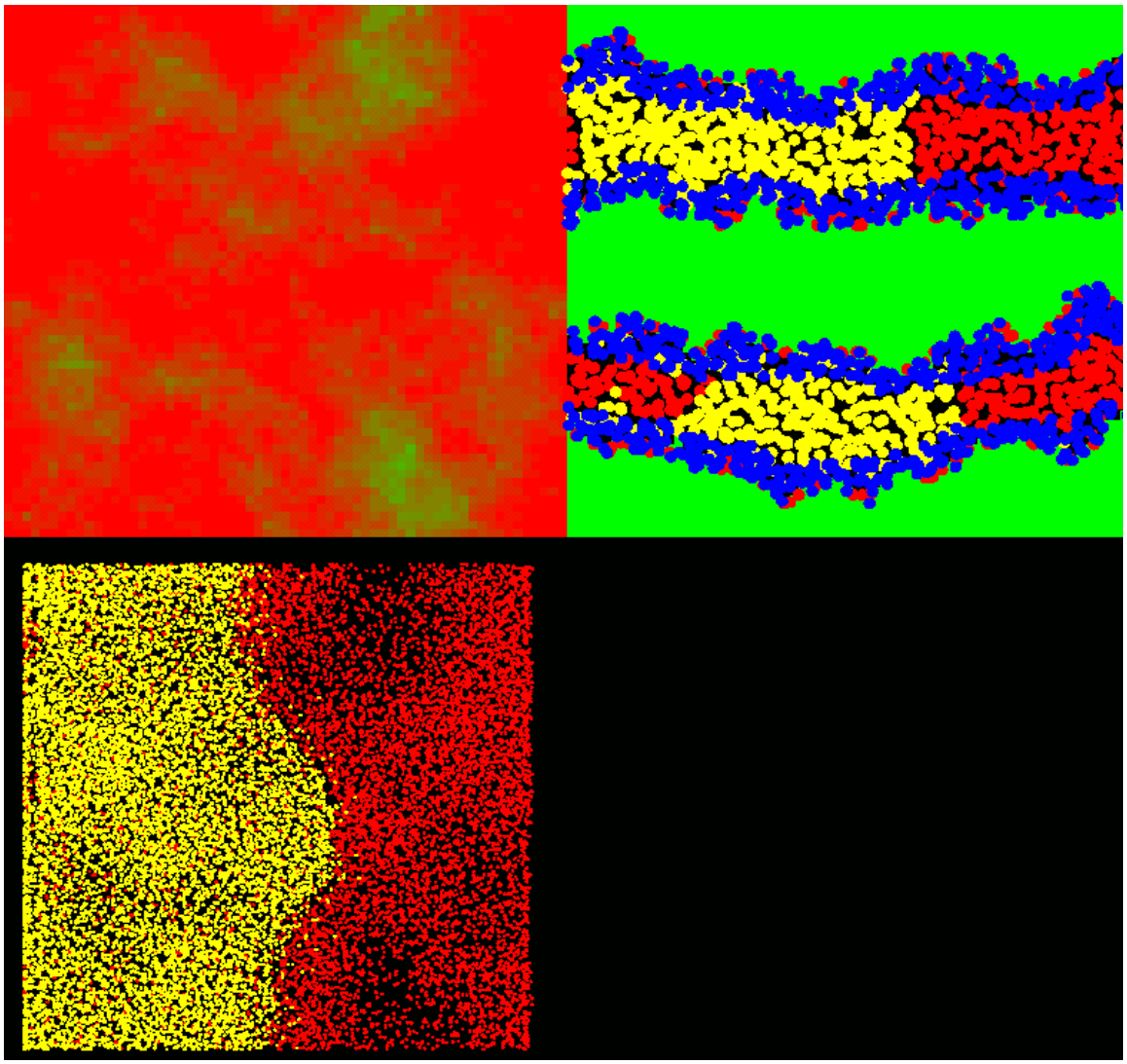

Figure 1a: Displacement of a fluid (red) by a somewhat more strongly wetting fluid (yellow) in a complex fracture aperture. The upper left corner shows the fracture aperture with a color scale that ranges from green to red with increasing aperture. The blue particles are 'boundary particles', and the interactions between these particles and the red and yellow particles determine the wetting properties of the two fluids. The upper right corner shows two cuts perpendicular to the plane of the cell; one parallel to the direction of flow (top) and the other perpendicular to the direction of flow. Both cuts pass through the center of the cell. The lower left corner shows a view from the top of the cell. The more wetting fluid (yellow) is injected at a uniform rate along the left-hand edge of the cell. The 'cell' containing the fluids was constructed from a self-affine fractal surface with a Hurst exponent of 0.7. The aperture is the gap between this surface and a replica that is translated both horizontally and vertically (without rotation) using periodic boundary conditions.

