CCSI™
Carbon Capture Simulation Initiative

Uncertainty Analysis for the Full-scale Regenerator Model as a Post-combustion Carbon-Capture Unit

Emily Ryan, Boston University
Bledar Konomi, Avik Sarkar, Guang Lin, Xin Sun
Pacific Northwest National Laboratory

U.S. DEPARTMENT OF ENERGY

Carbon Capture and Sequestration (CCS)

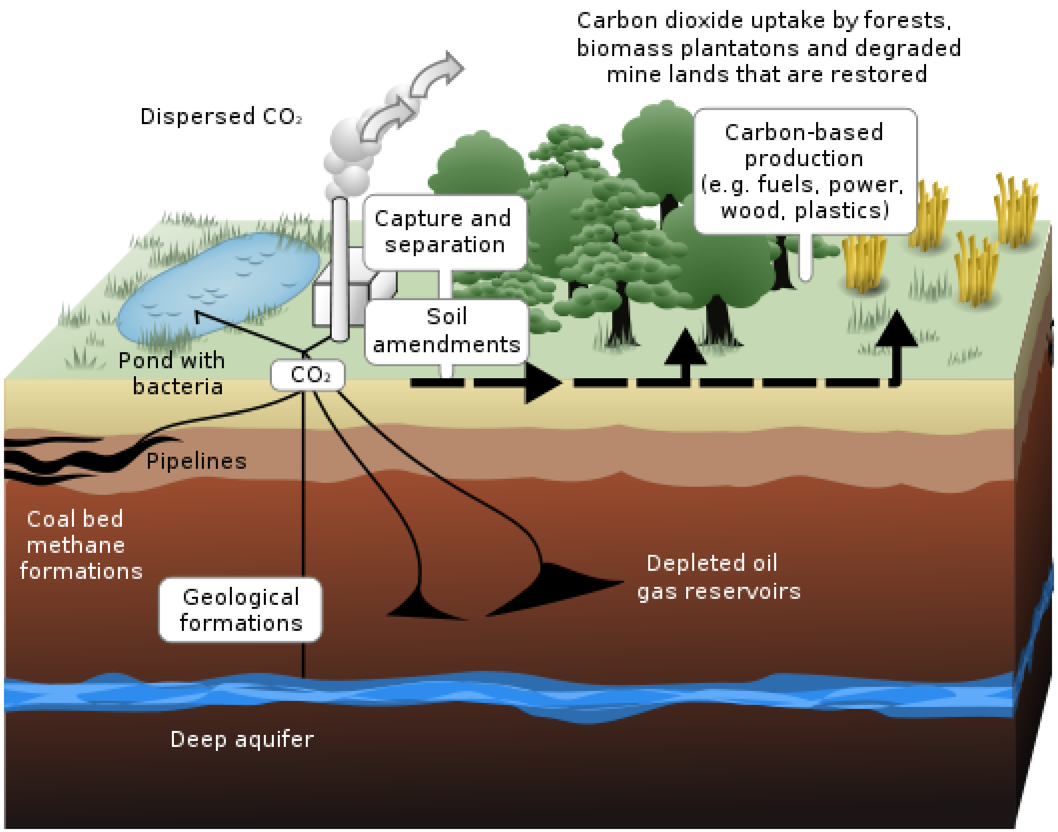
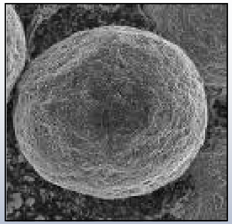
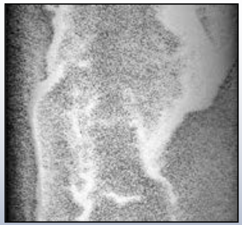
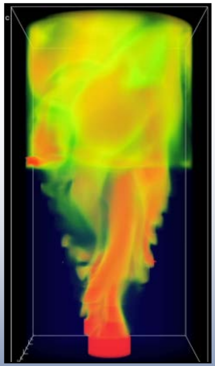


Image from wikipedia.

- ***Thermal power plants continue to produce CO_2.***
- ***To reduce emissions,***
  - *Chemically extract CO_2 from power plant exhaust.*
  - *Utilize or store CO_2 elsewhere.*
    - *E.g., pump it underground.*
- ***CCSI Objectives***
  - *Promote faster commercialization of CCS.*
  - *Develop CFD-based predictive models.*
  - *Uncertainty and risk analysis.*
  - *Develop tools for end-users (industry).*

Carbon Capture Simulation Initiative


Identify promising concepts → Reduce the time for design & troubleshooting → Quantify the technical risk, to enable reaching larger scales, earlier → Stabilize the cost during commercial deployment

National Labs

Berkeley Lab
Pacific Northwest National Laboratory
NETL
Los Alamos National Laboratory EST. 1943
Lawrence Livermore National Laboratory

Academia

Carnegie Mellon
Princeton University
West Virginia University
Boston University
Institute for Clean and Secure Energy, The University of Utah

