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

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FY 2004 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 numerical 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 heavily 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, particle-based methods rigorously conserve mass because each particle represents a fixed mass of fluid and the number of particles does not change unless particles leave or enter the computational domain (to represent fluid flow into or out of the system). 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/multicomponent flow under a wide range of flow conditions for a wide range of fluid properties.

In the second year of the program, we have also begun to investigate the possibility of developing grid-based (finite difference) methods coupled with the level-set method 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.

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

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 themselves.

Research Progress and Implications

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

Computer modeling

Our research approach is based on smoothed particle hydrodynamics, dissipative particle dynamics and lattice Boltzmann methods. All three of these methods rigorously conserved 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. This is illustrated in Figure 1, which shows a smoothed particle hydrodynamics simulation of the injection of a mixture of immiscible liquids into an initially empty complex fracture aperture. The liquids have different wetting properties (controlled by the interactions between the fluid particles and the barrier particles).

In these simulations, the fluid undergoes phase separation as it is injected into the aperture. The complex coupling between phase separation and multiphase flow cannot be simulated with grid-based methods, and this simulation illustrates the power of particle-based methods. However, other particle-based methods can also be used to simulate processes such as coupled flow and phase separation, and we have obtained similar results using dissipative particle dynamics and lattice Boltzmann simulations.

Despite the advantages of ‘particle based’ methods we have also been investigating the combination of level-set interface capturing with finite-difference numerical solution of the Navier Stokes equations. This method is more computationally efficient than the particle based methods, and it can handle large density contrasts and incompressible fluids. Another advantage of this approach over most particle-based methods is that fundamental fluid properties such as the viscosity and surface tension can be used directly as model parameters. In dissipative particle dynamics, for example, the basic model parameters are particle-particle interactions, and properties such as the fluid viscosity and surface tension cannot be calculated accurately from these interactions. Consequently, properties such as the viscosity must be determined from computer simulations under simple flow conditions. Smoothed particle hydrodynamics simulations can be carried out using a viscosity equation in which the fluid viscosity is a model