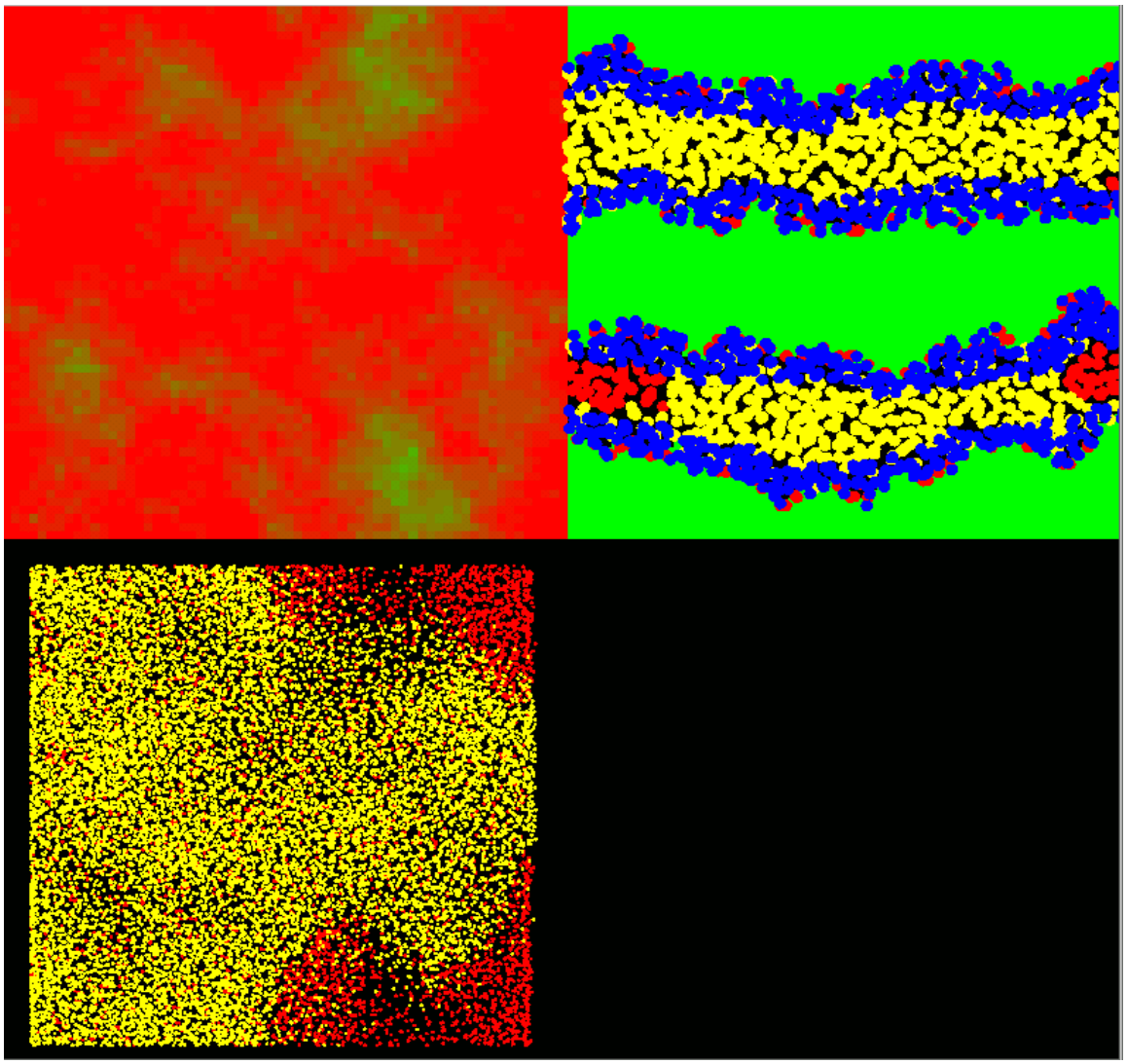

Figure 1b: A later stage of the simulation shown in figure 1a.

Figure 2 shows a similar simulation in which the displacing fluid is less strongly wetting than the fluid which initially fills the cell.

