



Pore-scale characterization of shale and reactive transport for geological carbon storage



Center for Frontiers of Subsurface Energy Security

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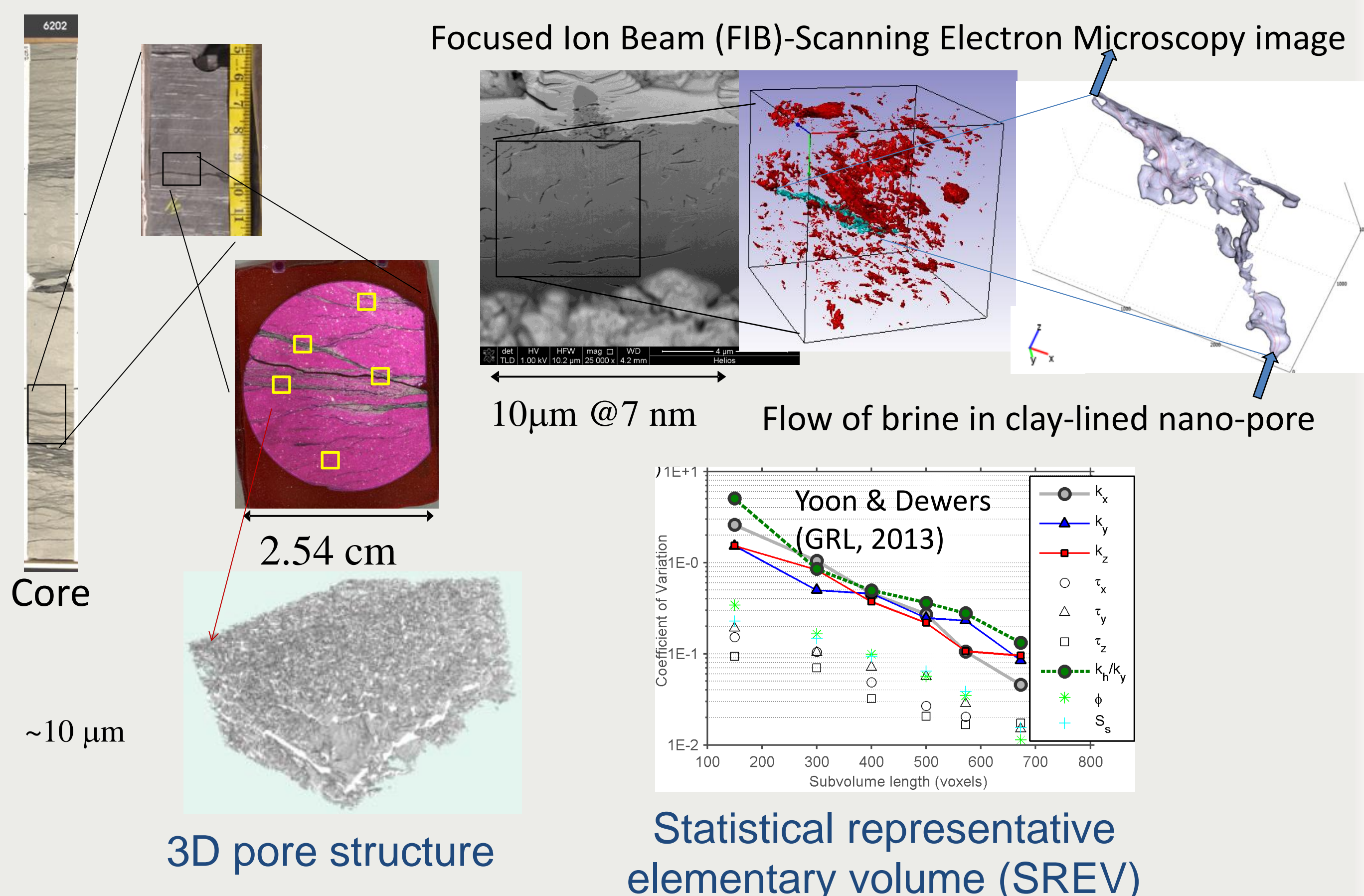
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We combine laboratory micro-scale and rock core-scale experimental and modeling efforts to examine:

- What are the characteristics of caprock materials for geological carbon storage? [Fundamental material characterizations]
- What are the relevant physics of dissolved CO₂ transport? [reactive transport and rock-fluid interactions]
- How can pore scale processes be synthesized and upscaled into more powerful continuum models? [upscaling]