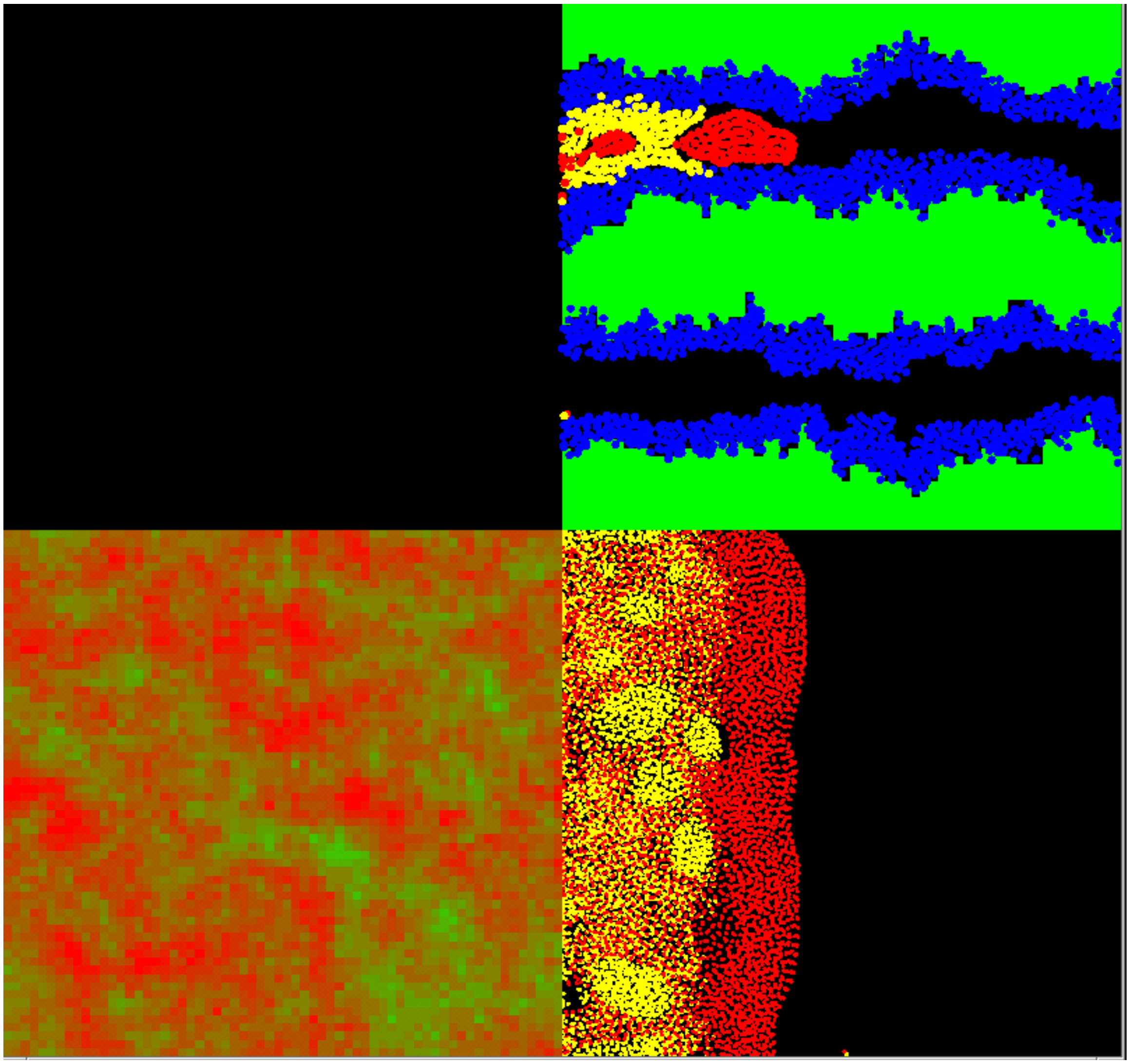

Figure 1a: The injection of a mixture of immiscible liquids into an open fracture aperture filled with a very low viscosity fluid. The lower left corner shows the aperture field using a color scale that varies from green to red as the aperture increases. The aperture is the gap between a self-affine fractal surface with a Hurst exponent of 0.4 and a replica of the surface that has been translated both horizontally and vertically, without rotation and with periodic boundary boundaries in the directions parallel to the plane of the fracture. The upper right corner shows two cross-sections through the system parallel (top) and perpendicular (bottom) to the flow direction. The blue particles are stationary 'boundary particles', and the interactions between these particles and the (red and yellow) particles representing the two fluids determine the wetting behaviors of the fluids. Both cross-sections are in planes perpendicular to the plane of the fracture. In this simulation, the yellow fluid is much more strongly wetting than the red fluid.