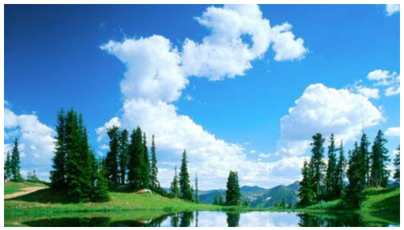
Industry

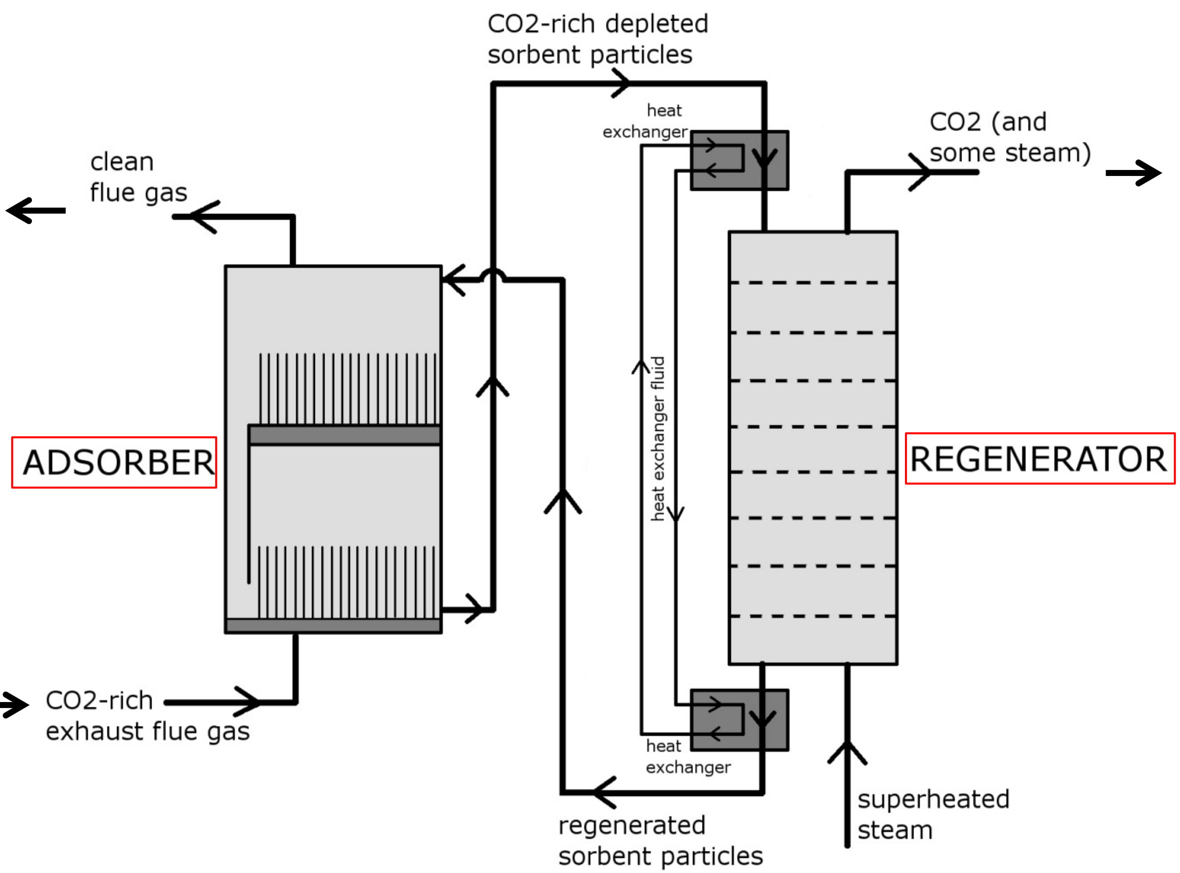
Fluor
ADA Environmental Solutions
B&W the babcock & wilcox company
GE
EPRI Electric Power Research Institute
Air Products
URS
Alstom
Burns & McDonnell Since 1898
Duke Energy
Southern California Edison, An Edison International Company, San Onofre Nuclear Generating Station
Southern Company
Boeing
Chevron
Eastman
ExxonMobil
WorleyParsons resources & energy
DuPont

CCSI™ Carbon Capture Simulation Initiative

NETL · Berkeley Lab · Lawrence Livermore National Laboratory · Los Alamos National Laboratory EST. 1943 · Pacific Northwest National Laboratory · U.S. Department of Energy

