Pr Michel LOUGE

Cornell University

"Statistical mechanics of unsaturated porous media"

Abstract:

Unsaturated porous media are ubiquitous in agriculture, natural resources and industry (e.g., soils, mining, oil reservoirs, fuel cells, mercury porosimetry). The main challenge is to predict how a wetting phase permeates the porous matrix in response to an applied capillary pressure.

Although recent progress in numerical simulations and X-ray tomography at 3SR have revealed the detailed behavior of unsaturated porous media, the current state-of-the-art in practical applications is to perform experiments on a porous sample and to fit parameters of the "retention curve" relating fluid saturation and capillary pressure, from which permeability can be evaluated.

Our objective is to predict the retention curve directly from known surface energies and dry void geometry without further empirical input. To that end, we derive an equilibrium mean-field theory of fluid retention in porous media near saturation using statistical mechanics. In the limit of vanishing inertial and viscous forces, the theory predicts the fluid retention curve that relates saturation of the porous matrix to applied capillary pressure.

To avoid complicated calculations, we deliberately adopt the simplest statistical mechanics, in which a unit cell is made up of a single cavity interacting with its neighbors through narrow openings called "links", while possessing only two energy states that are either full or empty of fluid. We show how the resulting retention curve can be calculated from the statistical distribution of two dimensionless parameters measuring the areas of, respectively, link cross-section and wetted cavity surface with respect to cavity volume.

We illustrate the theoretical predictions with a porous domain consisting of a random packing of spheres. The theory attributes hysteresis of the retention curve to collective first-order phase transitions in the ensemble of cavities. We show that hysteresis strength grows with relative link cross-section and weakens as the joint distribution of relative link cross-section and cavity wetted area broadens. We suggest that abrupt phase transitions on the mesoscopic scale are the origin of "Haines jumps", which we model and compare with recent data.

An estimate of the correlation length among neighboring cavities implies that experimental reproducibility of the fluid retention curve worsens at intermediate saturation as capillary pressure is applied across distant boundaries. This suggests that the Richards equation capturing the spatio-temporal evolution of saturation in porous media should be integrated with a retention curve measured for a mesoscopic domain of relatively small size. The theory also provides a framework for interpretating numerical simulations and X-ray tomographic data.