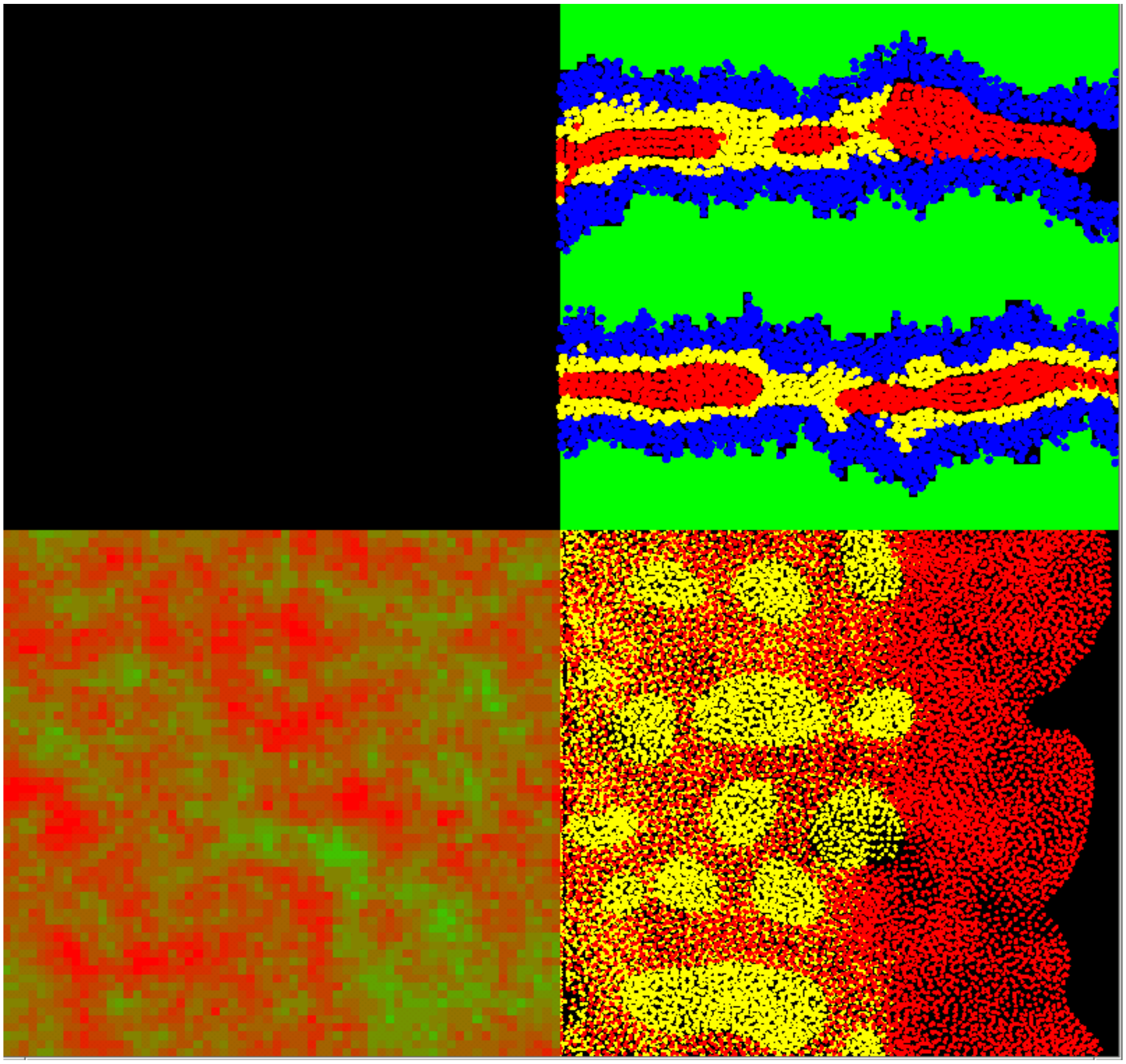

Figure 1b. A later stage in the simulation illustrated in Figure 1a.

parameter. Unfortunately, the motion of the particles results in momentum transfer between adjacent regions with different flow velocities, and this adds to the effective viscosity. However, the finite-difference/level-set method does not rigorously conserve mass, and it is difficult to apply this method to geometrically complex systems such as porous media and fracture apertures with realistic geometries. The finite-difference/level-set method is illustrated in Figure 2.

As Figure 1 shows, it is possible to use smoothed particle hydrodynamics to simulate fluids that do not fill the space that they occupy, but there are no particles in the low density 'vapor' phase and the effects of the pressure associated with the low density fluid are not included in the simulation. It is also possible to simulate liquid/vapor systems using a Van-der-Waals equation of state, but large density ratios cannot be simulated using this approach. We have been evaluating the approach of Colagrossi and Landri

(Journal of Computational Physics 191, 448-475 (2003)), which employs particles of different mass for the liquid (water) and gas (air) phases. Using this method, we expect tobe able to simulate multiphase fluid flow with density ratios of the order of 1000 (the water/air density ratio is approximately 750 at standard temperature and pressure).