The CCSI Carbon Capture Unit

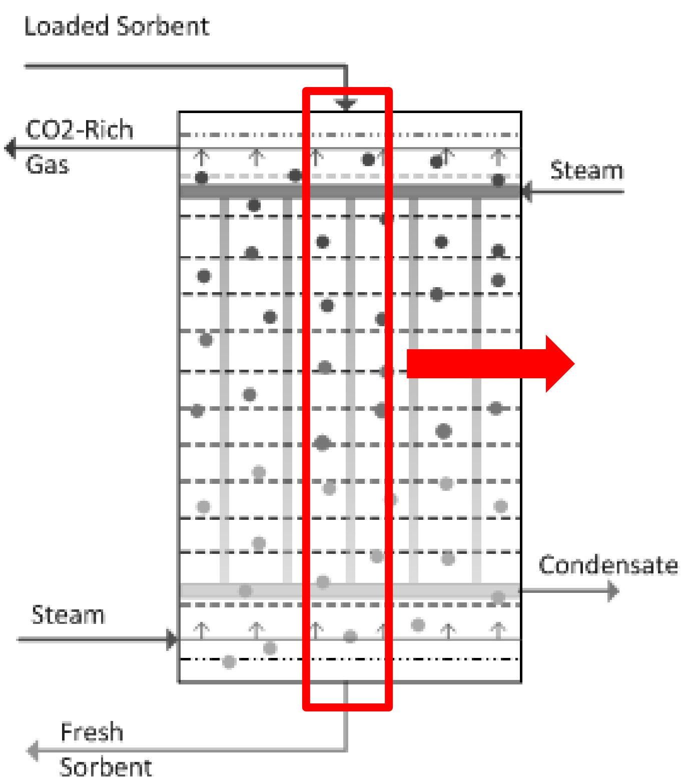




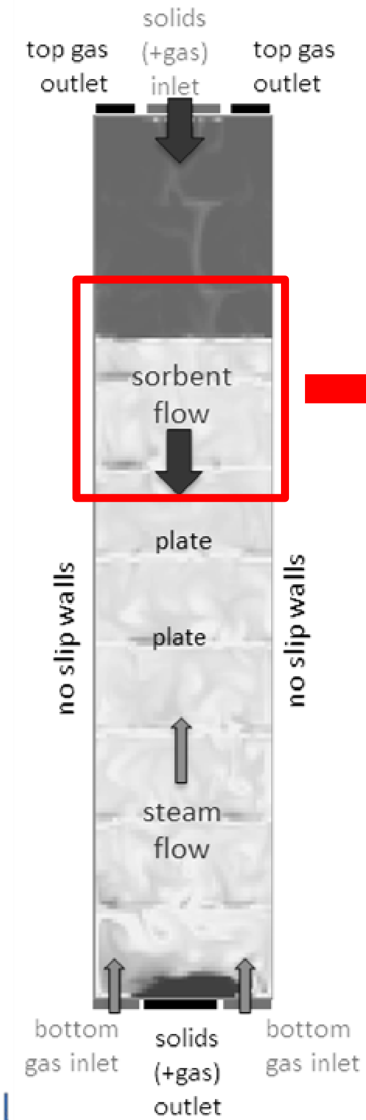
underground sequestration of CO_2

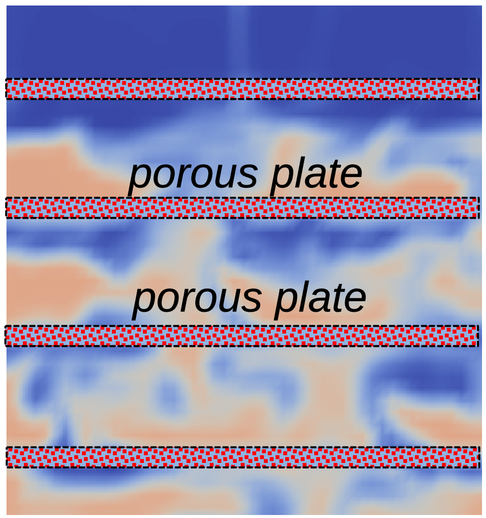
Modeling the Regenerator

***Full-scale regenerator design** (10 m × 10 m)*



***Regenerator model** (2 m × 10 m)*





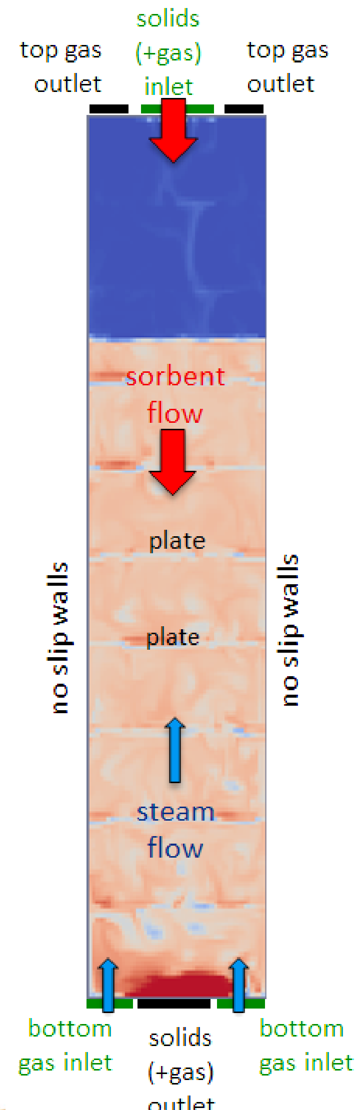
Porosity fixed at 80% for this work.

CCSI™ Carbon Capture Simulation Initiative
NETL
Berkeley Lab
National Laboratory
Los Alamos National Laboratory EST. 1943
Pacific Northwest National Laboratory
U.S. Department of Energy

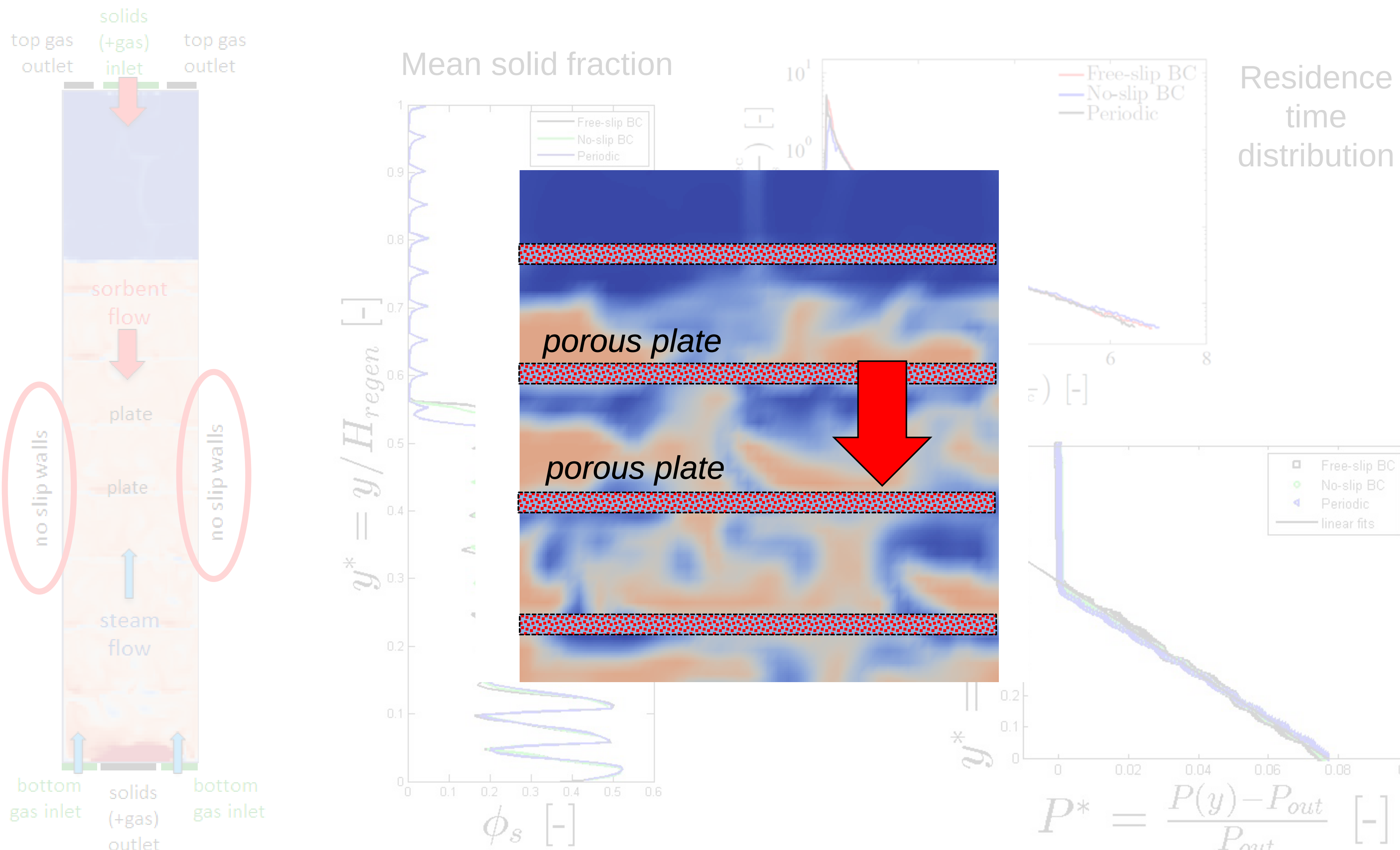
Regenerator Parameters

- Preliminaries
  - Side-wall boundary conditions
  - Grid size

- Operating conditions
  - Sorbent holdup (fill level)
  - Sorbent particle size
  - Inlet steam velocity



