PNNL SFA: Role of Microenvironments and Transition Zones in Subsurface Reactive Contaminant Transport

Facies-based Characterization of Hydrogeologic Structures and Reactive Transport Properties

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Project Objectives and Scope

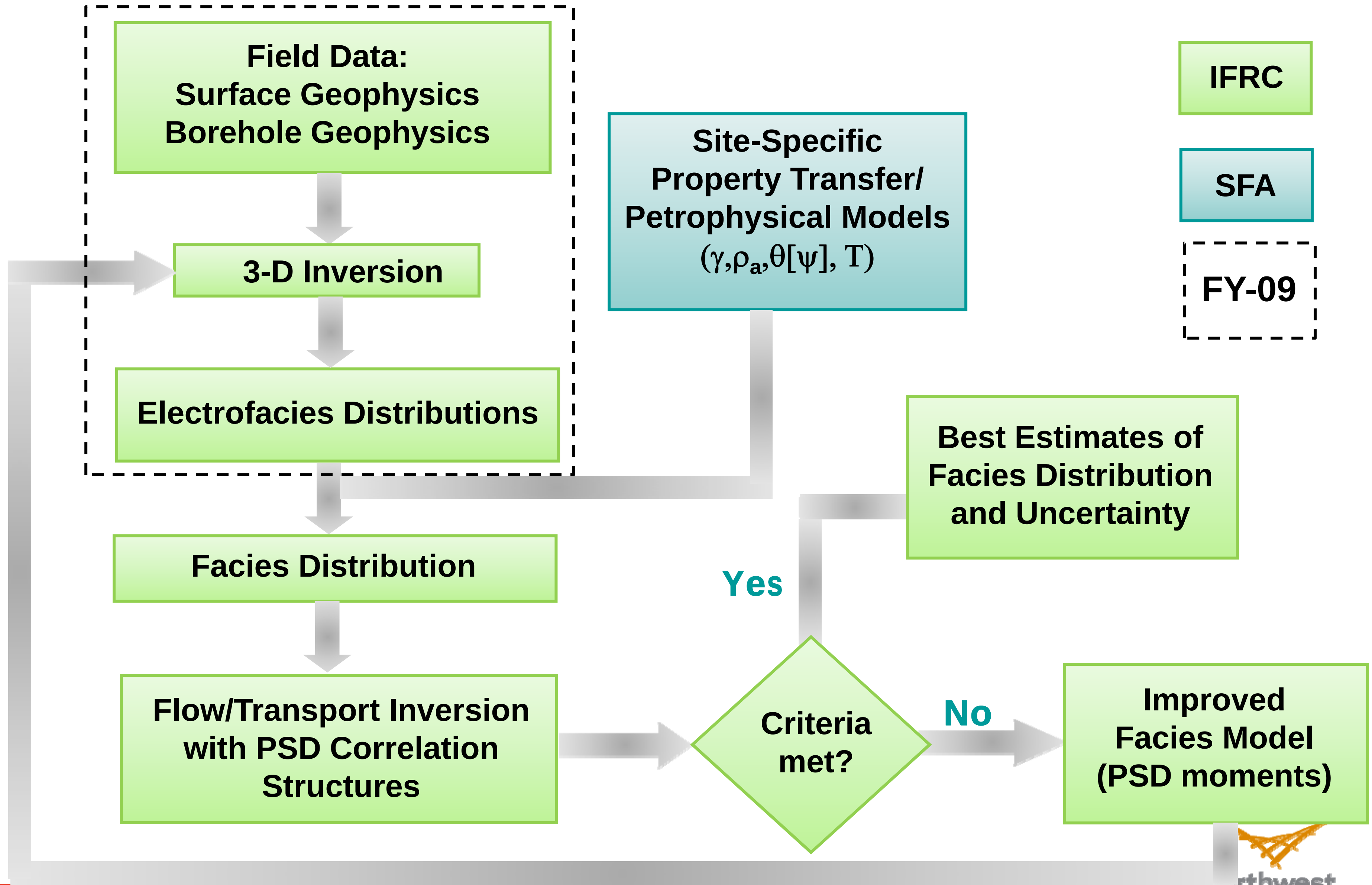
Objective

- Develop 3-D facies models that reflect variations in the depositional environment and the associated subsurface heterogeneity

