UNIVERSITY of HOUSTON

CULLEN COLLEGE of ENGINEERING

Department of Civil & Environmental Engineering

CIVE 6111 Graduate Seminar Series

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Atomic - to Pore-Scale Understanding and Prediction of Mineral Precipitation

Monday, November 24, 2014

10:30 am - 11:30 am

Room: D3 W205

Abstract

The ability to predict and control the nucleation and growth of minerals is important for a variety of applications such as disposal of spent nuclear fuel, scale formation during oil, gas and geothermal production, remediation of contaminants such as toxic metals and sequestration of carbon dioxide. Macroscopic net mineral reaction rates morphologies are ultimately driven by atomic-scale reactions on surfaces, but determining precise atomic-level reaction mechanisms and discovering how these translate to macroscopic observables such as effects on porosity and permeability is a daunting task. In this talk, I will focus our recent work to understand the precipitation of two minerals important industrially and environmentally, barite ($BaSO_4$) and calcite ($CaCO_3$). The talk will range from the atomic-, meso- and pore-scales using atomistic computational simulation, atomic force microscopy, interferometry and small angle neutron and X-ray scattering. Rare event theory can be used to model reactions at the atomic-scale thought to control rates of monomolecular step velocity at the mesoscale measured by microscopy on single crystals. Rate expressions from these can be derived to predict macroscopic growth rates as measured by changes in solution composition. Precipitation in pores leads to a pore-size dependence depending on the interaction between the substrate and precipitate.

About the speaker:

Dr. Andrew G. Stack is a Senior R&D Staff Member in the Geochemistry and Interfacial Sciences Group, Chemical Sciences Division at Oak Ridge National Laboratory. He is a geochemist who specializes in understanding the kinetics and mechanisms of mineral reactions, and how these inherently molecular-level processes manifest themselves at larger scales. Reactions he has examined include mineral growth and dissolution, incorporation of impurities, electron transfer and ligand exchange. He studies these using a variety of computational, experimental and theoretical approaches. He is currently the Division Chair for the American Chemical Society, Geochemistry Division.

Atomic- to pore-scales of mineral surface structure and reaction