Preliminaries: Effect of Side Wall Boundary Conditions



CCSI™ Carbon Capture Simulation Initiative
NETL
Berkeley Lab
Lawrence Livermore National Laboratory
Los Alamos National Laboratory EST. 1943
Pacific Northwest National Laboratory
U.S. Department of Energy

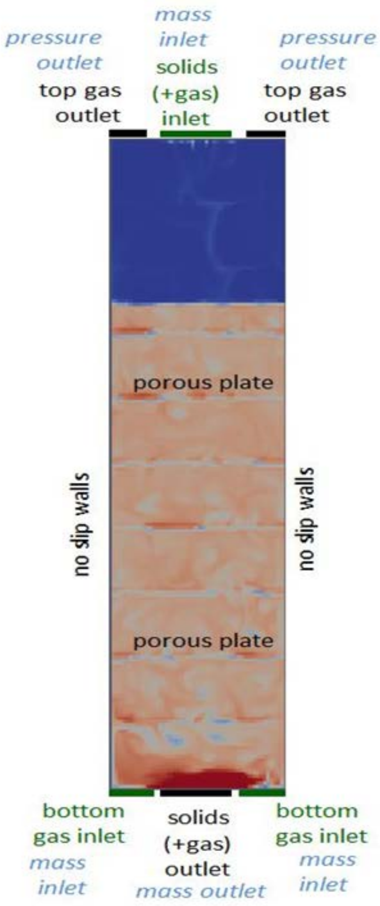
Uncertainty Quantification

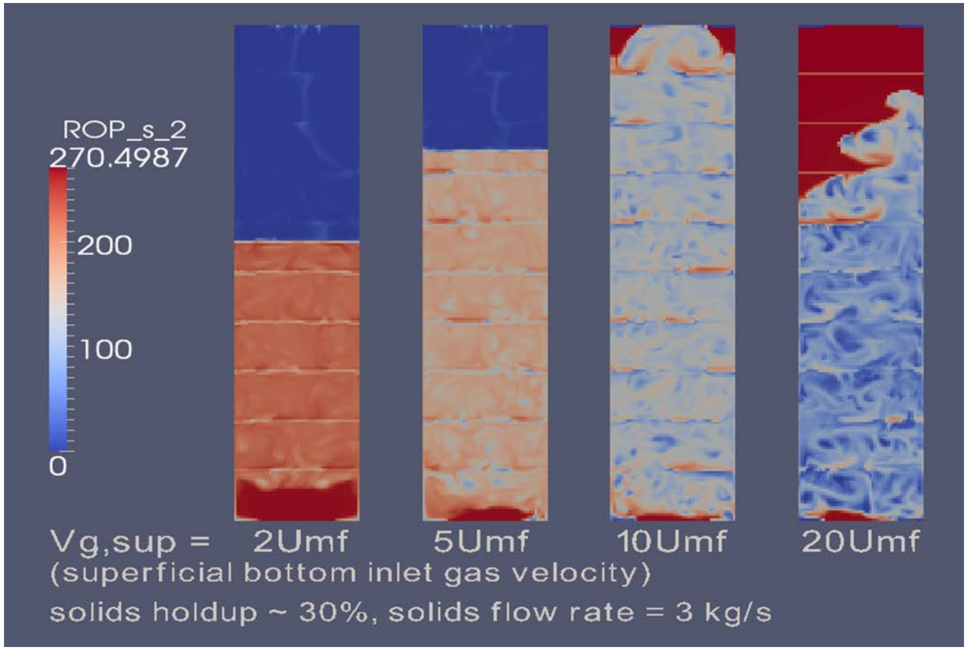
- UQ broadly: includes methods and tools to identify and quantify uncertainty at all levels of a system and incorporate that uncertainty in system performance analyses.
- UQ capability: is critical to simulation based analysis of carbon capture systems due to complexity and high cost of implementation of candidate systems.
- UQ needs: to understand and manage economic impact of incorporation of carbon capture systems in current industry operations.

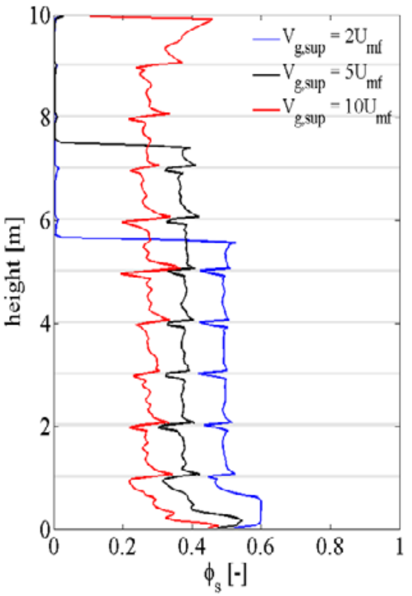
Immediate objectives

- Illustrates the use of a few UQ concepts in early stage development and evaluation of requirements for developing a full scale simulation.
- Input sensitivity and uncertainty: identify appropriate input ranges and impacts on simulation code results.
- Input calibration: estimate 'best' simulation input or parameters that determine equilibrium constants consistent with physical experimental results.
- Quantify the uncertainty: evaluate the posterior distribution of the parameters and the model.