Rock Samples and Multiscale Imaging

Characterization of pore structures and surface properties (optical microscopy, microCT, FIB-SEM, TEM, EDS)

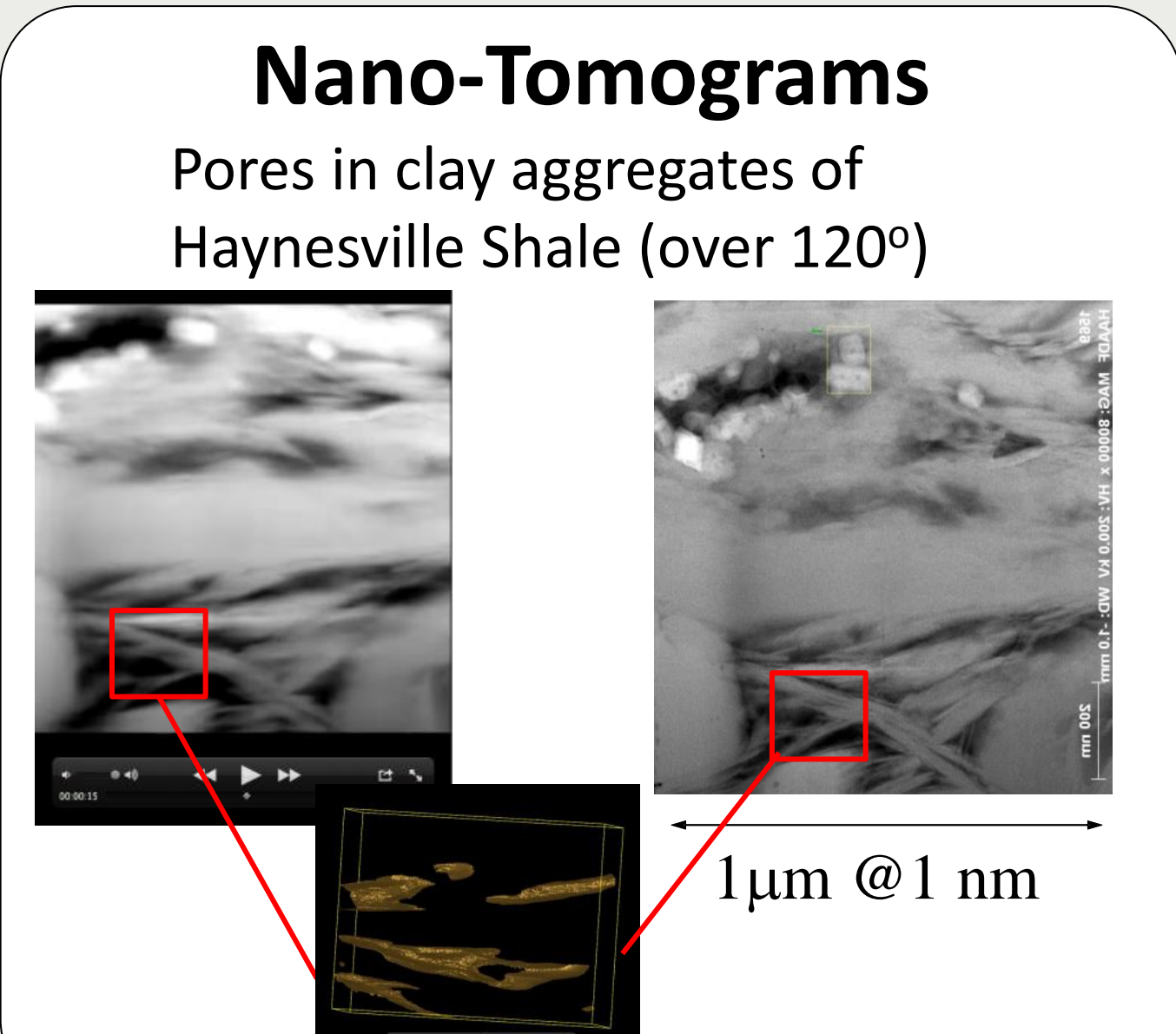