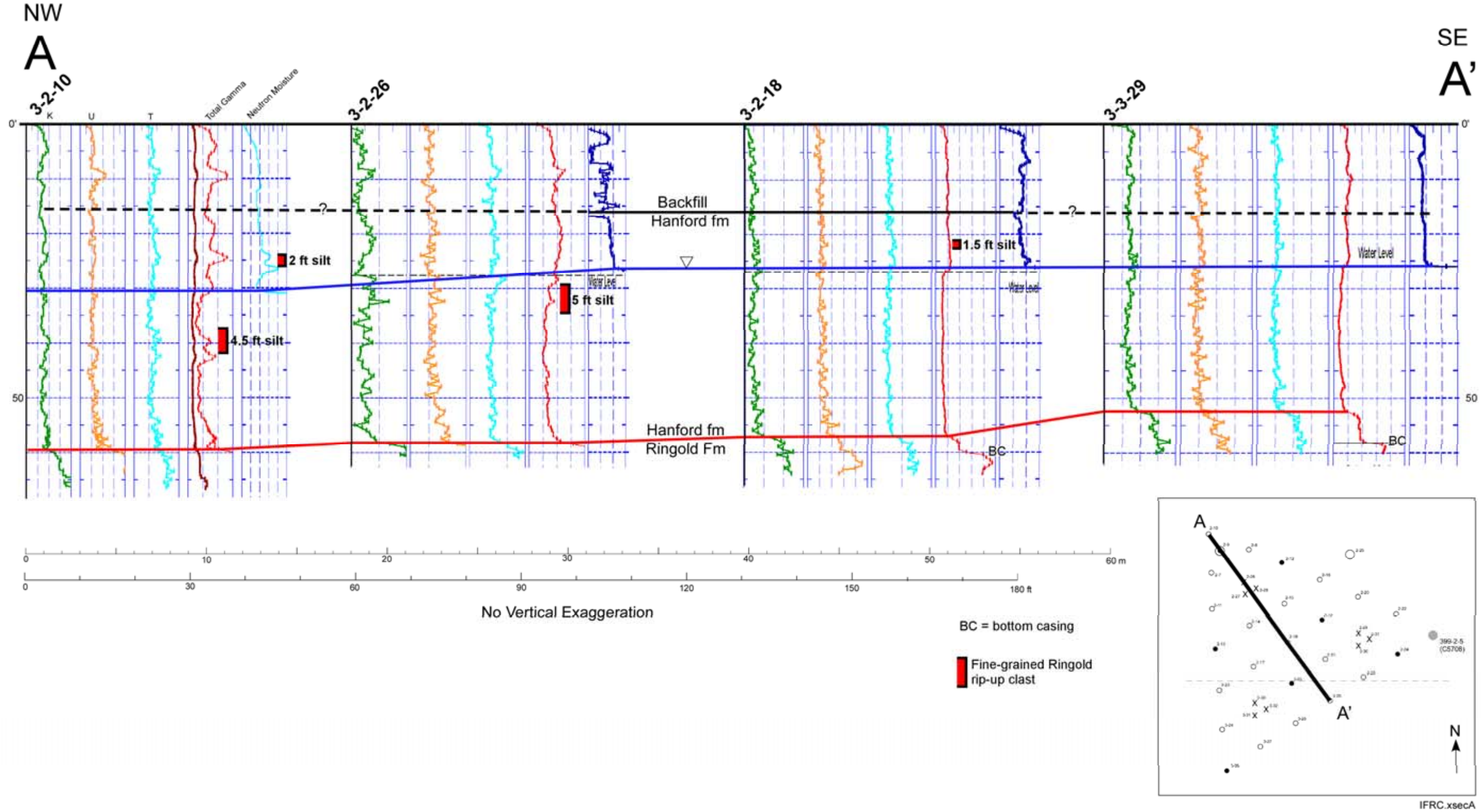
Scope

- Establish quantitative links between sedimentary facies and primary hydrophysical properties
  - requires higher level of sediment characterization
  - whole sediments and size fractions
  - lithocomponents of size fractions