Full-scale Regenerator Model



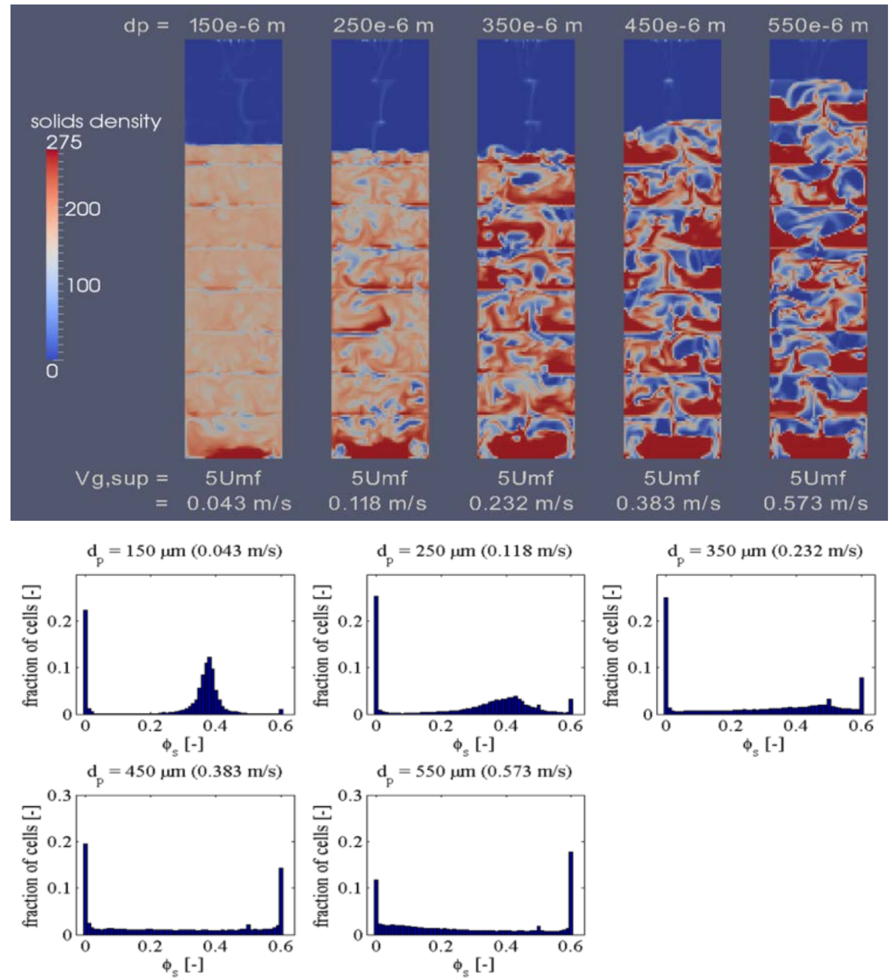




CCSI™ Carbon Capture Simulation Initiative
NETL
Berkeley Lab
Lawrence Livermore National Laboratory
Los Alamos National Laboratory
Pacific Northwest National Laboratory
U.S. Department of Energy

Frequency Distribution of the Solids Fraction (φ_s) for Different Particle Size and Inlet Gas Velocity

- Frequency distribution of the solids fraction (ϕ_s) in all the cells.
- For smaller sorbent diameters, most of the particles are uniformly fluidized at an intermediate solids fraction of ϕ_s~0.4.
- For larger diameters, two distinct modes are seen at ϕ_s= 0, representing the stream only regions, and ϕ_s= 0.6, indicating a densely packed bed of sorbents.



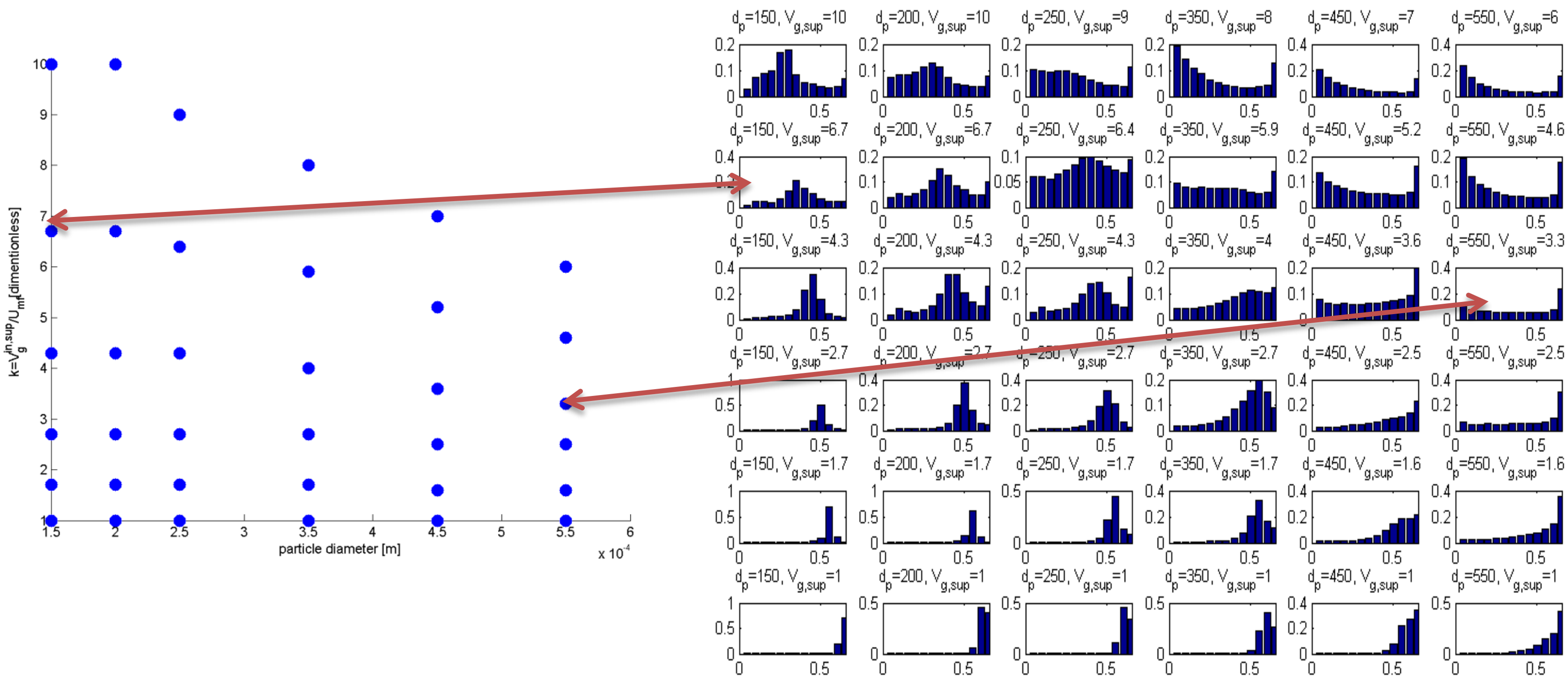
Building Statistical Model for Uncertainty Quantification

Use Gaussian process (GP) to model for the pressure drop gradient and the odds frequency distribution logarithm of the solid fraction.