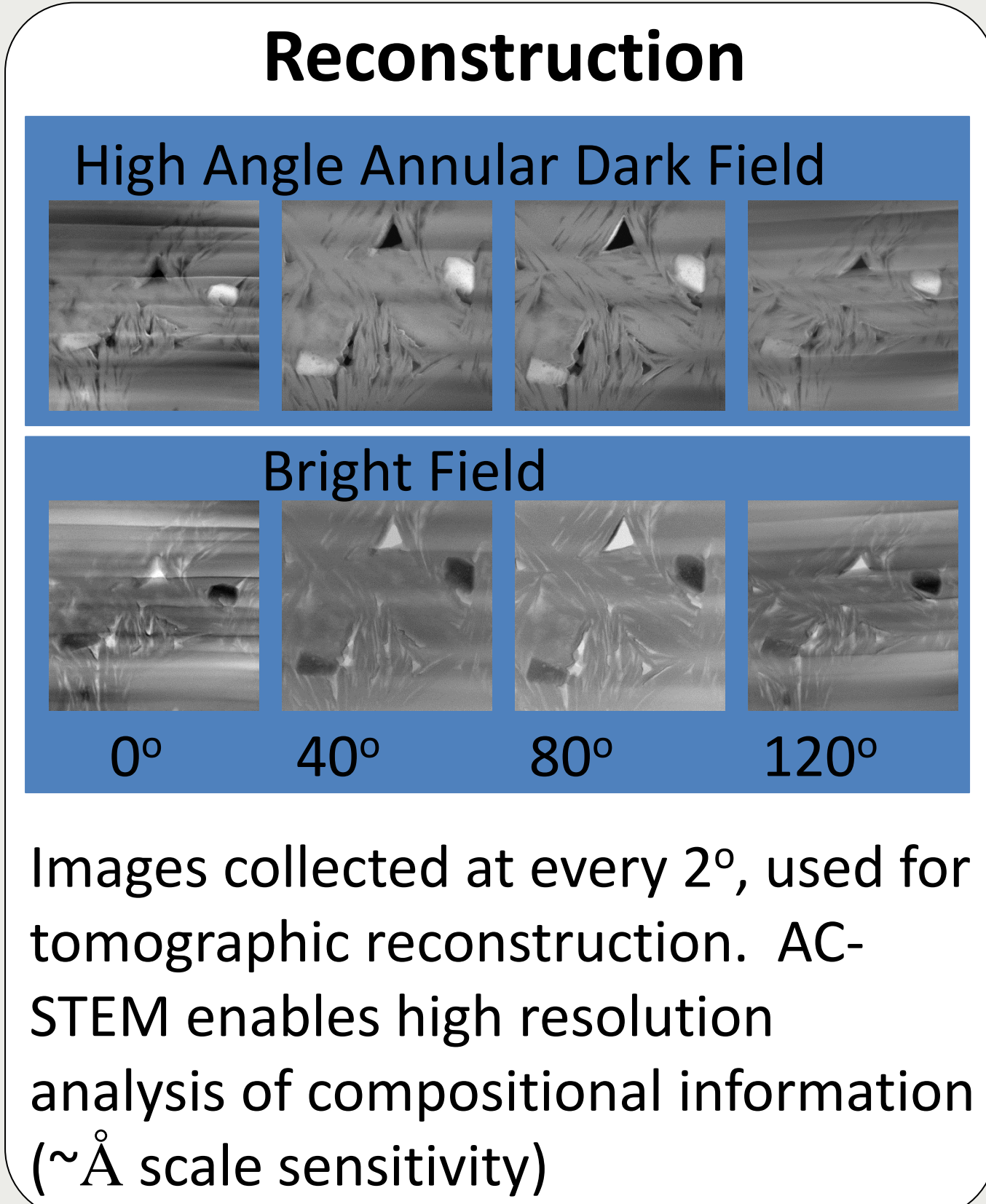
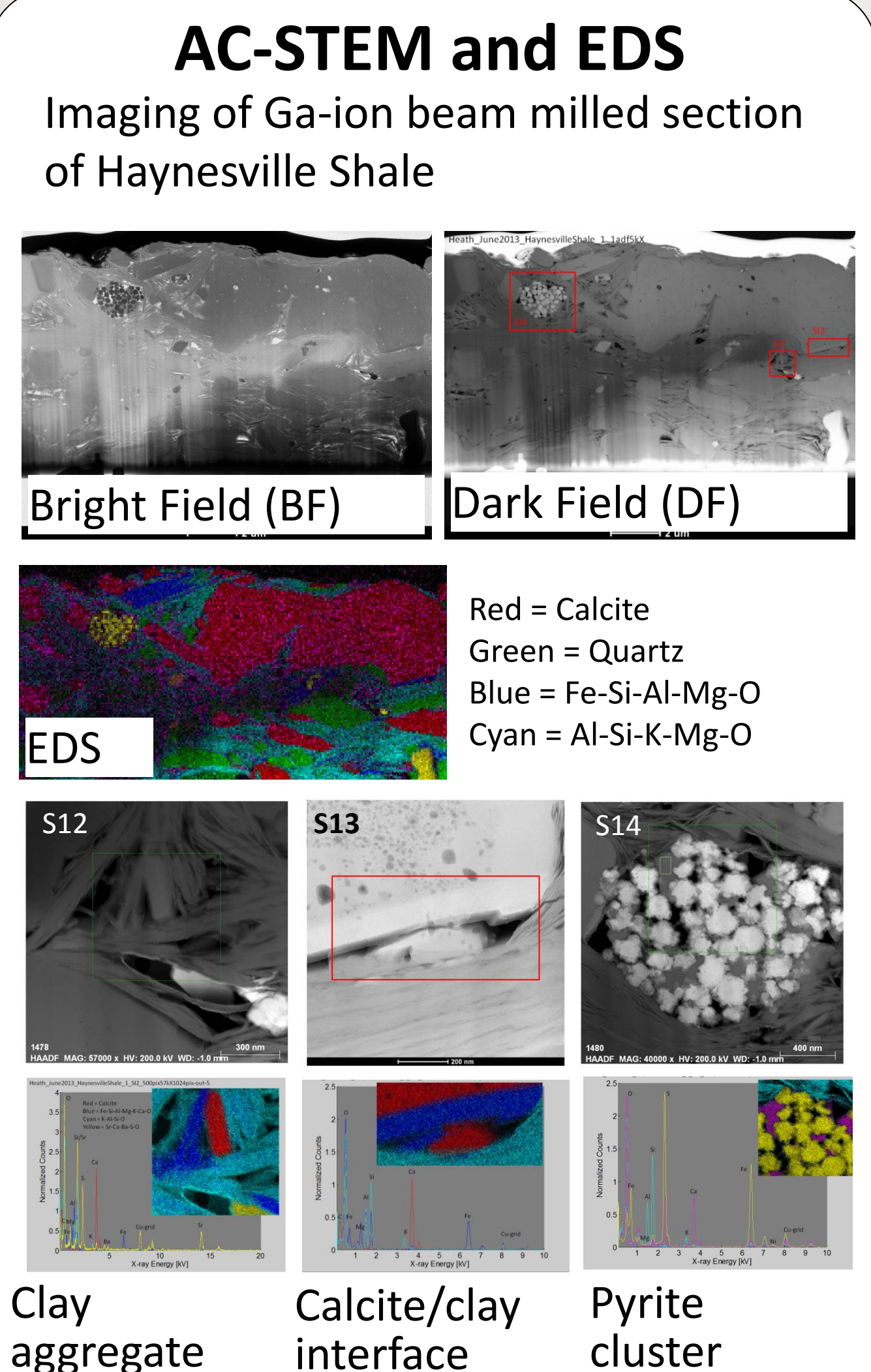