IFRC Linkage

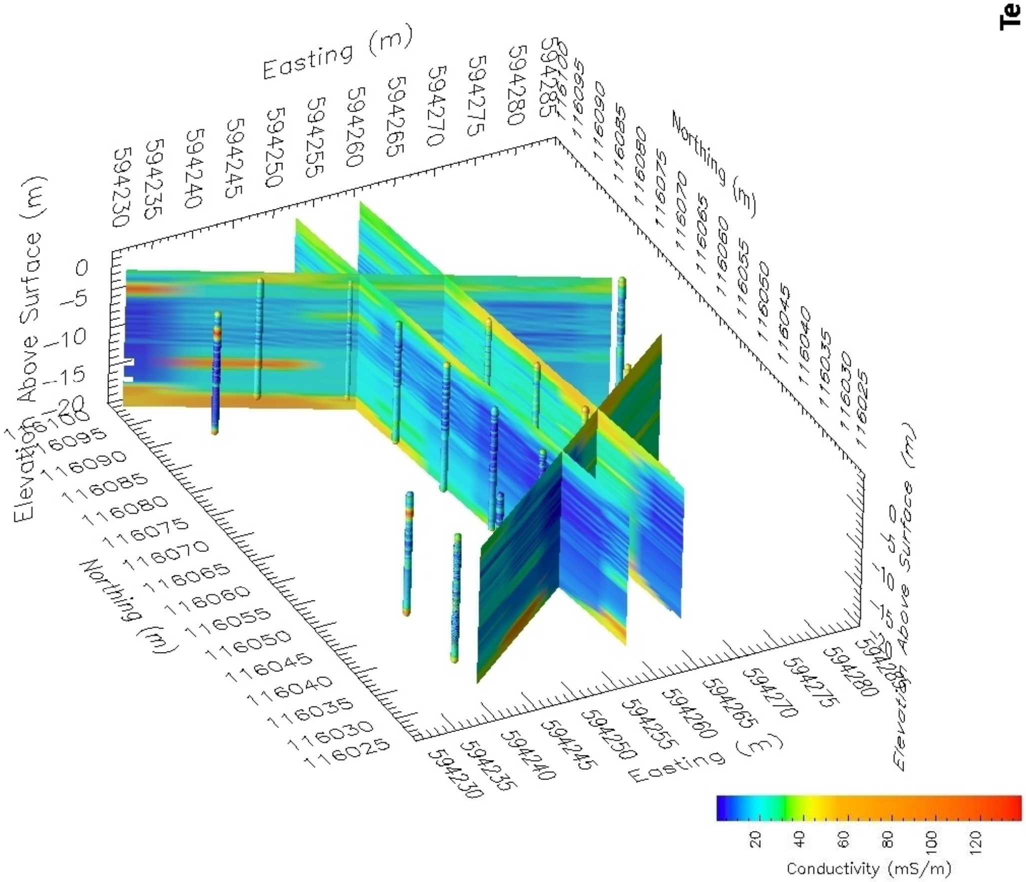


Multi-scale Heterogeneity

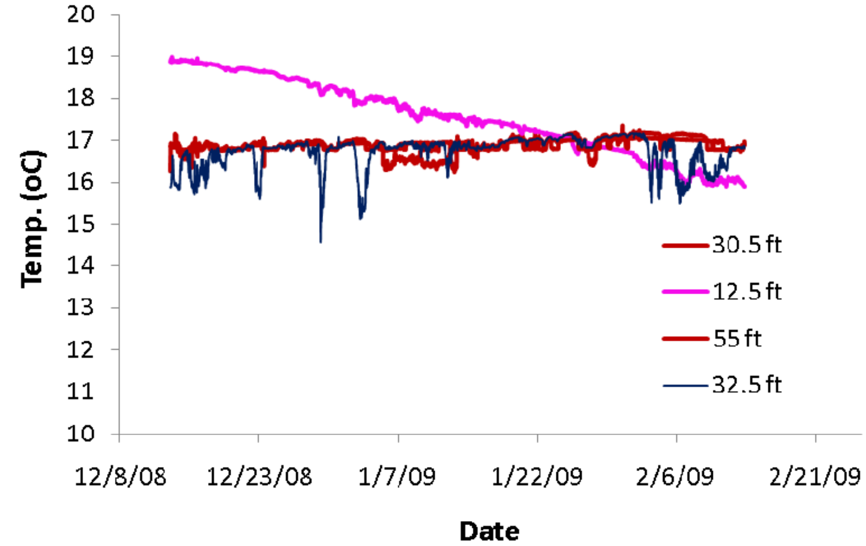


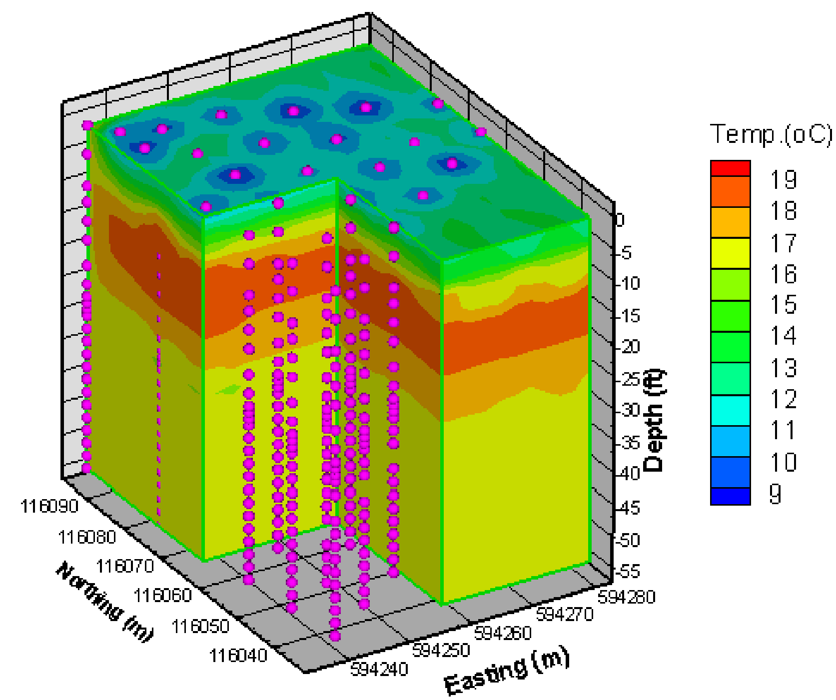
Field Characterization and Monitoring

Borehole Electrical Conductivity



Subsurface Temperature





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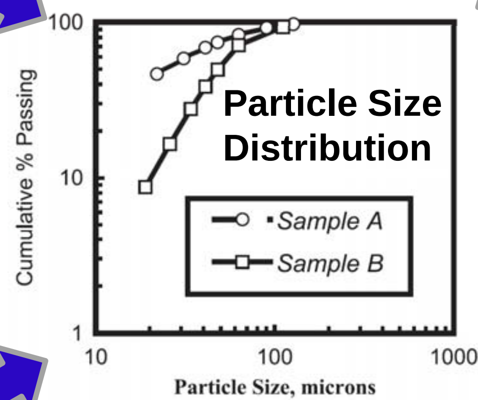
Project Premise

Primary sediment properties are controlled by facies distributions, which in turn are controlled by grain size distributions resulting from the depositional environment

Natural Isotope Abundance
- ^{40}K, ^{238}U, ^{232}Th
- Gross γ-ray response

Electrical Properties
- Dielectric Spectroscopy
- Surface conductivity
- Formation Factor
- Chargeability

Hydraulic Properties
- Bulk density
- Porosity
- Residual water content
- Water retention
- Relative Permeability



Reactive Properties
- Specific surface area
- CEC_{por}
- S_{por}
- Reaction Kinetics

Transport Properties
- Tortuosity
- Intrinsic Permeability
- Dispersivity
- Formation Factor