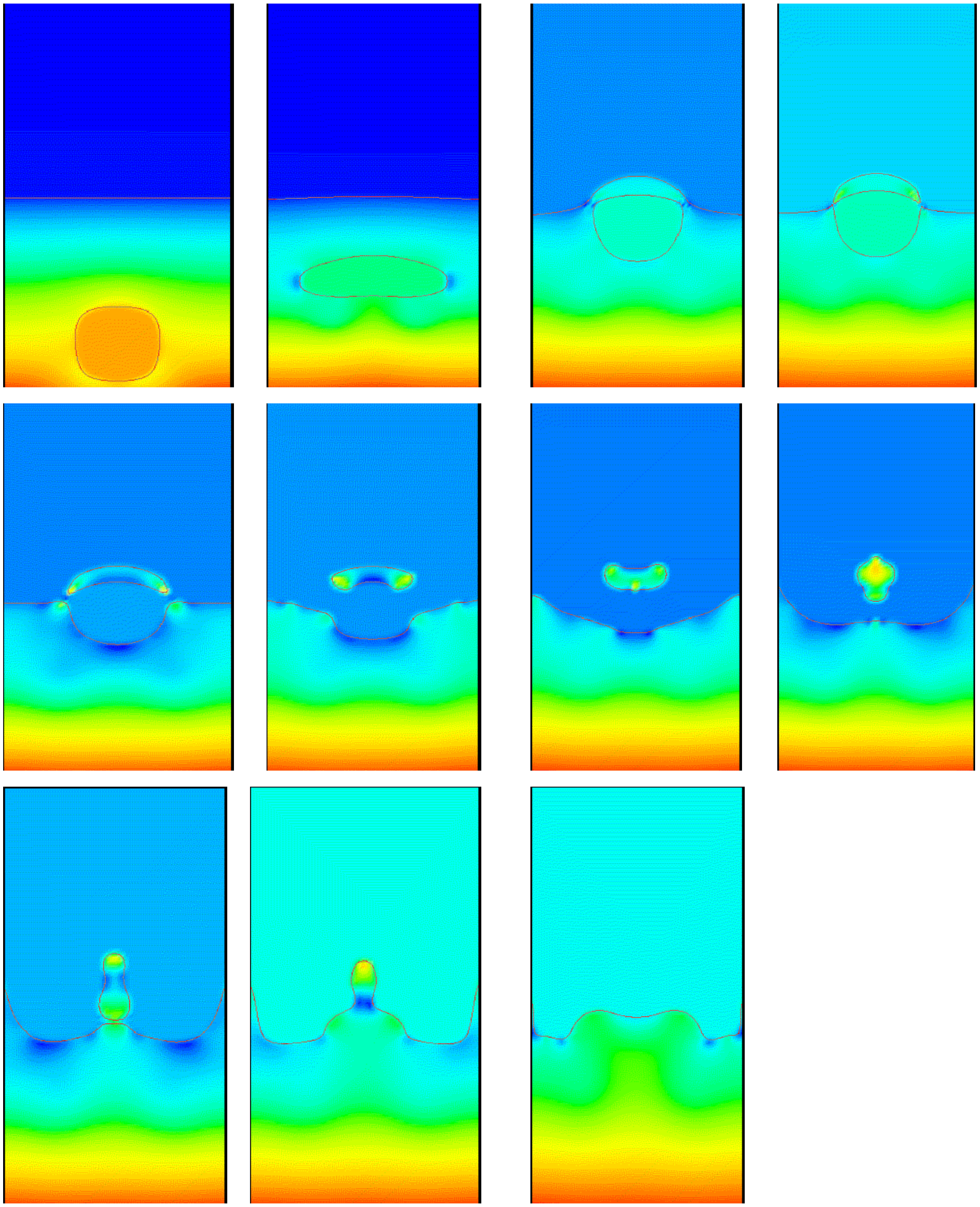

Figure 2. A two-dimensional finite-difference/level-set simulation of the rise and bursting of a bubble of air in water. The color scale shows the pressure field. This simulation demonstrates that the level-set method can be used to capture fluid-fluid interfaces during both fragmentation and coalescence processes.