- FIB-SEM sample volume has a size of SREV at ~10 μm
- 4-6 regions selected (e.g., principal component analysis) can be used to represent the properties of thin section image
- Multi-scale rocks can be reconstructed from nano- to core- scales

Nano-pore and surface characterizations

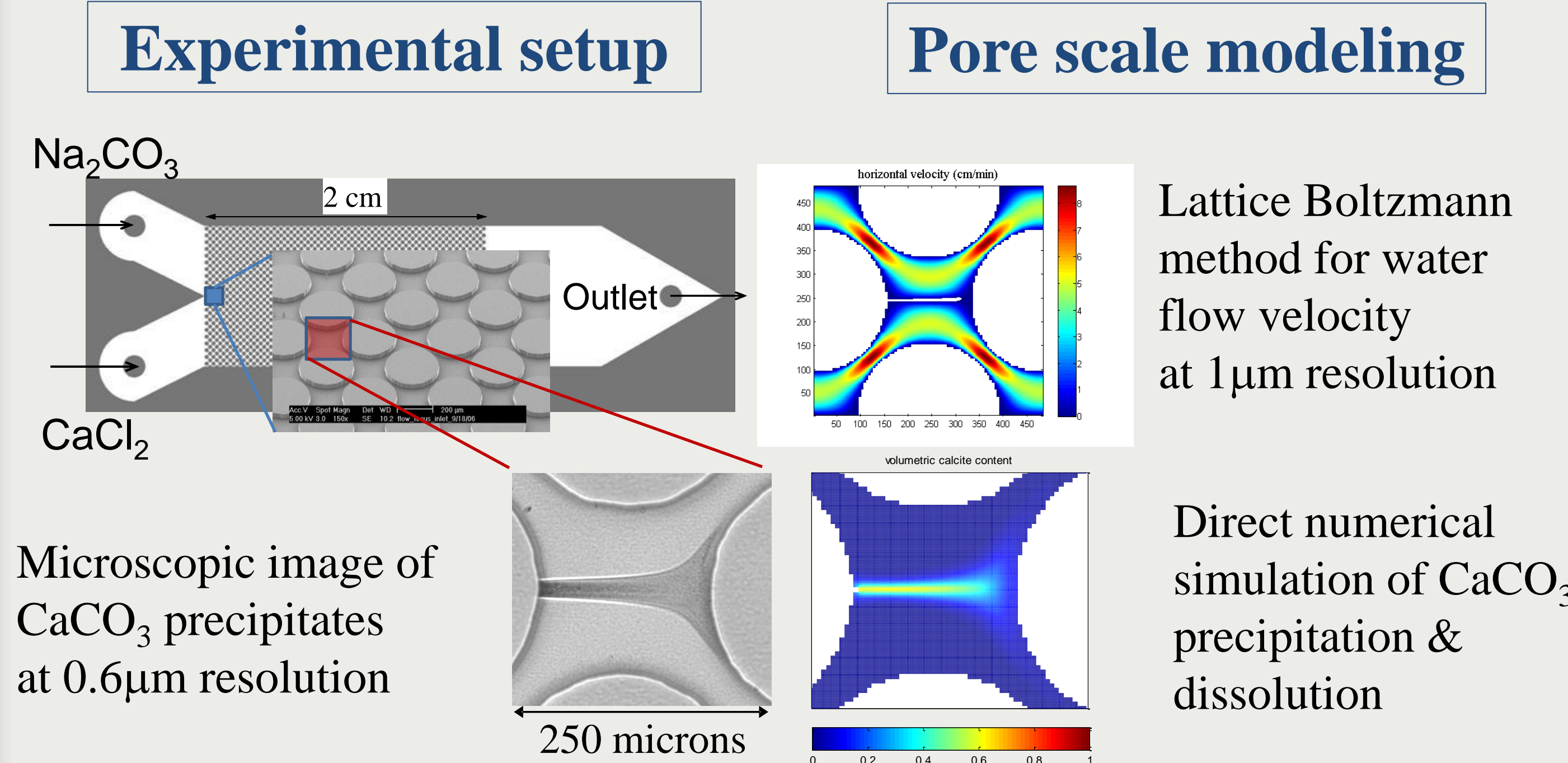
3D tomography using Aberration Corrected Scanning Transmission Electron Microscopy (AC-STEM) and chemical analysis by X-ray energy dispersive spectroscopy (EDS)

A state-of-the-art technique for visualizing 3D connectivity and structure of the <10nm pore population in gas shales coupled with composition analysis of pore-lining phases at ~ 1 nm resolution