Thermal Properties
- Heat Capacity
- Thermal conductivity

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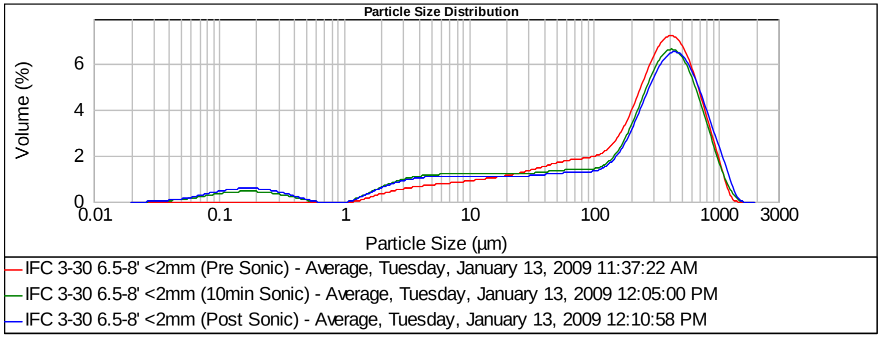
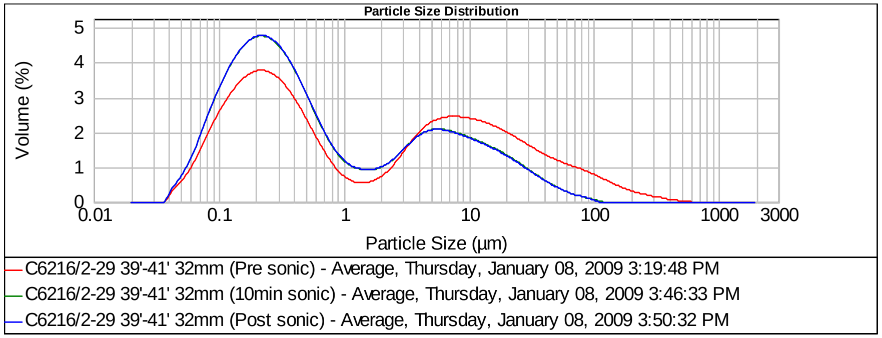
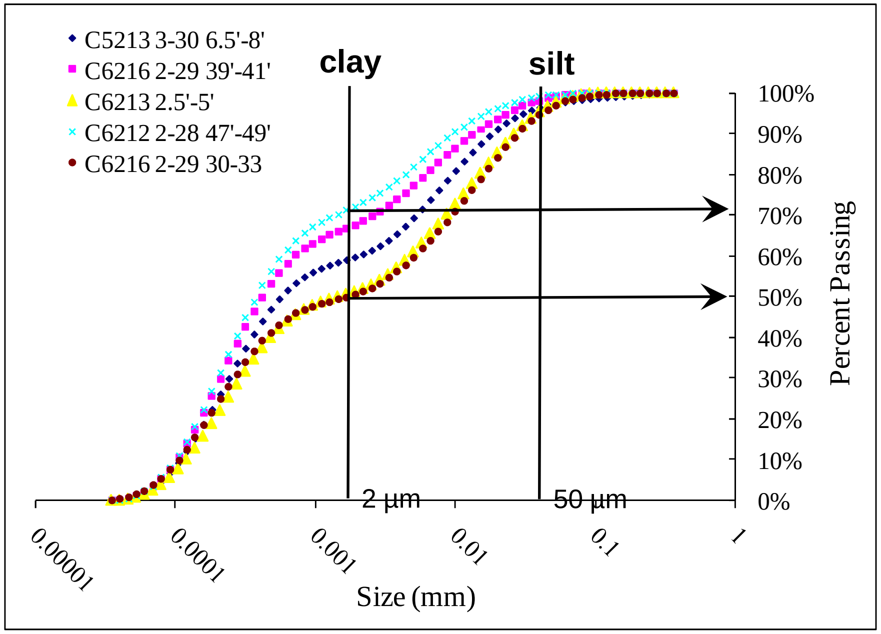
Sediment Characterization

- Establishing such linkages requires higher level of characterization
  - whole sediments
  - size fractions
- Size analysis
  - Dry/wet sieve
  - Hydrometer
  - Laser particle size
  - Mineralogy of size fractions
- Continuous size distributions
  - Differences in coatings on different size gravel
  - Differences in coatings on same size from different depths
  - Could impact variability in sorption





Particle Size of Coatings on 32 mm Gravel



γ-ray Dependence on Grain Size

Goal

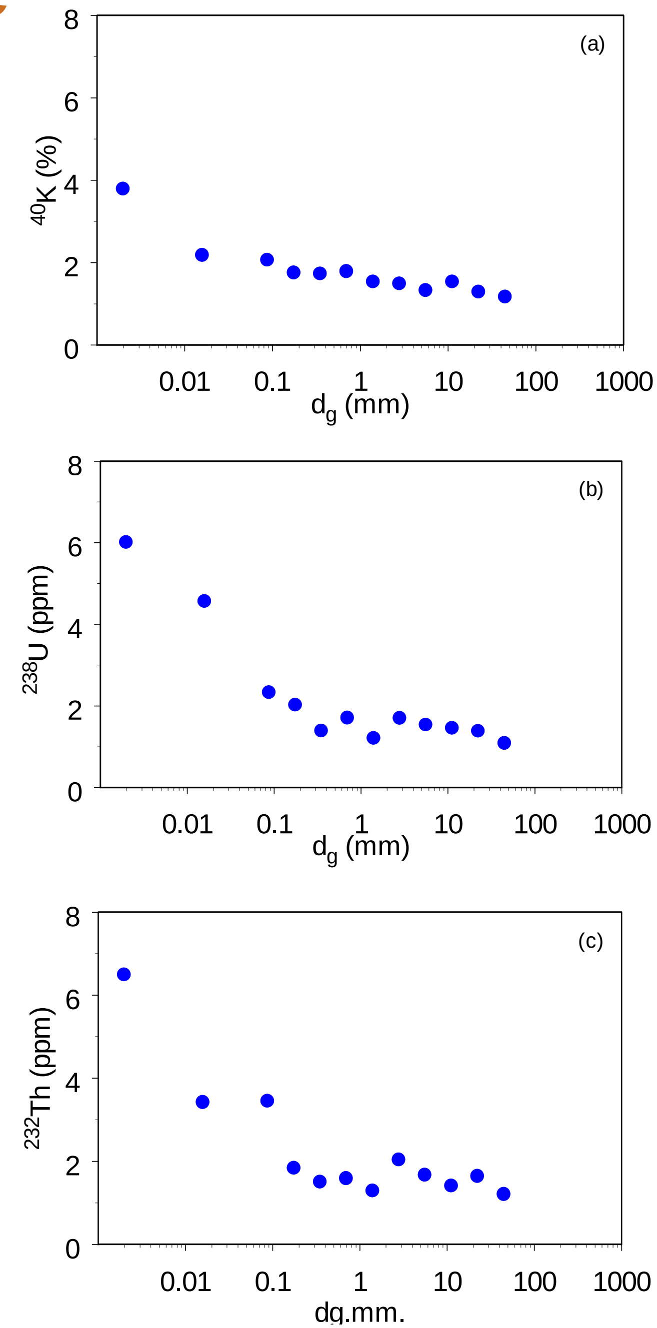
- Establish basis for using ^{40}K, ^{238}U, ^{232}Th logs to quantify grain size distributions and spatial variations