Experiments

A series of experiments was conducted to characterize the flow regimes for flow in parallel-wall channels with aperture widths varying from approximately 0.15 mm to 3.0 mm and flow rates varying from approximately 10 ml/hr to 8200 ml/hr. The experiments were carried out using the setup shown in Figure 3.

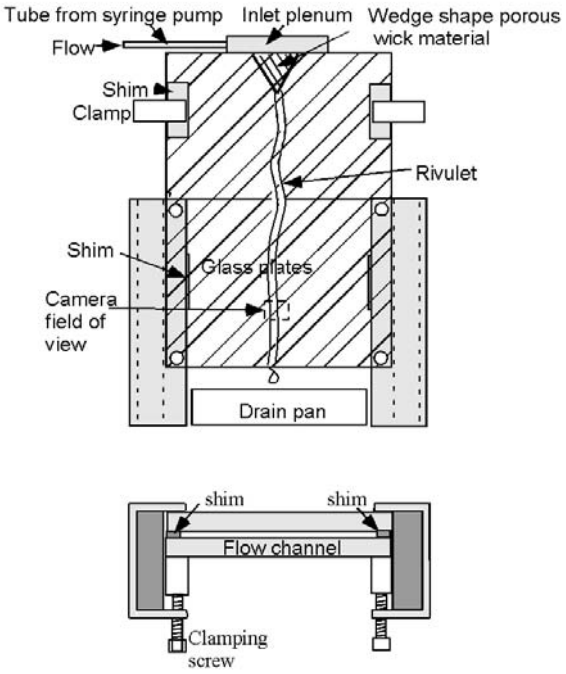

Figure 3: The experimental setup used to investigate fluid flow in a uniform aperture.

Under low flow rate conditions, the liquid enters the channel as separate drops that wet either one or both walls, depending on aperture width and flow rate. At higher flow rates, the liquid forms rivulets. A critical flow rate separates a high flow rate/small aperture regime in which the rivulet wets both walls from a low flow rate/large aperture regime in which the rivulet wets only one wall. An initially two-sided rivulet will transition to a one-sided rivulet if the flow rate is reduced below a critical value, and an initially one-sided rivulet will transition to a two-sided rivulet if the flow rate is increased above a critical value. Both one-sided and two sided rivulets follow essentially vertical paths below a critical flow rate. Above this critical flow rate, the linear rivulet becomes a stable meandering rivulet, like that shown in Figure 4. The stable meandering rivulet becomes unstable above a higher critical flow rate. The trajectory of an unstable meandering rivulet is transient and the rivulet may split into separate branches. Figure 5 illustrates some of the behavior observed in this highly dynamical regime. Under these