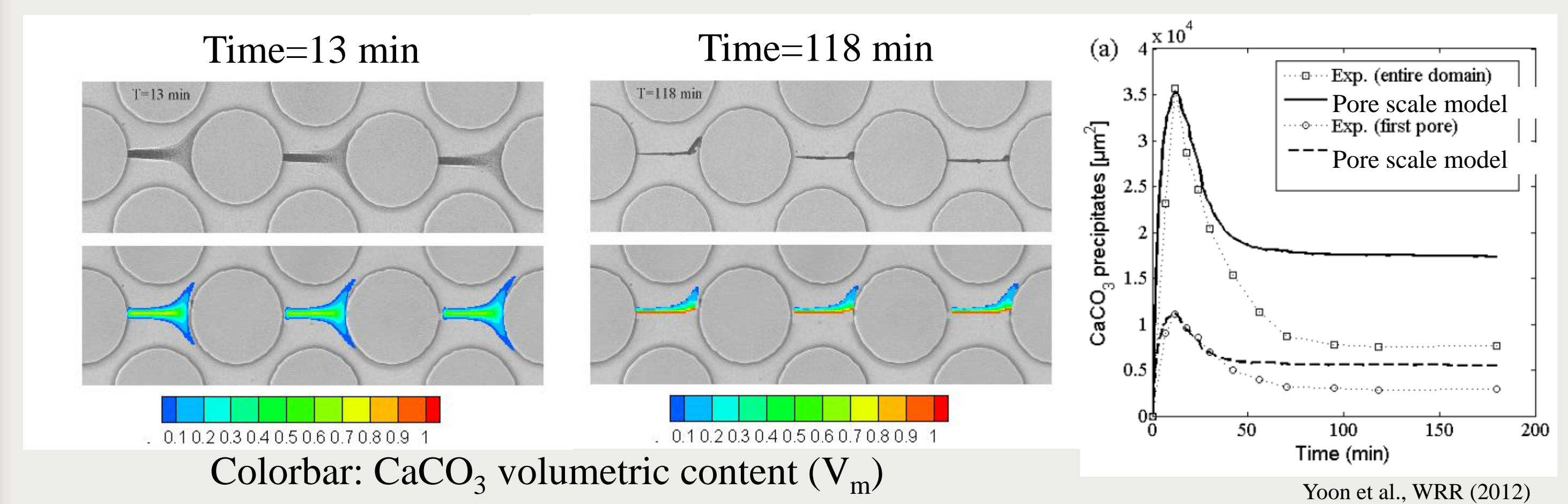


Pore Scale Experiment and Modeling for Reactive Transport

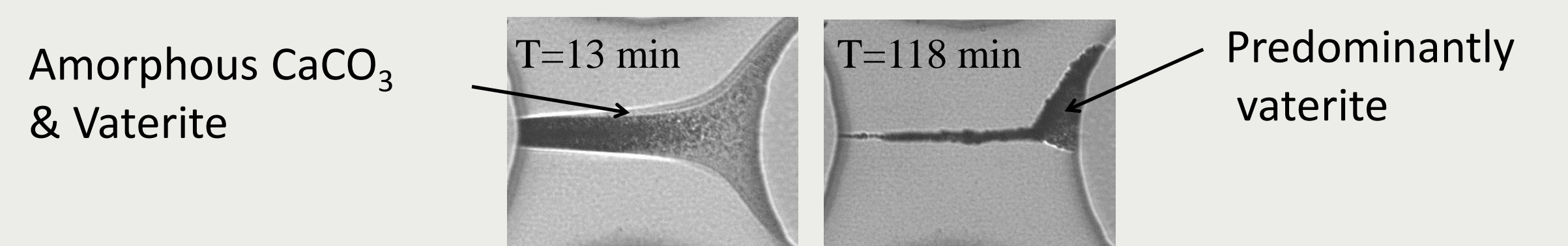
- Transverse mixing-induced calcium carbonate (CaCO₃) precipitation