Measurements

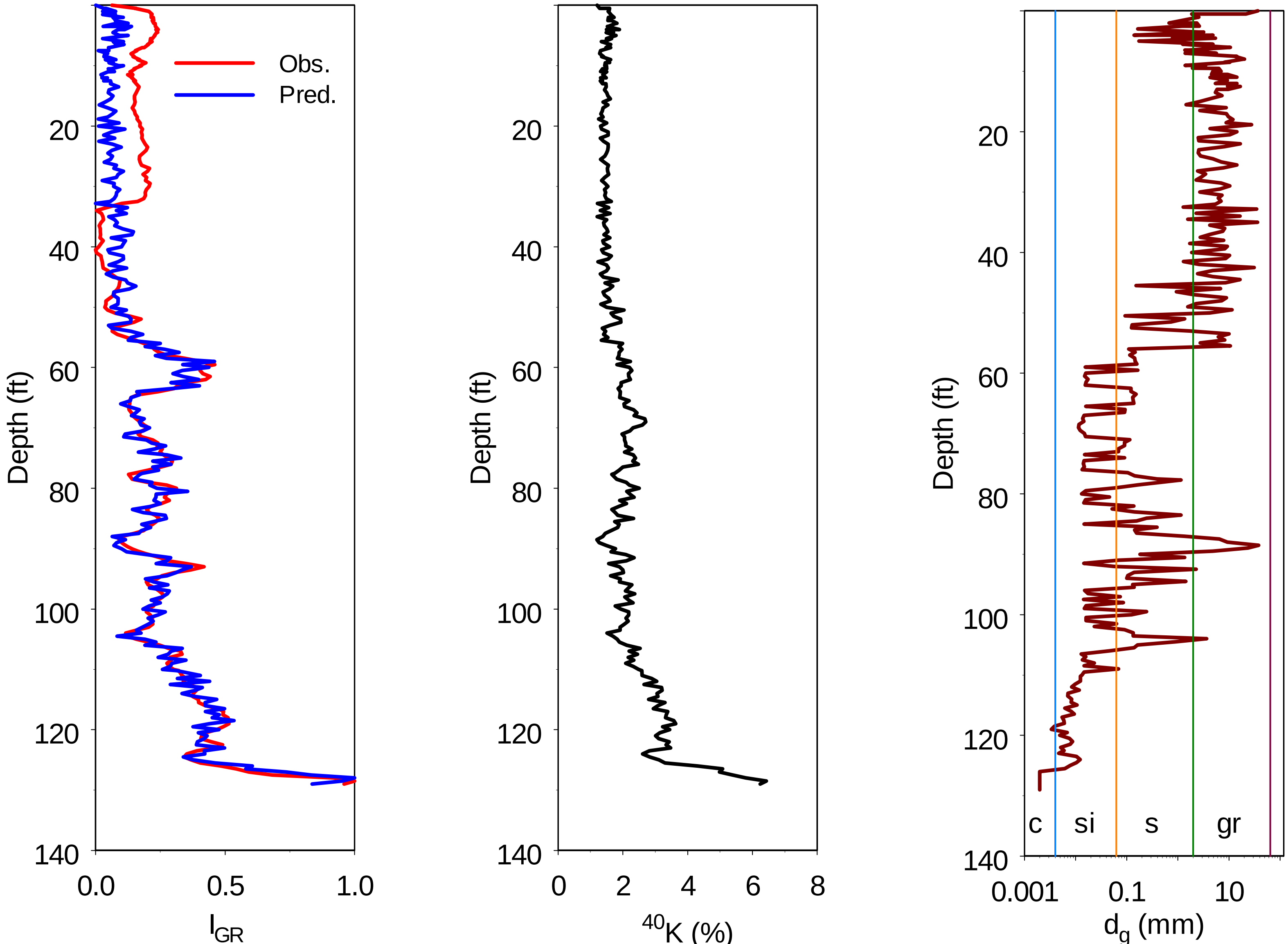
- GEA Analysis on samples from C5708
- strong relation between GEA response and grain size statistics
  - Observed on samples from Hanford and Rifle

