A Pore-Scale Analysis of the Electrical Properties of Partially Saturated Porous Media and Implications for Scaling Reactive Transport

Andy Ward*[1], Nazmul Hasan[1], Alexandre Tartakovsky[1], and Roelof Versteeg[2]
[1]Pacific Northwest National Laboratory, Richland, WA 99354; [2]Idaho National Laboratory, Idaho Falls, ID 83402

Pacific Northwest NATIONAL LABORATORY

INTRODUCTION AND OBJECTIVES

There have been numerous attempts to relate flow and transport properties to other characteristic material properties in heterogeneous, unconsolidated, partially saturated porous media. Most have failed to give satisfactory results by trying to relate transport properties to macroscopic geometric properties of smooth spherical grains and by failing to recognize the physical significance and sensitivity to the length scale in the predictions.

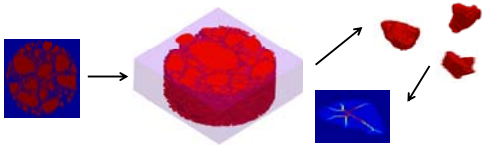
The interaction between the solid matrix, pore space, and pore fluids at the microscopic scale is critical to the development of the robust petrophysical relationships for predicting macroscopic flow and transport properties. Complex conductivity holds promise for characterizing the 3D distribution of permeability and its evolution over time; for detecting the presence of contaminants, and for monitoring reactions.

The objectives of this study are:

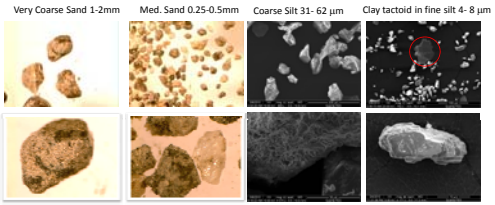
- To extend current pore-scale reactive transport theories and simulators to the prediction of pore-scale electrical properties
  - near-term focus compares empirical surface conductivity models
- Explore relationships between the effective electrical properties of unconsolidated porous materials as a function of porosity, saturation, clay content, and pore water composition
- Compare model predictions with laboratory complex conductivity measurements made on two cores from the Hanford and Ringold Formations at the IFRC site.

APPROACH

- Particle size distributions (psd), shape indices (sphericity and angularity) and packing efficiencies measured on representative facies from the IFRC Site
- Distribution of coordination numbers (number of contacts) , local void ratio, and packing efficiency derived from reconstructed X-ray CT images
- Smooth particle hydrodynamics (SPH) methods used to simulate multi-component flow, including water-air-solid interactions, transport, and reactions in realistic geometries
- Finite element (FE) techniques are used to solve the Laplace equation for electrical conductivity, including the effects of multiple fluid phases, double layer length, and counter-ion mobility
- Predict distributions of water, solute, and mineral precipitates as well as the current flow field at each pixel (2D) or voxel (3D)
- Effective hydraulic and electrical properties then calculated for each domain



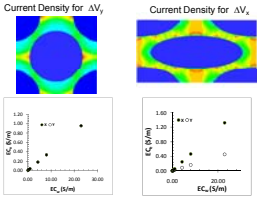
SEDIMENT CHARACTERIZATION



Optical and Scanning Electron Microscope Images of Selected Particle Size Classes

IFRC sediments are comprised of angular particles with low sphericities in all size classes that give rise to complex pore topology. Rough surfaces in all non-clay size classes are consistent with the underestimation of calculated geometrical properties like porosity, specific surface area, and surface area per unit pore volume. The clay fraction is mostly comprised of smectite and interstratified illite-smectite clays with small amounts of kaolinite. Clay minerals form tactoids of 10-50 μm that contribute to the underestimation of specific surface area of clay fractions. Effective characterization of complex microstructure is critical to accurate prediction of hydrogeophysical properties.

EFFECT OF PARTICLE SHAPE

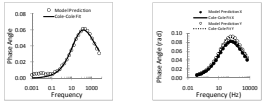


Maximum current density occurs orthogonal to applied field for both spherical and ellipsoidal particles

Bulk conductivity is a tensor controlled by particle shape. Conductivity is highest along the direction of lowest tortuosity.

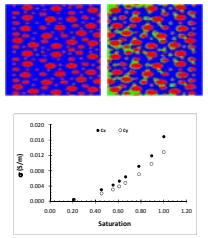
The presence of clay coatings influence the d.c conductivity as well as the complex conductivity and is compounded by particle shape. Conventional Cole-Cole models that assume spherical particles may not be applicable.

