

1. Summary

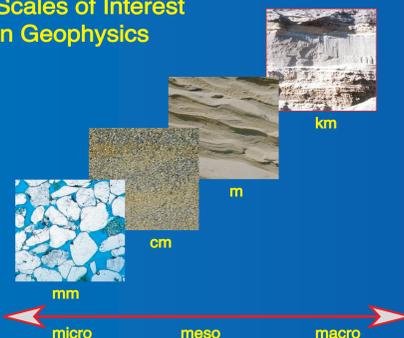
The accurate characterization and remediation of contaminated subsurface environments requires the detailed knowledge of subsurface structures and flow paths. Enormous resources are invested in scoping and characterizing sites using core sampling, 3-D geophysical surveys, well tests, etc.... Unfortunately, much of the information acquired is lost to compromises and simplifications made in constructing numerical grids for the simulators used to predict flow and transport from the contaminated area to the accessible environment. In rocks and soils, the bulk geophysical and transport properties of the matrix and of fracture systems are determined by the juxtaposition of geometric features at many length scales. In the interest of computational efficiency, recognized heterogeneities are simplified, averaged out, or entirely ignored in spite of recent studies that recognize that:

- (1) Structural and lithologic heterogeneities exist on all scales in rocks.
- (2) Small heterogeneities influence, and can control the physical and chemical properties of rocks.

In this work we propose a physically based approach for the description and treatment of heterogeneities, that highlights the use of laboratory equipment designed to measure the effect on physical properties of fine scale heterogeneities observed in rocks and soils. We then discuss the development of an integration methodology that uses these measurements to develop and upscale flow and transport models. Predictive simulations are "calibrated" to the measured heterogeneity data, and subsequently upscaled in a way that is consistent with the transport physics and the efficient use of environmental geophysics. This methodology provides a more accurate interpretation and representation of the subsurface for both environmental engineering and remediation. We show through examples, (i) the important influence of even subtle heterogeneity in the interpreting of geophysical data, and (ii) how physically based upscaling can lead to a different and more accurate description of a heterogeneous system, when compared to a more traditional upscaling approach that combines averaging and the application of core-based models. This may be of particular significance in bio-remediation studies where the link between microorganism activity and mesoscale flow through geologic structures, resides in the integration of multiscale processes.

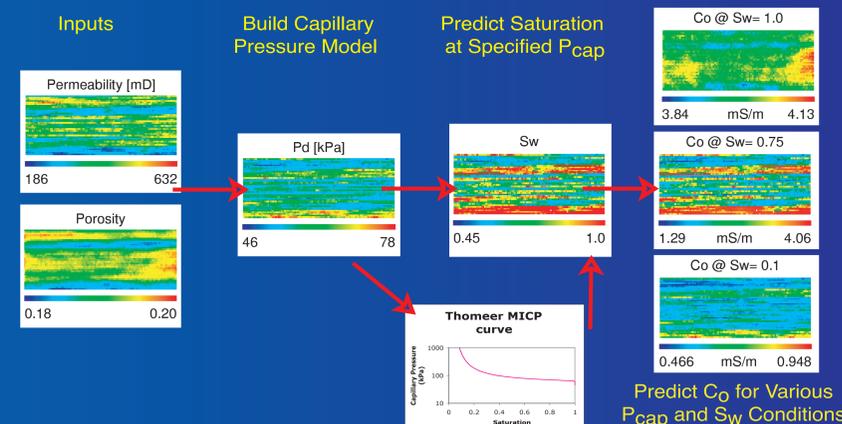
2. Problem Statement

Scales of Interest in Geophysics



- Geophysical measurements are commonly made at the micro- and macro- scales.
- Current measurement and modeling techniques ignore or simplify physical properties at the mesoscale.
- When do mesoscale heterogeneities control physical properties at the macroscale?
- How do we upscale microscale properties to the macroscale while honoring meso-scale heterogeneity?

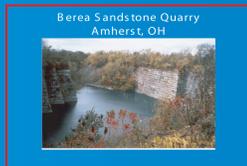
4. Comparing Standard and Physical Upscaling: An Example using Berea Sandstone



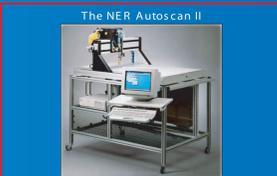
Workflow showing the process of calculating electrical conductivity (C₀) from maps of partial water saturation (S_w), employing the capillary pressure (P_{cap}) model of Thomeer and the partial-saturation Waxman-Smiths model.