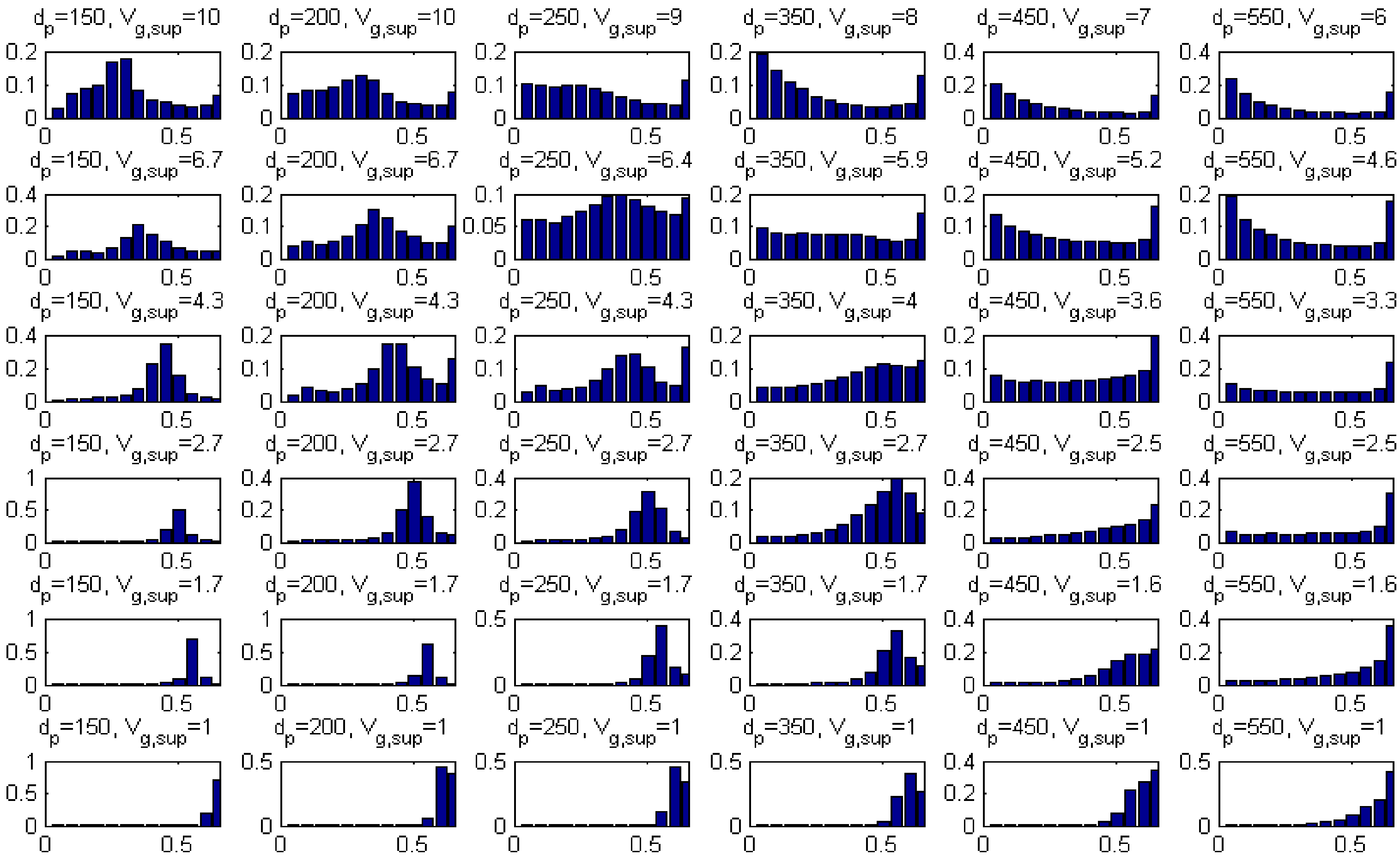
$$\ln\left(\frac{\pi_i(s)}{1-\pi_i(s)}\right) = \mu_i(s) + w_i(s) + \epsilon_i(s)$$

- $\pi_i(s)$ **probability of the i^{th} bin.**
- **s represent the input variables.**
- **i represent the i^{th} cell.**
- **$\mu_i(s)$ is a generalized regression.**
- **$w_i(s)$ is the spatial error and $\epsilon_i(s)$ is the nugget error.**