Pore Scale Reactive Transport Modeling Results

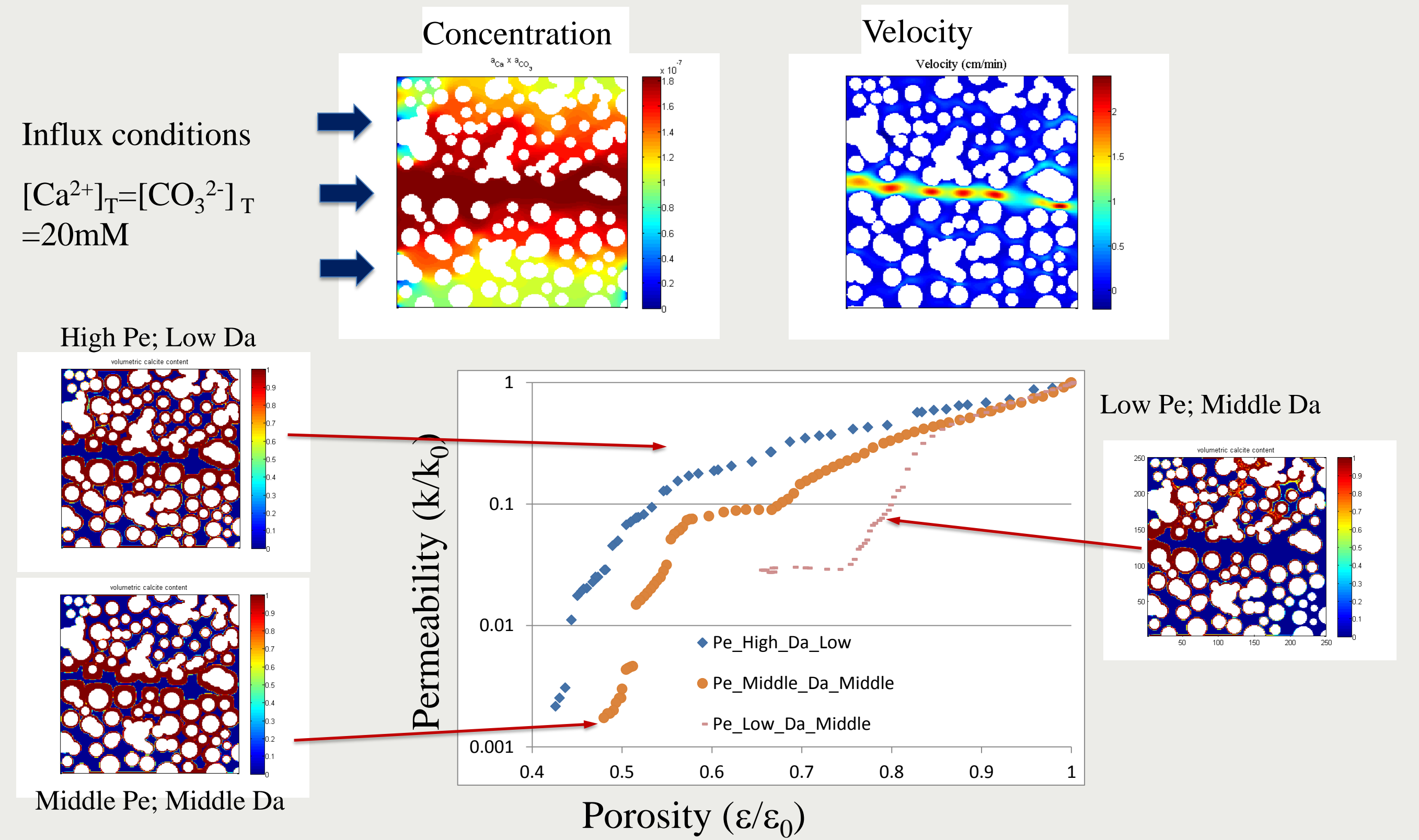


- Simulations capture precipitation & dissolution patterns observed in the micromodel
- A decrease of precipitate area (dissolution) was captured by using a dissolution factor which accounts for high surface area of nano-particles, transformation to different forms of CaCO₃, and stability of nano-particles after pore blocking as shown below



Response Function based on Pore Scale Simulations

- Phenomenological power law relations for continuum scale model can be derived from pore scale simulations (permeability-porosity, tortuosity-porosity, surface area-porosity)



Current and Future Works

- Vigorously tested pore-scale model can be used to develop a response function (or dimension reduction model) for continuum-scale relationships
- Image analysis methods will be developed to combine BF, HAADF, and EDS images to reconstruct complex pore structures with surface and material properties
- Pore scale CFD models for Knudsen gas diffusion and solute reactive transport that are dependent on pore characteristics and pore-lining phases will be developed

References

- Yoon, H., A.J. Valocchi, C.J. Werth, and T. Dewers (2012), Pore-scale simulation of mixing-induced calcium carbonate precipitation and dissolution in a microfluidic pore network, Water Resour. Res., 48, W02524.
- Yoon, H. and T. Dewers (2013), Nano-pore structures, statistically representative elementary volumes, and transport properties of chalk, Geophysical Research Letters, 40, 4294-4298.
- Dewers, T. et al. (2012), Three-dimensional pore networks and transport properties of a shale gas formation determined from focused ion beam serial imaging, Int. J. Oil Gas Coal T., 5(2-3), 229-248.



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