Predictions

- MCNP model of γ-ray spectrometer
  - MCNP model of borehole log
  - Neural network to predict size moments from KUT



Predicted Grain size (C5708)



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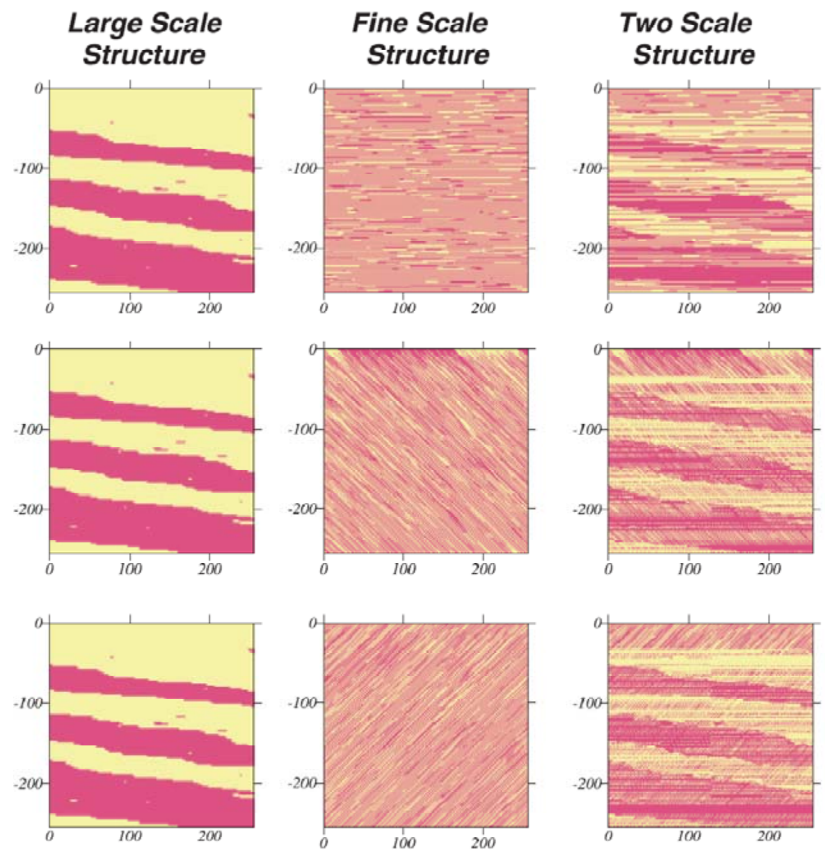
Integrating Multi-scale Heterogeneities

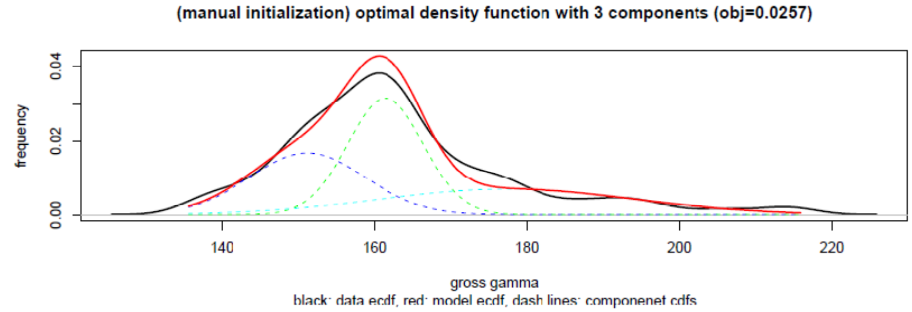
- Vertical variation in lithology
  - Generation of fine-scale heterogeneity patterns
  - Borehole logs for vertical transition probabilities and conditioning
- Horizontal continuity
  - large-scale architectural structure
  - surface geophysics
- Merge fine- and large-scale heterogeneities
  - TPROGS algorithm of Carle et al. (1998)
  - Coupled Markov chain (Dekking et al. 1999)
  - Sequential indicator simulation (SISIM) from GSLIB library

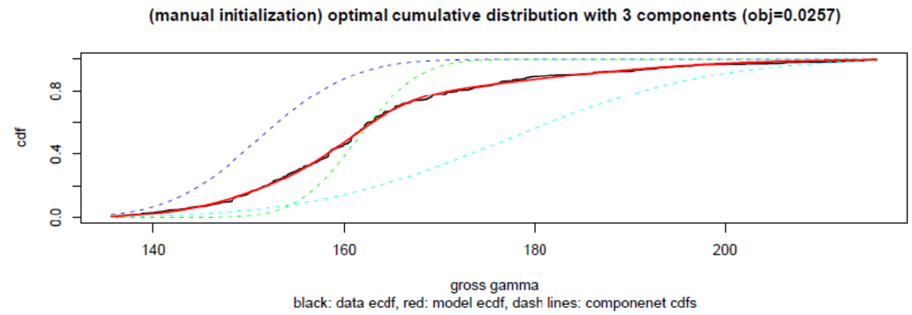


From Elfeki et al. 2002, Petroleum Geoscience, 8:159-165

γ-ray Properties of Geologic Units

- Assume global histogram of total γ is sum of *n* normal populations
  - One normal distribution for each lithofacies
  - Optimize fit of lithofacies to global histogram of γ data
- Three lithofacies identified
- Use spectral γ ^{40}K, ^{238}U, ^{232}Th
  - Extend to all logged IFRC wells
  - Neural network approach for identification of facies
  - Calibrate with grain size data
- Extend lithofacies simulation to three dimensions
  - Algorithm employed will be based on comparison of 2-D results





