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The project used numerical and analytic techniques to study a number of problems involving transport of fluids in porous media, with application to subsurface fluid dynamics in hydrocarbon reservoirs and aquifers.

1. Transit-time distributions in source-sink flows

The long-time tail of the arrival-time distribution function for passive tracer released in a subsurface flow between a source and a sink was found to have universal properties which should be useful in reservoir diagnostics. Generally these distributions vary with time asymptotically as $p(t) \sim t^{-p}$ and the key observation is that the exponent p depends only on the multipole order of the source-sink distribution, but is independent of the precise geometry of the fluid-occupied region and the spatial location of sources and sinks. The results were obtained first by explicit computation and then more generally by a scaling analysis, and were verified by experiments and numerical simulations.

- Anomalous dispersion in a dipole flow geometry, P. Kurowski, I. Ippolito, E. J. Hinch, J. Koplik and J. P. Hulin, *Phys. Fluids* **6**, 108 (1994).
- Tracer dispersion in planar multipole flows, J. Koplik, S. Redner and E. J. Hinch, *Phys. Rev. E* **50**, 4650 (1994).
- Universal and non-universal first-passage properties of planar multipole flows, J. Koplik, S. Redner and E. J. Hinch, *Phys. Rev. Lett.* **74**, 82 (1995).
- Tracer dispersion in three-dimensional multipole flows, M. Zhang and J. Koplik, *Phys. Rev. E* **56**, 4244 (1997).
- The tracer transit time distribution in multipole reservoir flows, J. Koplik, *Transport in Porous Media* **42**, 1999 (2001).

2. Deep-bed filtration in porous media

In order to understand particle deposition in porous media, we first studied simplified lattice models of particle motion with trapping dynamics, and then carried out detailed pore-level calculations using the Stokesian dynamics method to track the motion of suspended particles through a fixed bed. The results of the latter were used to develop rules for the motion of finite-sized particles at junctions in the flow paths and to investigate possible cooperative trapping mechanisms.

- First passage time in a two-layer system, J. Lee and J. Koplik, *J. Stat. Phys.* **79**, 895 (1995).
- Simple model of deep-bed filtration, J. Lee and J. Koplik, *Phys. Rev. E* **54**, 4011 (1996).
- Microscopic motion of particles flowing through a porous medium, J. Lee and J. Koplik, *Phys. Fluids* **11**, 76 (1999).
- Network models of deep bed filtration, J. Lee and J. Koplik, *Phys. Fluids* **13**, 1076 (2001).

3. Nonlinear flow in porous media

In order to clarify competing predictions for the form of the finite Reynolds number generalization of Darcy's law, we conducted extensive finite element calculations of flow through model porous media. The result was that both previous proposals were correct in their appropriate parameter ranges: the pressure gradient is linear in average velocity at low Reynolds number (Darcy's law) and quadratic at high Reynolds number (Forcheimer's law), but these two behaviors are separated by a transitional region where the behavior is cubic.

- Non-Darcy flow in porous media, J. Koplik and S. Rojas, Phys. Rev. E **58**, 4776 (1998).

4. Permeability and hydrodynamic dispersion in self-affine fractures

We used numerical simulations and approximate analytical methods to study (Newtonian) fluid flow and passive tracer dispersion in self-affinely rough two and three-dimensional fractures. The fractures were generated by a Fourier synthesis method with the experimental value of the Hurst exponent, and flow and concentration fields within them were obtained by the lattice-Boltzmann method. In the case of fracture joints, both numerical results and effective medium analyses give consistent scaling laws for permeability and velocity fluctuations, involving the mean gap and Hurst exponent. For laterally-displaced fracture faults, the flow is distinctly channeled and anisotropic, with reduced permeability parallel to the shift and little change in the orthogonal direction. We then considered mechanical dispersion resulting from velocity variation in the plane of the fracture, showing first that this mechanism dominated Taylor dispersion for very narrow fractures, and then discussing diffusivity in terms of the velocity autocorrelation function. The effective diffusivity was found to decrease with mean aperture as observed experimentally, reflecting a competition between decreasing fluctuation magnitude and increasing correlation length, while the degree to which the transit-time distributions were Gaussian varied with the presence of low-velocity zones.

- Numerical study of geometrical dispersion in self-affine rough fractures, F. Plouraboué, J. P. Hulin, J. Koplik and S. Roux, Phys. Rev. E **58**, 3334 (1998).
- Permeability of self-affine rough fractures, G. Drazer and J. Koplik, Phys. Rev. E **62**, 8076 (2000).
- Tracer dispersion in two dimensional rough fractures, G. Drazer and J. Koplik, Phys. Rev. E **63**, 056104 (2001).
- Transport in rough self-affine fractures, G. Drazer and J. Koplik, Phys. Rev. E **66**, 026303 (2002).