EFFECT OF CLAY COATINGS

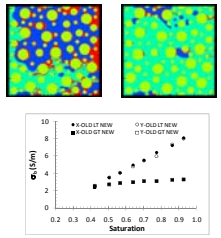


	Fitted Cole-Cole Parameters			
Shape	m	τ	c	k
Sphere	0.281	0.024	0.553	0.574
Ellipse-ΔV_y	0.356	0.032	0.584	0.533
Ellipse-ΔV_x	0.393	0.034	0.588	0.528

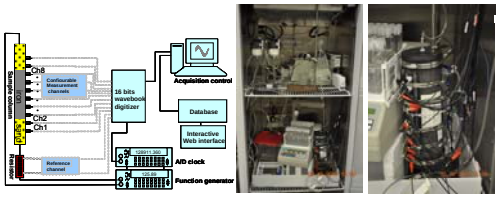
EFFECT OF SATURATION



PORE WATER COMPOSITION



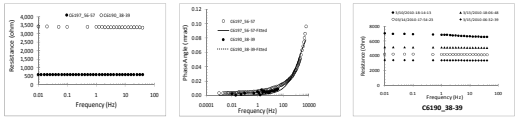
LABORATORY MEASUREMENTS



Schematic of INL complex resistivity system. The signal source is applied over the combination of the reference resistor and the sample, and full waveforms are collected for both the reference channel and the measurement channel(s). Subsequent processing gives the amplitude and phase for the measurement channel.

Cores instrumented Ag/AgCl current electrodes at the end of each core and with 9 electrodes along the core. Subsequent to this cores are placed in a temperature controlled chamber and a sequence of measurements is made including : 1) measurement in initial state, 2) measurement after saturation with synthetic Hanford groundwater, 3) measurement with water flowing through at 4 ml/minute, 4) measurement with the core at temperatures between 7.5 °C and 25 °C, and 5) measurement with the core saturated with groundwater with LiBr added (to simulate the effect of conductive tracers). Full waveform data is collected continuously by a dedicated computer according to user defined configuration files. Subsequent to data acquisition completion data is parsed into a MySQL relational database, and processed to extract phase and amplitude information for each frequency as well as real and imaginary conductivity.

LABORATORY RESULTS



Preliminary results of measurement on IFRC cores from the Hanford (C6190) and Ringold Formations (C6197) at the IFRC Site showing: (a) resistance as a function frequency for .Ringold and Hanford core, (b) measured phase and fitted Cole-Cole model; (c) resistance versus frequency for Hanford formation sediment in response to increasing LiBr concentration.

	Fitted Cole-Cole Parameters			
Formation	m	τ	c	k
Ringold	0.329	2.11E-04	0.683	0.505
Hanford	0.124	9.50E-02	0.584	0.533

Additional processing and interpretation is under way, but initial results show: 1) a modest but measurable IP signal associated with these cores; 2) a difference between the cores in terms of electrical properties, specifically, the core which appears finer grained has a larger IP signal. The introduction of the LiBr tracer causes a reduction in resistance, as would be expected. While further analysis is needed, these preliminary results support our contention that we can use spectral IP to enhance the mapping of facies and physical properties.

SUMMARY AND CONCLUSIONS

- IFRC sediments are comprised of angular particles with low sphericities in all size classes giving rise to complex pore topology and geometrical properties
- Aspherical particles result in an anisotropic response that is well described with a cementation index, *m* , tensor but not by traditional empirical complex conductivity models that assume smooth spherical particles.
- Desaturation causes a shift from a parallel-dominated to a series-dominated conductivity as the pore space becomes more tortuous, giving rise to a two-arc response at high frequencies.
- The history of saturation and pore water composition chemistry affects the conductivity response and this is reflected in different model parameters for empirical petrophysical relationships.
- The ability of the pore-scale model to correctly predict observed core-scale responses observed in validates the consistency of the approach and will allow investigation of the effects of system parameters on petrophysical relationships

FUTURE RESEARCH

- Reconstruction of complex pore topology from X-ray CT images and the generation of networks for pore-scale hydrogeophysical model simulations
- Implement mechanistic approach for electrochemical polarization effects in partially saturated media on the basis of pore-scale reactive transport theories and simple structural parameters
- Develop experimental methods and theory for predicting the time-dependent diffusive properties of partially saturated porous media, while accounting for heterogeneity of sorption and diffusion parameters

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