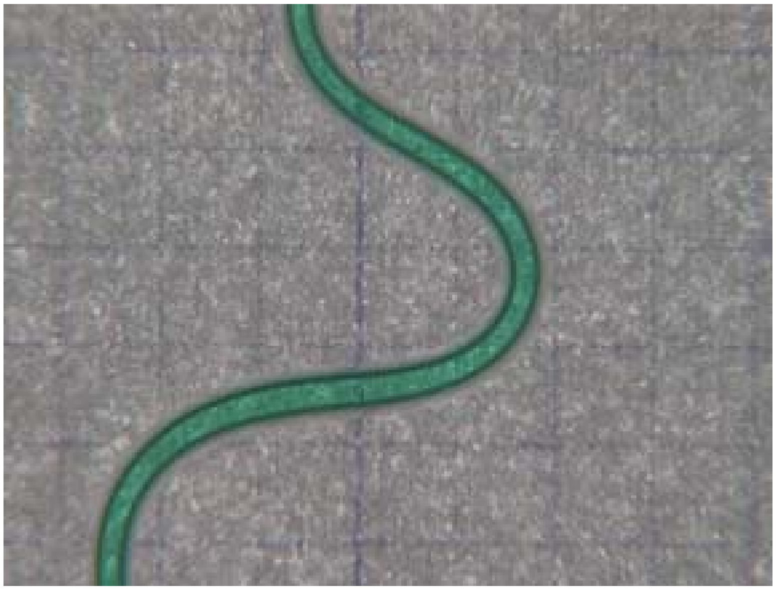

Figure 4: A two-sided stable meandering rivulet in a 0.9 mm aperture. The water flow rate was 500 ml/hr.

Figure 5: Unstable meandering rivulet flow showing the formation of a new rivulet. The liquid drops mark abandoned rivulet paths.

flow conditions, the rivulets dynamically come into contact with much of the fracture surface, and this will facilitate the exchange of materials between the aperture and the surrounding porous rock matrix.

Figure 6 shows how the likely flow behavior for water depends on the flow rate and aperture. A similar series of transitions occurs with different fluids. However, two-sided rivulets will not form if the aperture is too large.

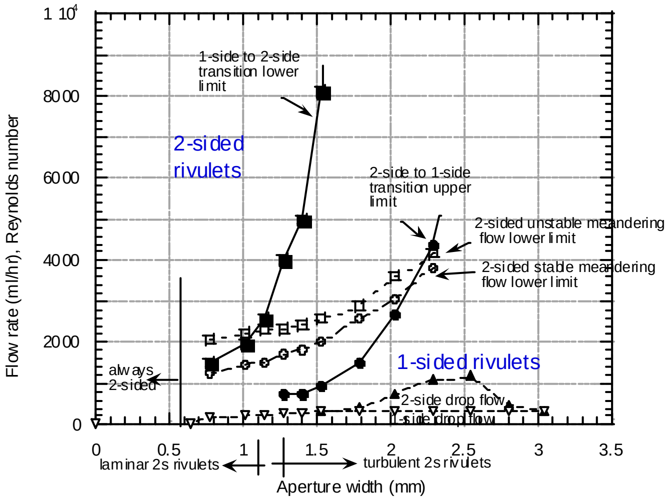

Figure 6: A 'phase diagram' showing how the flow behavior depends on flow rate and aperture for water in a uniform glass-walled aperture.