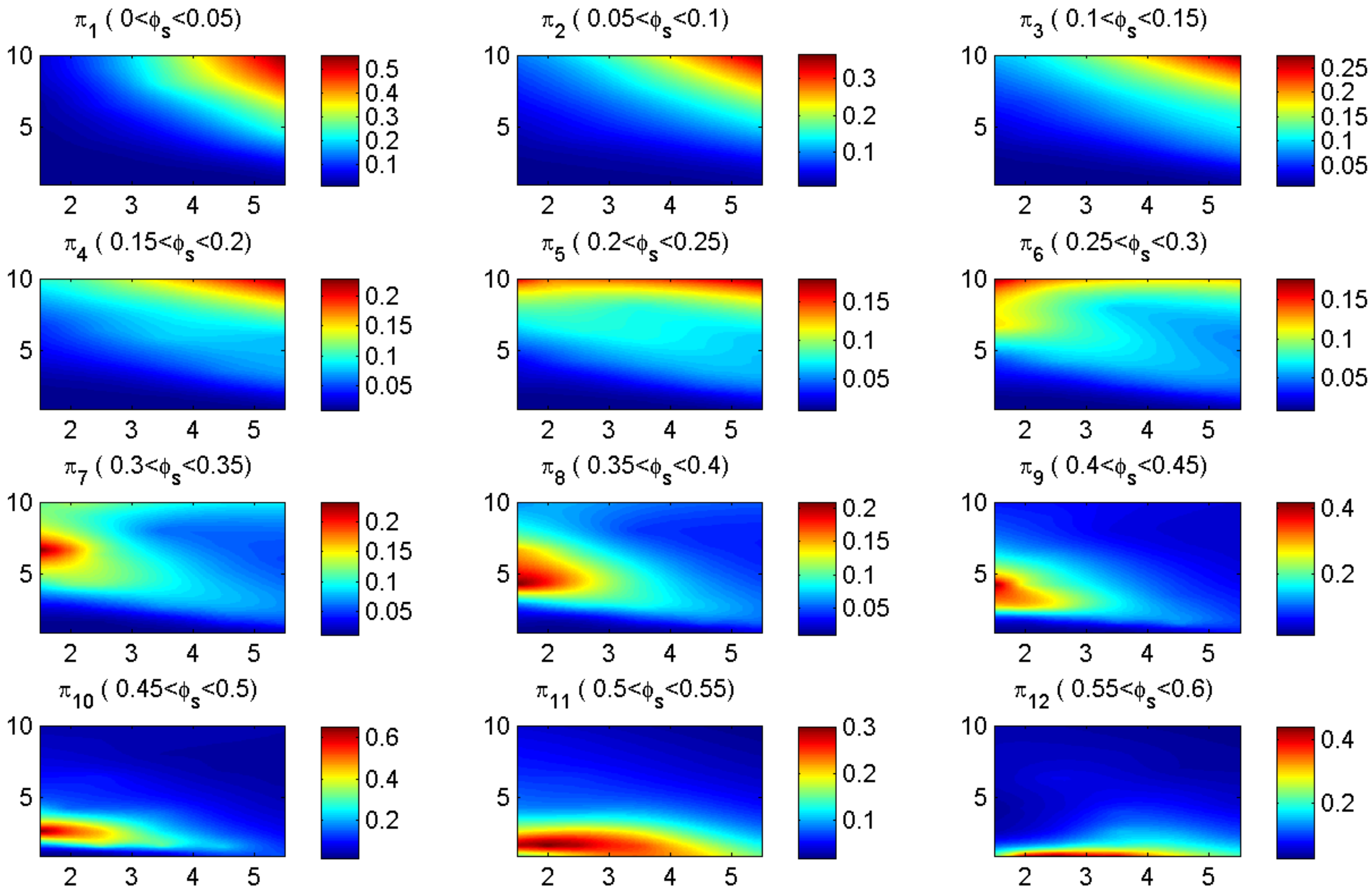
Simulated Cases & Corresponding Solid Fraction Distribution



Real Solid Fraction Distributions (36 observations)

