Final Report

NORTHWESTERN UNIVERSITY
Department of Civil and Environmental Engineering
Evanston, IL 60208

Grant: DE-FG02-08ER15980

Multiscale framework for predicting the coupling between deformation and fluid diffusion in porous rocks

José E. Andrade, (626) 395-4141, jandrade@caltech.edu
John W. Rudnicki, (847) 491-3411, jwrudn@northwestern.edu

Website: http://www.geomechanics.caltech.edu

Objective: To develop a predictive multiscale framework to hierarchically homogenize the constitutive behavior of fluid-saturated rocks, directly linking the continuum representation with granular processes, in areas of severe deformation, such as deformation banding, where phenomenology breaks down.

Project description: In this project, a predictive multiscale framework will be developed to simulate the strong coupling between solid deformations and fluid diffusion in porous rocks. We intend to improve macroscale modeling by incorporating fundamental physical modeling at the microscale in a computationally efficient way. This is an essential step toward further developments in multiphysics modeling, linking hydraulic, thermal, chemical, and geomechanical processes. This research will focus on areas where severe deformations are observed, such as deformation bands, where classical phenomenology breaks down.

Multiscale geometric complexities and key geomechanical and hydraulic attributes of deformation bands (e.g., grain sliding and crushing, and pore collapse, causing interstitial fluid expulsion under saturated conditions), can significantly affect the constitutive response of the skeleton and the intrinsic permeability. Discrete mechanics (DEM) and the lattice Boltzmann method (LBM) will be used to probe the microstructure---under the current state---to extract the evolution of macroscopic constitutive parameters and the permeability tensor. These evolving macroscopic constitutive parameters are then directly used in continuum scale predictions using the finite element method (FEM) accounting for the coupled solid deformation and fluid diffusion.

A particularly valuable aspect of this research is the thorough quantitative verification and validation program at different scales. The multiscale homogenization framework will be validated using X-ray computed tomography and 3D digital image correlation in situ at the Advanced Photon Source in Argonne National Laboratories. Also, the hierarchical computations at the specimen level will be validated using the aforementioned techniques in samples of sandstone undergoing deformation bands.

Results

We obtained samples of Aztec sandstone from the Valley of Fire (Nevada). Five were taken from inside a compaction band and four from outside the compaction band. Specimens were scanned at the synchrotron APS, at Argonne National Laboratory to obtain X-ray CT images. A sample slice of the images obtained is shown in Figure 1. By stacking images such as these we are able to non-destructively reconstruct the three-dimensional microstructure of sandstones inside compaction bands for the first time. We do this using new computational techniques that use level set methods and concepts from graph theory. We obtain not only porosity but also other important microstructural attributes, such as occluded/connected porosity and geometrical tortuosity.

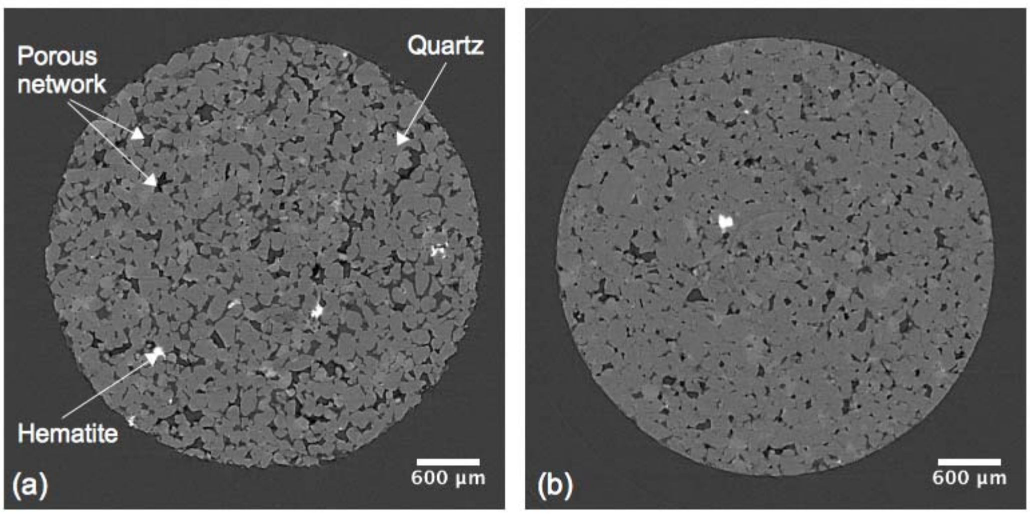

Figure 1. Sample horizontal CT slices from Aztec sandstone. (a) Outside compaction band and (b) inside compaction band.

To relate the microstructural structure obtained from the digital images to macroscopic fluid transport behavior we have developed a new computational multiscale framework. The framework uses a hybrid lattice Boltzmann/finite element scheme to obtain homogenized effective permeability at specimen-scale. We demonstrate the applicability and efficiency of this multiscale framework by two examples, one using a synthetic array and another using a sample of natural sandstone with complex pore structure.

Results obtained from the Aztec sandstone samples reveal approximately an order of magnitude permeability reduction within the compaction band. This is less than the several orders of magnitude reduction measured from hydraulic experiments on compaction bands formed in laboratory experiments and about one order of magnitude less than inferences from two-dimensional images of Aztec sandstone. Geometrical analysis concludes that the elimination of connected pore space and increased tortuosities due to the porosity decrease are the major factors contributing to the permeability reduction. In addition, the multiscale flow simulations also indicate that permeability is essentially isotropic inside and outside the compaction band.

These methods and results are explained in more detail in the publications listed below.

Publications

N. Lenoir, J.E. Andrade, W.C. Sun, and J.W. Rudnicki. Permeability measurements in sandstones using x-ray ct and lattice Boltzmann calculations inside and outside of compaction bands. Advances in Computed Tomography
for Geomaterials, pages 279–286. GEOX2010, ISTE & Wiley, 2010

W.C. Sun, J.E. Andrade, and J.W. Rudnicki. Multiscale method for characterization of porous microstructures and their impact on macroscopic effective permeability. International Journal for Numerical Methods in Engineering,
88:1260–1279, 2011.

W.C. Sun, J.E. Andrade, J.W. Rudnicki, and E. Eichhubl. Connecting microstructural attributes and permeability from 3d tomographic images of in situ shear-enhanced compaction bands using multiscale computations.
Geophysical Research Letters, 38, 2011.