Reactive Facies: An Approach for Parameterizing Plume-scale Reactive Transport Models Using Multi-type and Multi-scale Datasets

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ABSTRACT

The concept of reactive facies has been developed for tractably describing the subsurface heterogeneity and for improving the predictive capability of long-term plume behavior. Because geophysical attributes are often sensitive to bulk characteristics of such geological units, this concept allows us to take advantage of both geophysical and lithological datasets for characterizing the spatial distribution of reactive transport (RT) parameters. In this study, we first identified the reactive facies by statistical data mining, based on historical and recently collected hydrogeological, geophysical and geochemical datasets at DOE's Savannah River Site, F-Area. We then mapped the reactive facies and distribute the RT parameters over the local and plume scale, using the lithological and geophysical datasets. For mapping the reactive facies in the plume scale, we have developed a multiscale Bayesian estimation method to jointly invert wellbore and geophysical datasets in different types, resolution, and spatial coverage. The results show that our methodology effectively integrates different types of data, providing an approach for distributing critical information about properties that control flow and transport to the scales needed for simulating plume migration and remediation.

BACKGROUND & OBJECTIVE

1. Savannah River Site, F-Area

- Plutonium production waste
- U and nitric acid plume (~800m)

2. Reactive Facies Concept

- Unique and linked distributions of reactive transport (RT) properties; reactive surface area, sorption properties, permeability
- Extension of hydrofacies concept: Both hydraulic and reactive properties are related to reactive facies

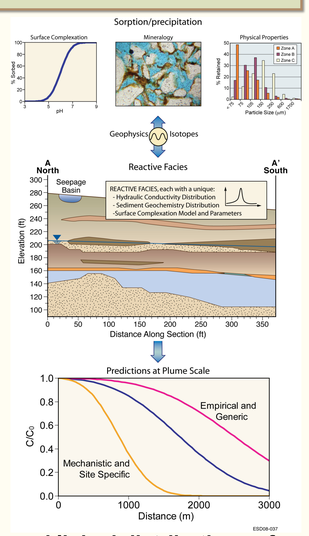
3. Geophysical Techniques

- Sensitive to bulk characteristics of geological units with different texture, porosity, and mineralogy

→ Map the reactive facies

4. Objective

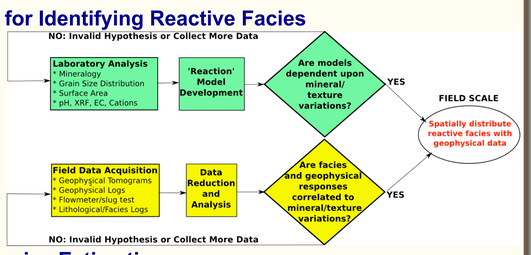
- Identify the reactive facies that have unique and linked distributions of RT properties
- Quantify the geophysical signature of each reactive facies type
- Use the spatially extensive geophysical and sparse wellbore data to map reactive facies and associated transport properties over the scale necessary for simulating long-term plume migration.



METHODOLOGY I

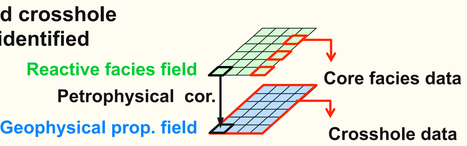
1. Statistical Data Mining for Identifying Reactive Facies

- Classification/cluster analysis of key RT parameters
- Correlation between co-located geophysical and lithological properties



2. Local-scale Reactive Facies Estimation

- Integrate core facies data and crosshole geophysical data, using the identified petrophysical relationship



- Posterior Distribution: P(reactive facies|all the datasets) ∝ P(crosshole data|geophy. prop.) P(geophy. prop.|facies)P(facies|core data)

METHODOLOGY II

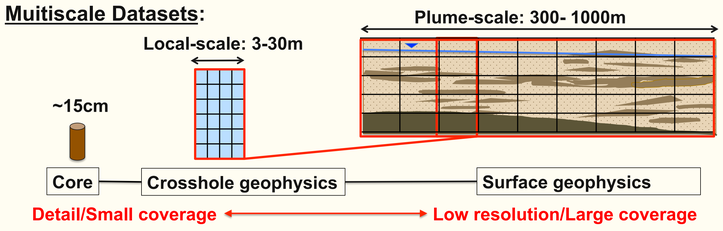
3. Bayesian Estimation for Plume-scale Mapping Reactive Facies

(1) Multiscale Concept

Muitiscale Heterogeneity: Nested structure

Large-scale structure (trend) + Small-scale variability (e.g., individual facies)

Muitiscale Datasets:

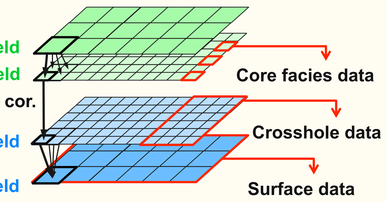


(2) Plume-scale Reactive Facies Estimation

Multiscale heterogeneity

Nested Model: Large-scale variability field; Reactive facies field

Multiscale data: Fine-grid geophy. prop. field → Upscaling → Coarse-grid geophy. prop. field



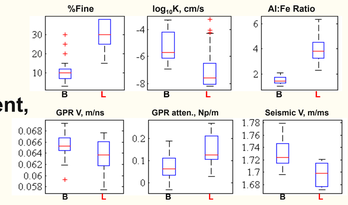
- Posterior distribution: P(reactive facies | all the datasets)
  - Marginal of P(reactive facies, trend, geophy. prop. | all the datasets)
- Break the posterior distribution into conditional probabilities
- Sample each field by the Markov-chain Monte-Carlo method