5. Fractal structure of dispersion fronts

We studied the fluctuations in the shape of a high-Péclet number dispersion front expanding radially in a self-affine fracture, and found that the front itself developed a self-affine structure with the same Hurst exponent as the fracture surface. In effect, a self-affine fractal

surface is able to “impose itself” on a flexible object moving through it. We used numerical simulations as described above to improve the resolution and statistical uncertainty of earlier experimental observations suggesting this behavior, and analyzed the front using an average wavelet analysis which is more suitable than box-counting for self-affine structures. The range of length scales over which the front was self-affine was bounded below by the mean fracture aperture and above, remarkably, by the entire width of the front (growing linearly with time), rather than the surface correlation length.

- Self-affine fronts in self-affine fractures, G. Drazer, H. Auradou, J. Koplik and J.-P. Hulin, *Phys. Rev. Lett.* **92**, 014501 (2004).

6. Permeability anisotropy in flow through fractures

The permeability anisotropy resulting from a shear displacement between the complementary self-affine walls of a rough fracture was investigated using experiments and lattice Boltzmann calculations. In the laboratory, a dyed fluid was radially injected into a transparent fracture and displaced a transparent one. A clear anisotropy is observed in the presence of shear displacements and allowed us to estimate the ratio of the permeabilities for flow parallel and perpendicular to the shift. Numerical simulations gave consistent results, and allowed us to explore the parameter space in more detail. A simple model was proposed which accounts for the development of channels perpendicular to the shift, which qualitatively explains these results and in particular predicts a permeability decreasing (increasing) linearly with the variance of the aperture field for flow parallel (perpendicular) to the shear displacement.

- Permeability anisotropy induced by the shear displacement of rough fracture walls, H. Auradou, G. Drazer, J. Koplik and J.-P. Hulin, *Water Resources Res.* **41**, W09423 (2005).
- Shear displacement induced flow channelization in a single fracture, H. Auradou, G. Drazer, A. Boschan, J.-P. Hulin and J. Koplik, submitted to *Geothermics*.

7. Particle motion and wall interactions in a flowing fluid

We studied the interplay of deterministic and stochastic behavior in the dynamics of a sheared suspension, using Stokesian dynamics methods. The specific goal was to understand the respective contributions of shear and viscous particle interactions to velocity fluctuations and the suspension microstructure. It was found that two-particle interactions dominate, and furthermore that the use of a short-ranged artificial repulsive force can efficiently model the effects of surface roughness. A second set of calculations used molecular dynamics simulations to investigate the interaction between a colloidal particle in a flowing fluid and a solid wall, with an emphasis on the effects of the degree of wetting of the fluid. A sharp transition between steady transport and adsorption and stick-slip motion was found, as the strength of the fluid molecule-solid atom interaction decreases. Above the transition, the particle’s behavior is in good agreement with continuum hydrodynamics despite substantial thermal fluctuations, whereas the adsorbed behavior seems to be a distinctive nano-scale effect. Hysteretic effects were observed in the particle adsorption process, and associated with long-term structural rearrangements in the fluid.

- Deterministic and stochastic behavior of non-Brownian spheres in sheared suspensions, J. Fluid Mech. **460**, 307 (2002), G. Drazer, B. Khusid J. Koplik and A. Acrivos.
- Adsorption phenomena in the transport of a colloidal particle through a nanochannel containing a partially wetting fluid, Phys. Rev. Lett. **89**, 244501 (2002), G. Drazer, A. Acrivos and B. Khusid and J. Koplik.
- Microstructure and velocity fluctuations in sheared suspensions, G. Drazer, J. Koplik, B. Khusid and A. Acrivos, J. Fluid Mech. **511**, 237 (2004),
- Wetting and particle adsorption in nanoflows, G. Drazer, J. Koplik, A. Acrivos and B. Khusid, Phys. Fluids **17**, 017102 (2004),
- Hysteresis, force oscillations, and non-equilibrium effects in the adhesion of nanoparticles to atomically smooth surfaces, G. Drazer, B. Khusid, J. Koplik and A. Acrivos, Phys. Rev. Lett. **95**, 016102 (2005).

8. Non-Newtonian flow

As an first step in considering the dynamics of non-Newtonian fluids in fractures, we developed and tested a numerical code based on a modified version of the lattice-Boltzmann method. The basic idea is due to Aharonov and Rothman and involves adjusting the relaxation time parameter in the BGK approximation to the Boltzmann equation locally, so that the viscosity has the correct (power-law) dependence on the strain rate. The code was tested on a non-trivial reentrant corner flow, which contains nearly-singular corner regions of high stress as well as channel-flow regions with mild linear stress variation, and the results agreed well with a finite element continuum calculation. Furthermore, even in the simplest version of the algorithm, the errors were found to decrease with increasing lattice resolution faster than $1/N$.

- Lattice-Boltzmann method for non-Newtonian (power-law) fluids, S. Gabbanelli, G. Drazer and J. Koplik. Phys. Rev. E **72**, 046312 (2005).