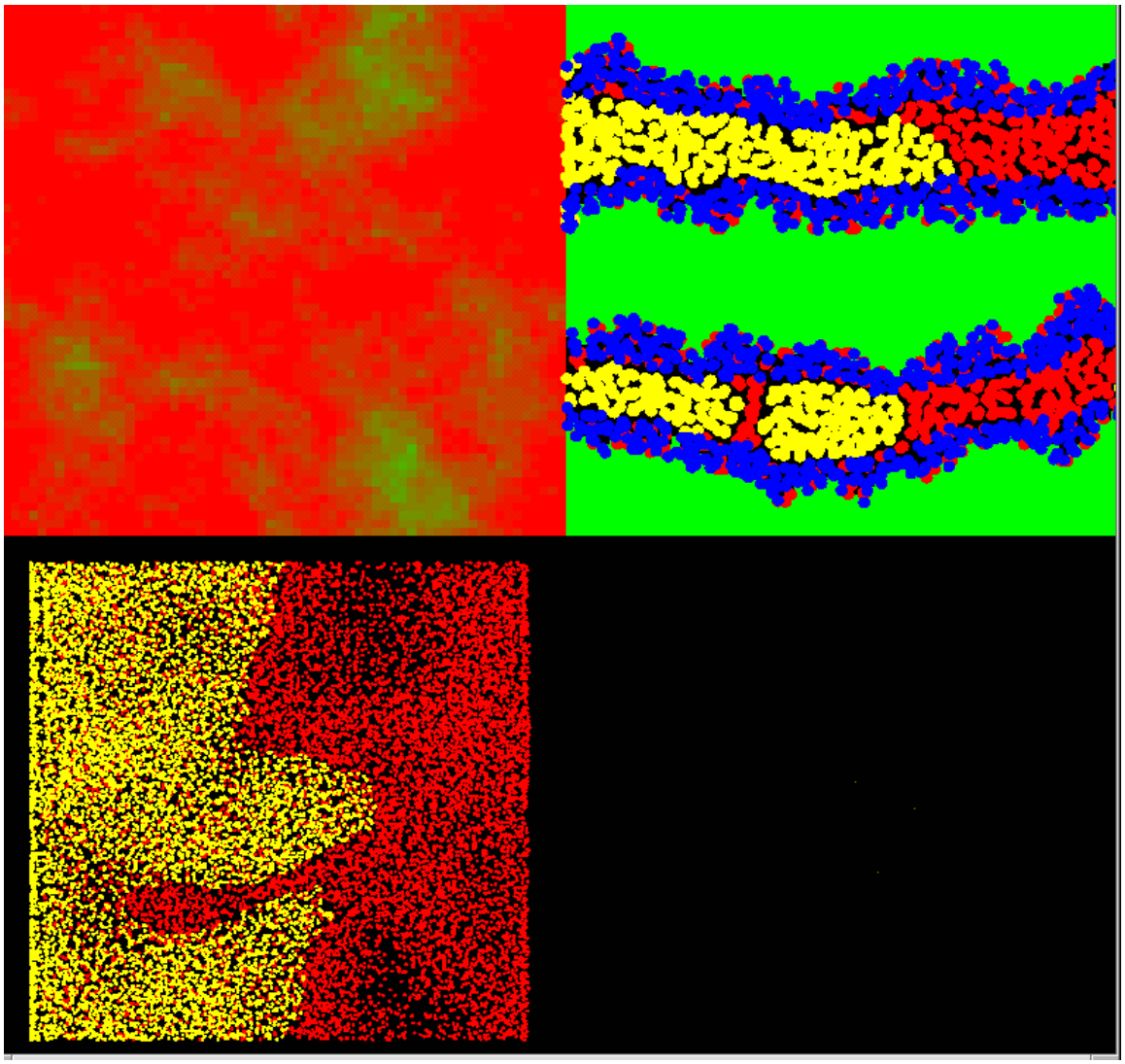

Figure 2a: Results of a simulation of the displacement of a more strongly wetting fluid by a less strongly wetting fluid in the model 'cell' that was used in the simulations illustrated in figure 1.

As a result of research carried out by Daphne Stoner, Vance Deason and Robert Stedtfeld at INEEL, we are able to use sterolithography (rapid prototyping) to fabricate fracture apertures enclosed by transparent polymers. These flow cell can be fabricated using actual fracture surfaces characterized by profilometry, or the cells can be designed entirely on the computer. This will provide us with the ability to carry out flow experiments and computer simulations with essentially the same fracture apertures geometries. Preliminary flow experiments have been carried out using a cell fabricated with random self-affine fracture surfaces.