3. Methodology/Workflow

Field Data (Macro scale)

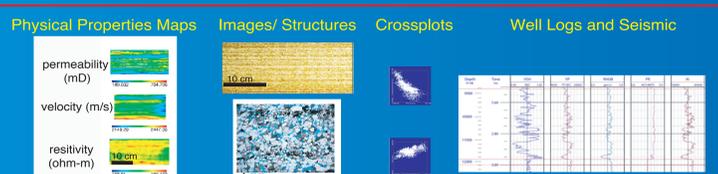


Lab Data (Micro/Meso scale)



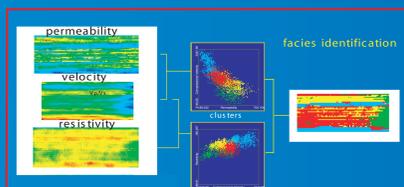
We have developed a multi-probe physical properties scanner that allows the mapping of geophysical properties on a slotted sample or core. This device permits the detailed study of heterogeneity at those length scales most difficult to quantify using standard field and laboratory practices. The measurement head consists of a variety of probes designed to make local measurements of various properties, including gas permeability, acoustic velocities (V_p, V_s), complex electrical impedance (4 electrodes, wide frequency coverage), and ultrasonic reflection (ultrasonic impedance and permeability). We can thus routinely generate detailed geophysical maps of a particular sample. We have been characterizing the heterogeneity of sandstones and unconsolidated soils and find that they exhibit complex heterogeneity at the centimeter scale.

Construct a Database



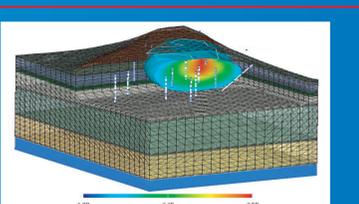
Data collected at a variety of scales are compiled in a database. The AutoScan II device enables the mapping of physical properties such as air permeability, complex resistivity, acoustic impedance, and ultrasonic velocity at the millimeter scale.

Build a Physical Model



In this example using Berea sandstone, cluster analysis is performed on the data in order to identify and map unique facies.

Apply the Model in the Field



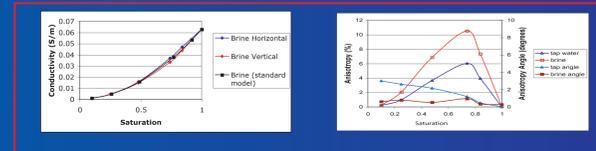
The resulting physical model can be incorporated into finite element flow and transport codes and applied at the field scale.

In this example, the FEHM flow and transport code is used to produce a realization of the dispersion of a groundwater contaminant plume.

Physically upscaled conductivity anisotropy is plotted as a function of saturation and fluid conductivity:

- Anisotropy increases rapidly from zero at full saturation to a maximum near 75% saturation.
- Standard upscaling predicts isotropic conductivity under all conditions.

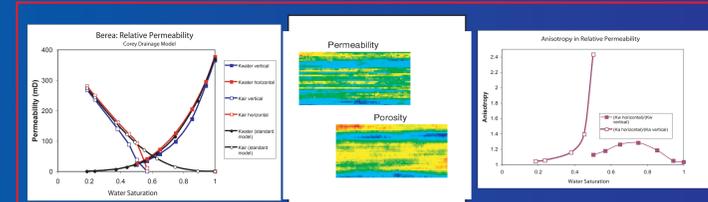
Upscaling Conductivity



Physically upscaled relative permeability is plotted as a function of saturation:

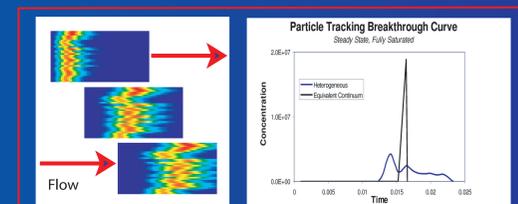
- Due to structural heterogeneities the non-wetting phase permeabilities go to zero by 60% partial saturation.
- For the wetting phase, relative permeability anisotropy is similar to, but stronger than the electrical conductivity case.
- Heterogeneities lead to significant anisotropy in the relative permeabilities for both phases.

Upscaling Relative Permeability



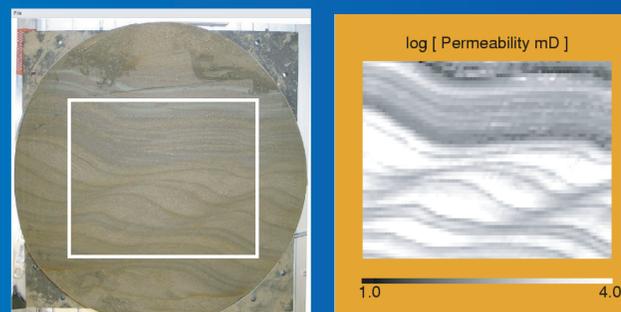
Details of the relative permeability curves can be understood by viewing the permeability maps as a function of saturation.

Upscaling Flow and Transport



Flow parallel to bedding with permeability heterogeneities measured by AutoScan II, leads to non-Fickian transport that causes the amplification and time dependence of longitudinal macrodispersivities commonly observed in field tests.

5. Unconsolidated Sands and Soils



The AutoScan II is now being used to collect permeability data on unconsolidated sands and paleosols from a Kame Quarry in Vermont. Permeability differences of up to 3 orders of magnitude are common, associated with cross beds and fine scale layering. These results imply that the upscaling methodology described above for consolidated rocks can be equally applied to unconsolidated samples.

6. Findings:

- Heterogeneities in a nominally homogeneous sandstone are observable at the mesoscale.
- These heterogeneities lead to anisotropic flow and transport behavior.
- Upscaling methods that explicitly include mesoscale heterogeneities lead to more robust predictive capabilities.
- These results are applicable to unconsolidated sands and soils.