Facies	Percent	Mean γ
1	32%	151.2
2	40%	161.5
3	29%	177.5

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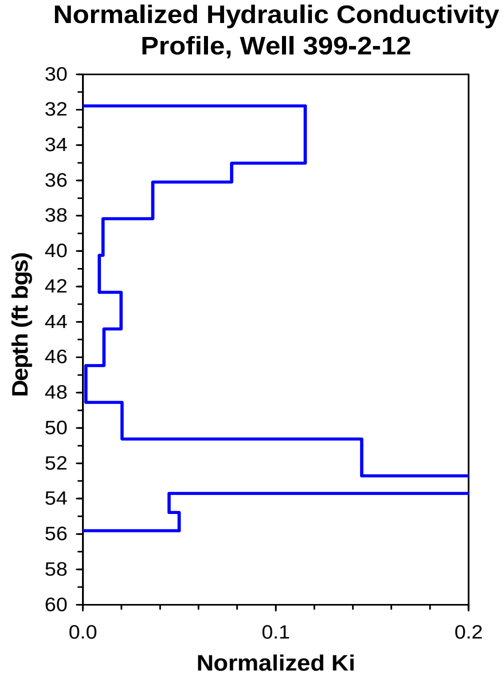
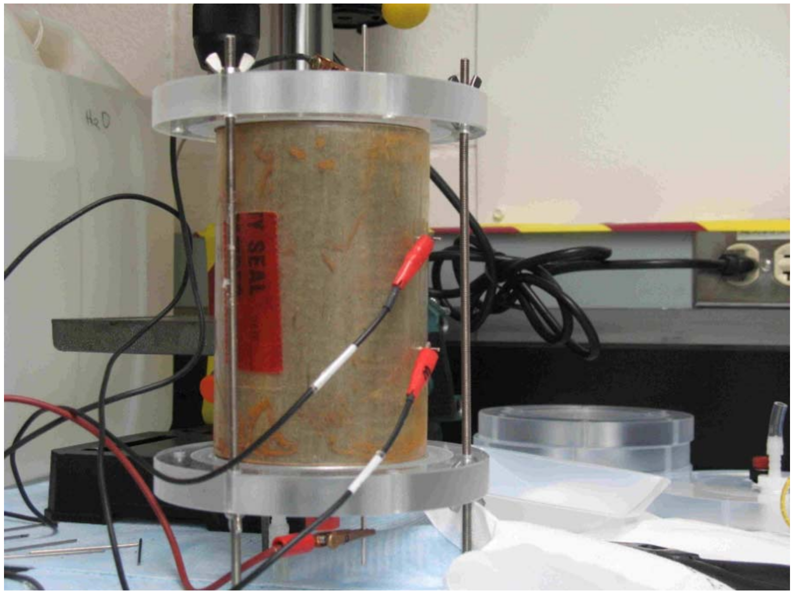
Electrical Properties of Geologic Units

- Selected 4 cores based on EBF-K_{sat}
  - 21-22’, 43-44’ 52-53’, 58-59’
- Instrumented for electrical measurements
  - Resistivity, chargeability (IP)
- Three major electrofacies identified
  - High resistivity, low chargeability
  - Intermediate resistivity, low chargeability
  - Low resistivity, high chargeability
- Low fines = low chargeability (<10 mV/V)
  - mineral type, grain size, S_{por}, pore water chemistry, physics of interaction between surfaces and fluids



Depth (ft)	Facies	ρ_a (Ω m)	*m* (mV/V)
21-22	1	2000	1.0
43-44	2	900	4.6
52-53	3	1500	2.0
58-59	4	110	13.0