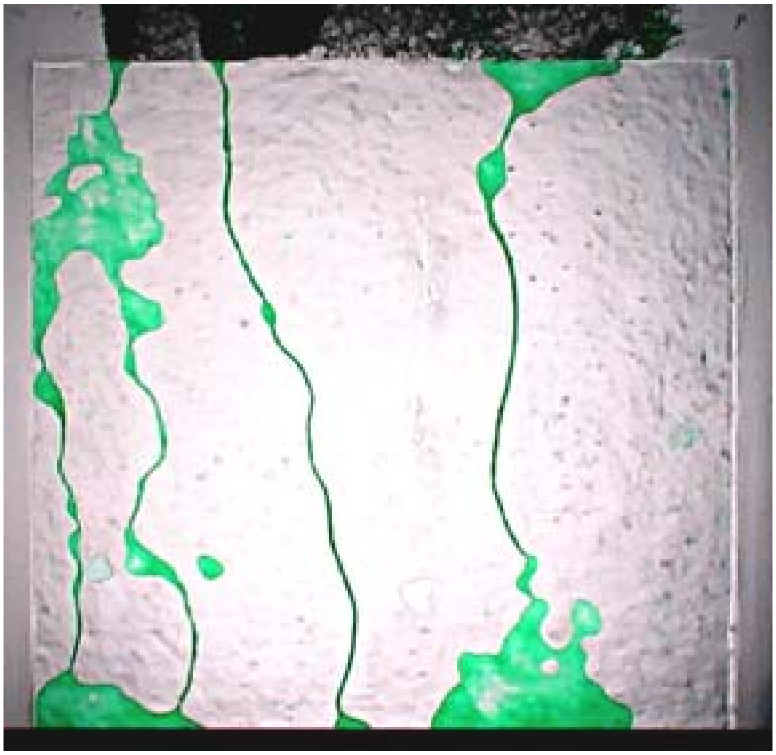

Figure 7: Rivulets in a synthetic fracture aperture fabricated using sterolithography.

On the other hand, the higher flow rates associated with unstable meandering will result in deeper and faster penetration through fractures in the unsaturated zone.

Experiments have also been conducted to investigate flow regimes in a simulated fracture aperture with a realistic geometry. As Figure 7 illustrates, the water forms rivulets similar to those observed in parallel walled channels. The widths of the rivulets vary due to variations in aperture spacing, and the water pools in areas where the walls are close to touching due to capillary forces. The average aperture in this experiment was approximately 0.5 mm.

The experiments with parallel walled fractures are an important step towards developing a better understanding of flow in apertures with realistically complex geometries. The experiments with parallel walled fractures can be more easily understood, and they provide a basis for understanding the behavior observed in experiments carried out with more complex systems.

Theoretical work

A simple theoretical model for rivulet flow in a smooth-walled fracture aperture was developed. The model predicts that the width of the rivulet is given by

$$W = \frac{12Q\nu}{g\delta^3}, \qquad [1]$$

where Q is the volumetric flow rate, ν is the kinematic viscosity, g is the acceleration due to gravity and δ is the full width of the aperture. The approximate theoretical model is based on mass conservation and a balance between friction (viscous) forces and body forces due to gravity acting on the difference in density between the liquid in the rivulet (water, for example) and the surrounding fluid (air, for example). The model applies for steady laminar flow of an incompressible fluid surrounded by an inviscid fluid. Equation [1] is applicable to rivulet flow in narrow apertures, and it is important because the width of the rivulet is one of the factors controlling the exchange of fluid and contaminants between the fracture aperture and the surrounding porous matrix in the subsurface. The variations in the rivulet widths shown in Figure 9 are qualitatively consistent with equation 1.

In follow-on work, the predictions of equation [1] were tested by comparison with experiments. A rivulet consists of an inner region, which is completely filled by fluid, and this is extended by wetting and capillary effects. It is assumed that essentially all of the flow occurs in the central region, and the width W in equation [1] is the width of this inner region (the 'inner width' W_i in Figure 8). The total width (the 'outer width' W_o in Figure 8) can be calculated by adding twice the depth of the meniscus, calculated geometrically from the aperture and the contact angle, to the inner width.

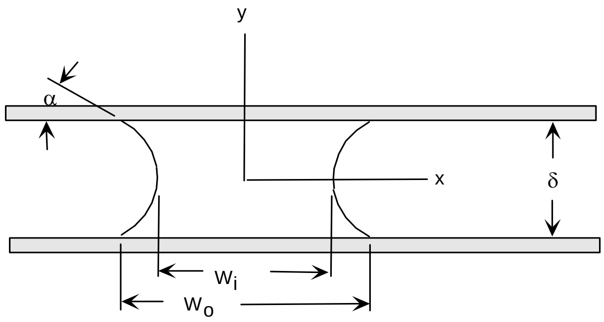

Figure 8: The cross-section geometry of a rivulet confined between two parallel planar surfaces. The inner width W_i is the width W in equation [1], and W_o is the outer width. The flow is in the downward z direction, perpendicular to the plane of the Figure.