RESULTS: Local Scale Modeling

1. Identified Reactive Facies

Two reactive facies in the Barnwell (main) formation, which correspond to depositional facies:

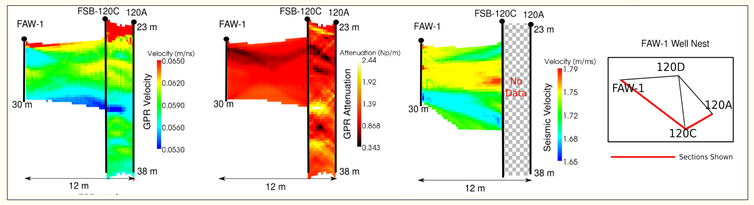
- Lagoonal Facies (L): High clay content, low hydraulic conductivity, high Al:Fe ratio, low radar velocity, high radar attenuation, low seismic velocity
- Beach Barrier Facies (B): low clay content, high hydraulic conductivity, low Al:Fe ratio, high radar velocity, low radar attenuation, high seismic velocity



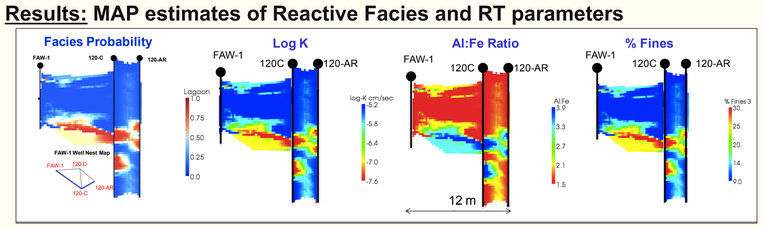
2. Local-scale Reactive Facies Estimation

Datasets:

- Well bore lithology
- GPR and seismic crosshole data



Results: MAP estimates of Reactive Facies and RT parameters



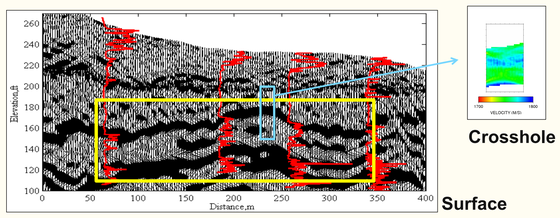
Reactive Transport Modeling → See Poster by Bea et al.

RESULTS: Plume Scale Modeling

3. Plume-scale Reactive Facies Estimation

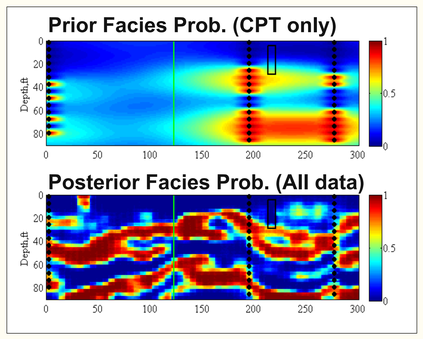
Datasets:

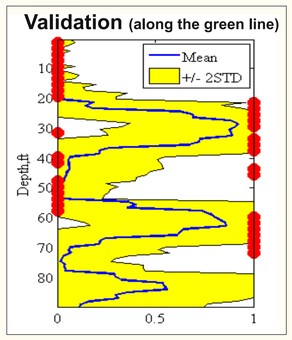
- Surface seismic data (reflective series)
- Crosshole seismic data (first arrival time)
- CPT data (point measurements: facies calibrated to core data)



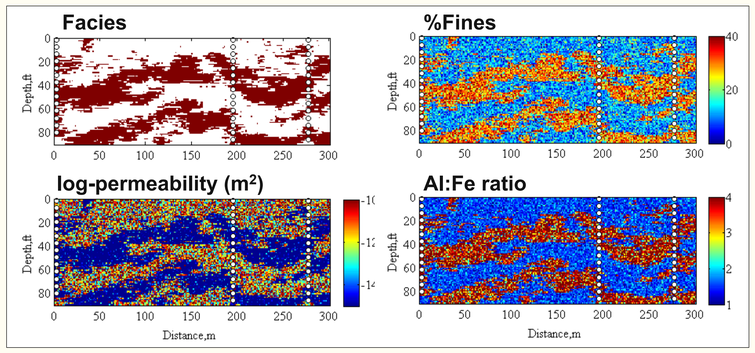
Results:

- Reactive Facies Estimation





- One realization of Reactive Facies and RT Parameters



SUMMARY

(1) We have identified two reactive facies, having distinct distributions of flow and reactive transport properties: %fines, permeability, and Al:Fe ratio (proxy for kaolinite:geothite ratio).

(2) The Bayesian assimilation of crosshole radar and seismic data revealed detailed maps of the reactive facies transport properties at the local scale. The surface seismic data, on the other hand, was useful to identify large-scale heterogeneous structures over the plume scale.

(3) Multiscale Bayesian method can consistently assimilate multi-type multiscale geophysical and wellbore datasets, making it suitable for mapping the reactive facies over the plume scale.

REFERENCES

D. Sassen, S. S. Hubbard, N. Spycher, S. Bea, J. Chen and M. Denham, Reactive facies: An approach for parameterizing field-scale reactive transport models using geophysical methods, accepted in WRR.

H. M. Wainwright, D. Sassen, J. Chen, S. S. Hubbard, Multiscale Hydrogeophysical Joint Inversion for Plume-Scale Subsurface Characterization Based on Reactive Facies, in preparation.

Funding for this study was provided by the U.S. Department of Energy, BER Program Contract DE-AC020SCH11231 to the LBNL Sustainable Systems Scientific Focus Area