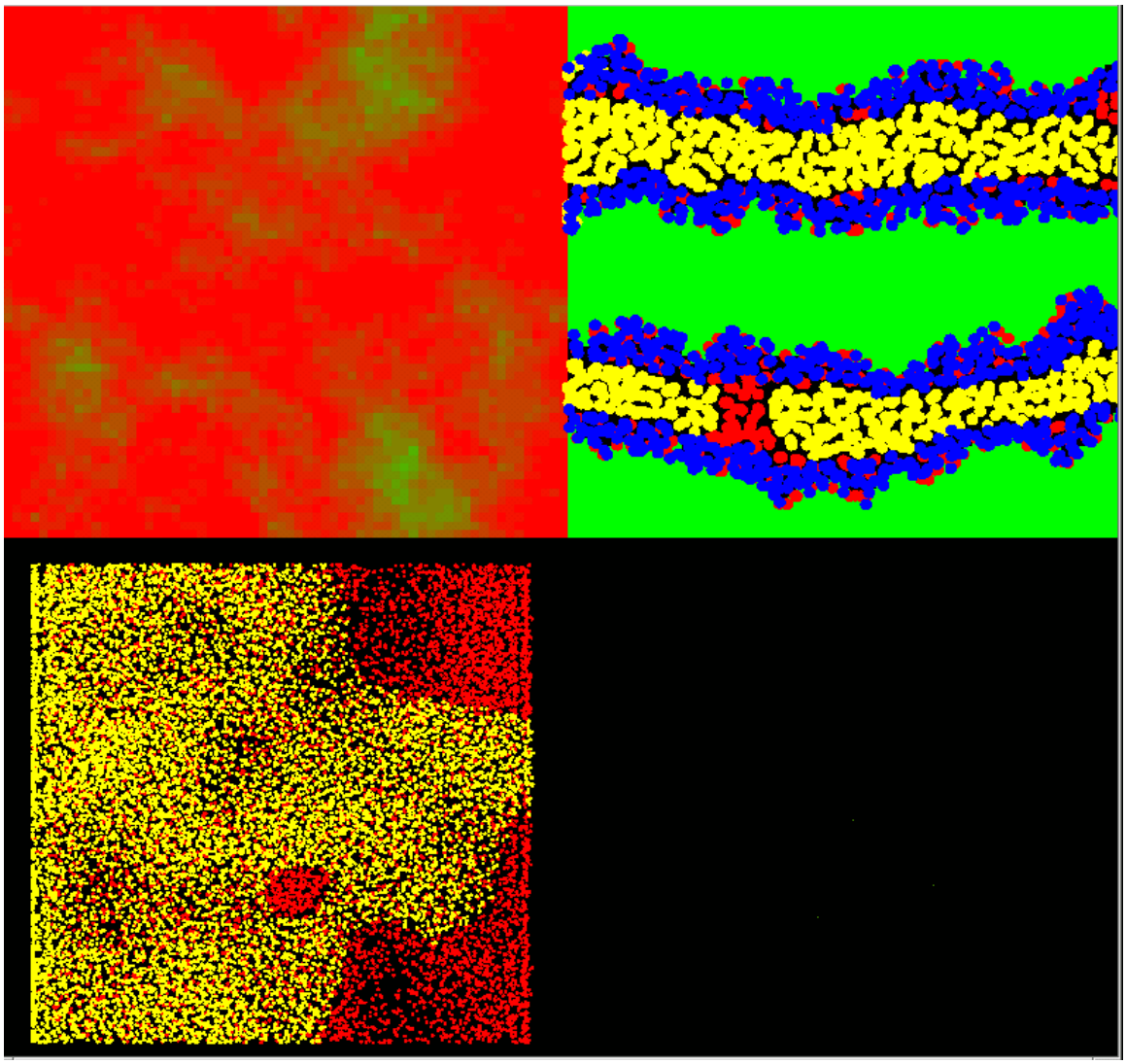

Figure 2b: A later stage in the simulation illustrated in figure 2a. A bubble of wetting fluid has been surrounded by the invading non-wetting fluid. Similar 'trapping' of wetting fluid occurs during the displacement of a wetting fluid by a non-wetting fluid in a porous medium. This type of process is very difficult to model using grid-based methods.

Planned activities

During the next year, we will use the basic computer models developed during the first 8 months of this project as a basis for computer models with enhanced capabilities that can be applied under a wider range of flow conditions and a wider range of fluid properties (viscosity ratios, wetting behavior, density ratios ….). The models will be tested against analytical results (where available) and simple experiments.

Towards the end of this period, we will begin to make detailed comparisons between computer simulations and experiments carried out with more complex flow conditions and/or more complex fracture geometries. A preliminary assessment of the dissipative

particle dynamics and smoothed particle hydrodynamics codes indicates that advanced multiprocessor computers will be needed for this purpose, and suitable code will be developed when the reliability of single-processor models has been demonstrated.

Collaboration with the University of Oslo Center for the Physics of Geological Processes is a component of this project. Paul Meakin will be visiting the University of Oslo in June to establish this collaboration.

Information Access

An account of progress in this project was presented at the FY2003 EMSP Principal Investigator Workshop held at the Pacific Northwest National Laboratory, May 6—7, 2003. http://www.pnl.gov/emsp/fy2003/presentations/meakin_paul_86977.pdf