Figure 9 compares the rivulet width predicted by equation 1 with the results of experiments. The agreement between the experiments and Figure 1 is within the estimated uncertainties expected from the uncertainty in the determination of fundamental variables such as the width of the aperture and measurement errors.

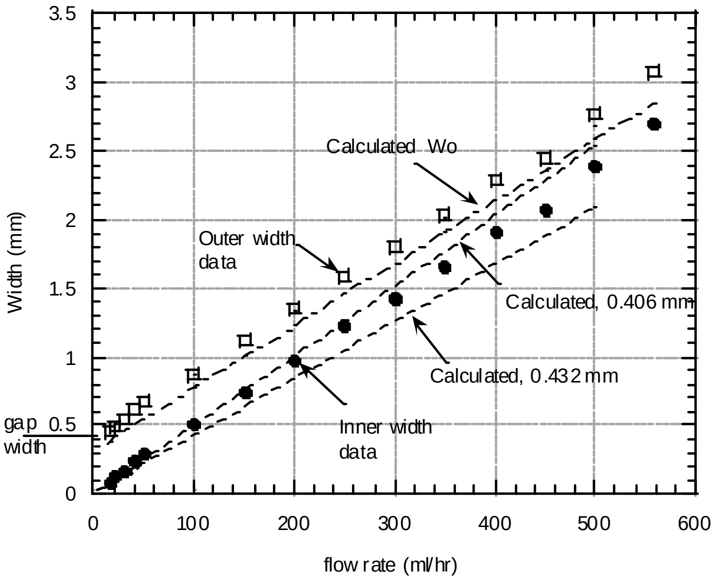

Figure 9: A comparison between the measured inner and outer rivulet widths and the predictions of the simple theoretical model for water in a 0.419 mm aperture. Similar results were obtained using ethanol, mineral oil and water with a wetting agent.

Planned activities

During the remaining 15 months we will focus on additional development of the numerical methods and detailed comparison between experiments and computer simulations. We will begin by trying to reproduce the results observed in the experiments carried out using parallel walled apertures, and proceed to testing the results of the simulations against experiments carried out using apertures with known geometries fabricated using sterolithography. Because of limited computer resources, we have been confined to two-dimensional simulations and relatively small-scale three-dimensional simulations. The laboratory expects to acquire a Beowulf cluster with 460 64 bit AMD Opteron processors and 12Tb of additional storage. This system should be operational early in FY05, and it will be available to the foreign national postdoctoral associates who will be working on this program. This new computer system will make it possible for us to carry out simulations on a substantially larger scale.

We plan to further investigate the use of level-set interface capturing, volume-of-fluid interface tracking and a combination of these approaches to perform grid-based multiphase flow simulations. These simulations will provide us with an alternative approach to the simulation of multiphase flow in fractures and will enable us to assess the effects of compressibility on simulations carried out using the particle based methods. The primary challenge will be the extension of our two-dimensional simulations to three dimensions and the development of methods that include realistic contact-line dynamics in systems with complex geometries.

The main focus will be on the quantitative comparison of different modeling methods and experiments. We plan to use experiments carried out in our own laboratory – like those shown in Figures 3-8, and experiments reported in the literature. In particular, we plan to simulate rivulet flow, film flow and flow through fracture junctions.

Additional experiments will be carried out using a variety of aperture geometries and apertures with fill materials. So far our work has focused on vertical fractures. We plan to investigate inclined fractures during the next year.

Information Access:

Publications:

1. Transition to Meandering Rivulet Flow in Vertical Parallel-Plate Channels. Glenn E. McCreery and Donald M. McEligot., Accepted for publication in the Journal of Fluid Engineering.

2. Rivulet flow in vertical parallel-wall channels. Glenn E. McCreery, Paul Meakin, and Donald M. McEligot. Submitted to the International Journal of Multiphase Flow.