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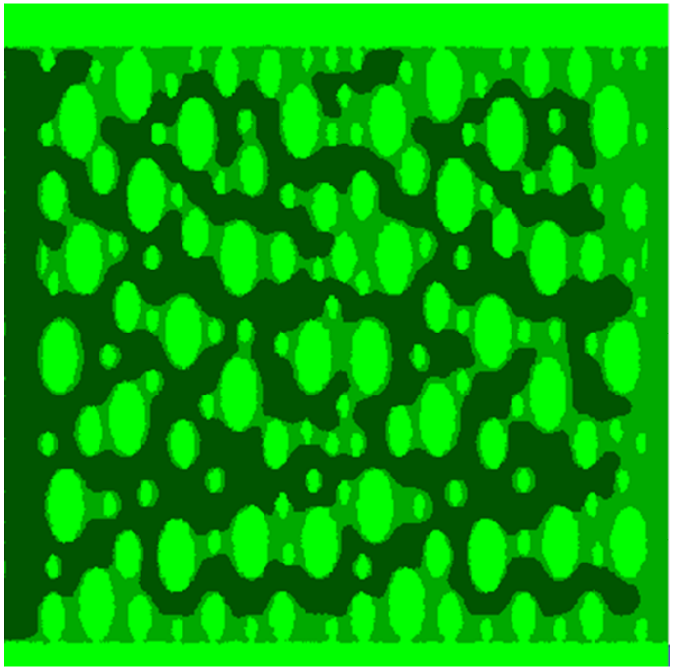
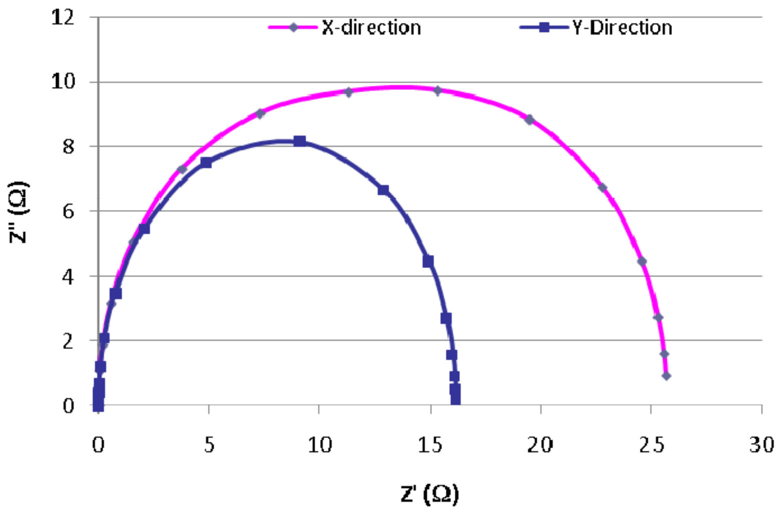
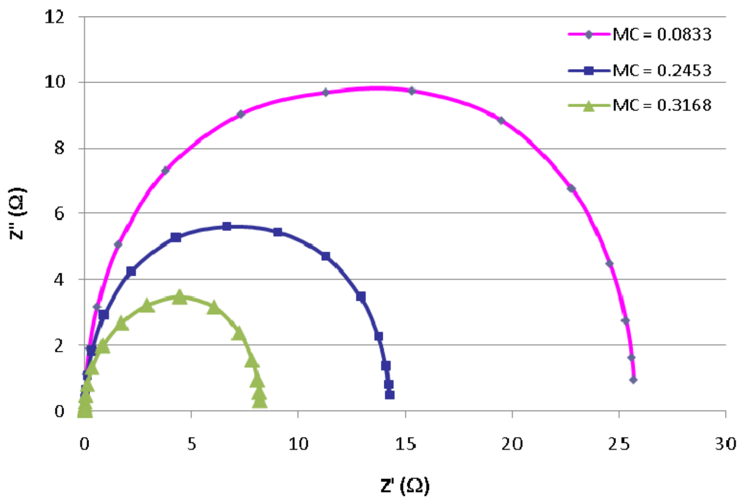
Porescale

- Smooth particle hydrodynamics
  - Aspherical particles
  - Packing based on IFRC sediments
  - Reactive chemistry
- Impedance spectroscopy
  - Solve 3-D Poisson equation
  - Multiple phases
- Important factors
  - Particle size
  - Particle shape
  - Surface area/ surface charge





x-direction



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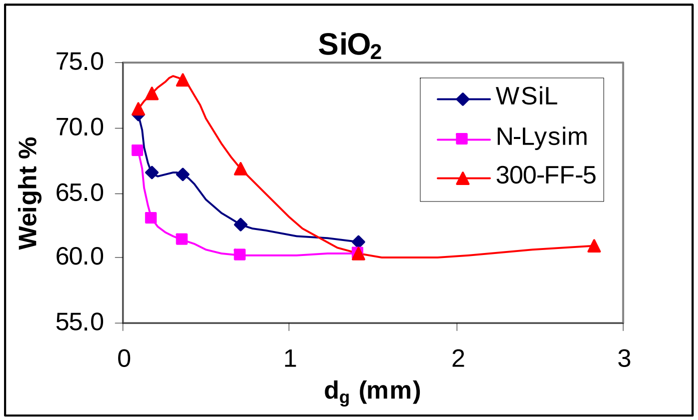
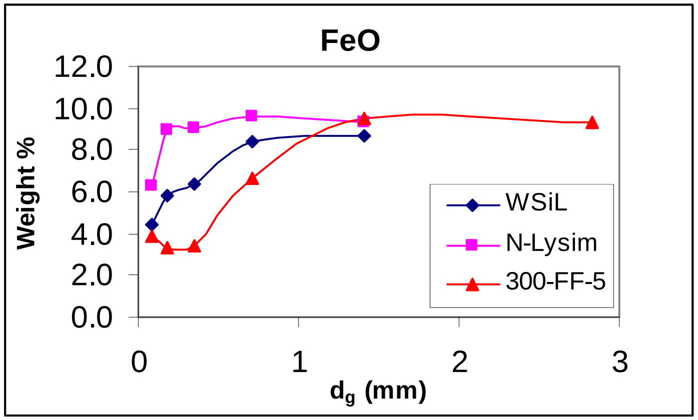
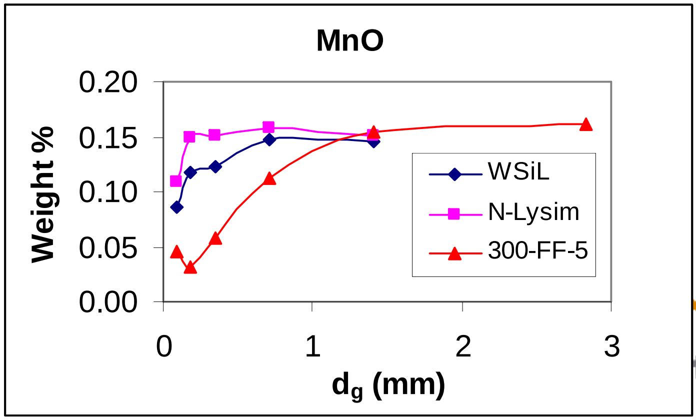
FY 2009 Science Deliverables

- Property Transfer Models for IFRC Sediments
  - Spectral gamma logs
- 3-D electrofacies model reflecting heterogeneity at IFRC well field
- 3-D lithofacies model reflecting heterogeneity at IFRC well field

Backup Slides- Mineralogy







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