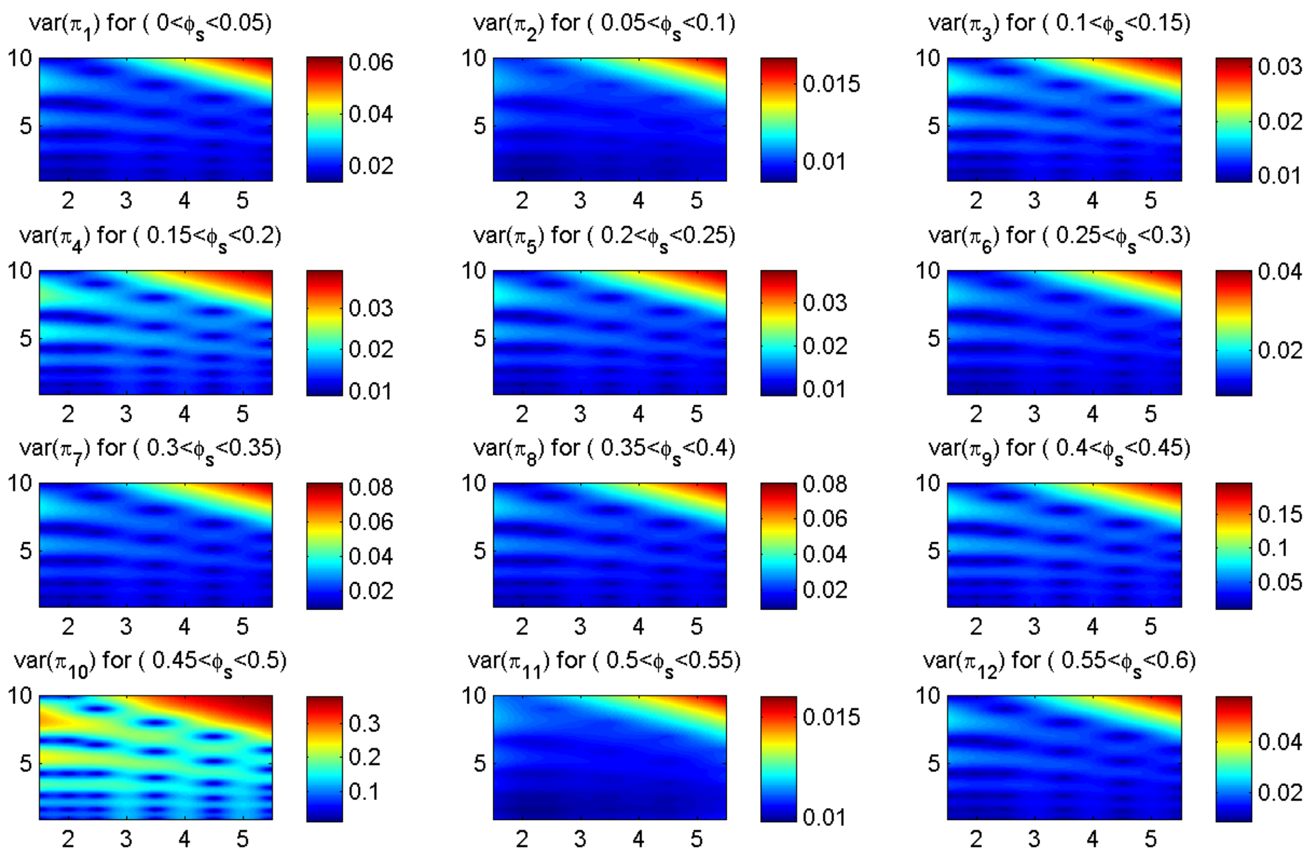


Predicted Probabilities of Solid Fraction Distribution Bin Magnitudes

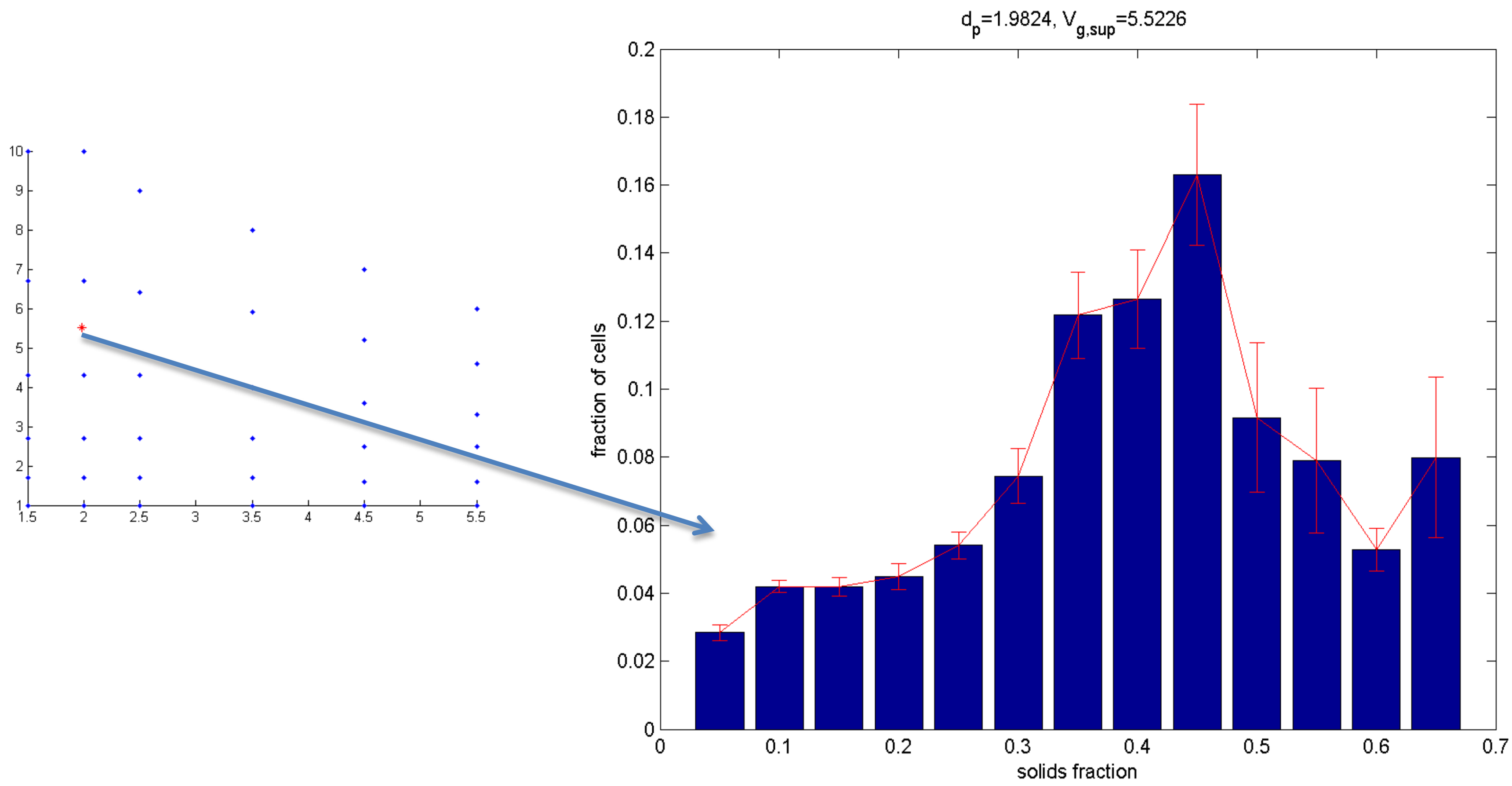


CCSI™ Carbon Capture Simulation Initiative | NETL | Berkeley Lab | Lawrence Livermore National Laboratory | Los Alamos National Laboratory | Pacific Northwest National Laboratory | U.S. Department of Energy

Variance of Predicted Probabilities of Solid Fraction Distribution Bin Magnitudes

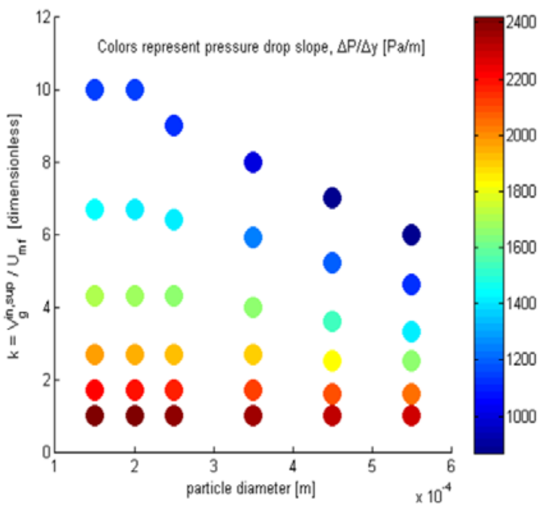


Example of Predicted Solid Fraction Distribution with Error Bars



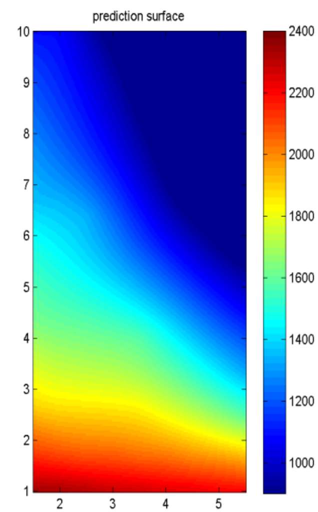
Predicted Probabilities for Pressure Gradient

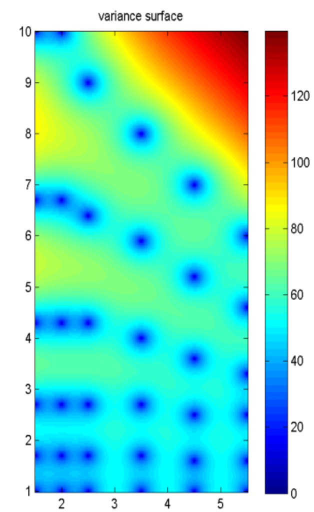
- **Find the posterior distribution of the parameters.**
- **Find the response surface and its uncertainty.**
- **Construct confident intervals.**



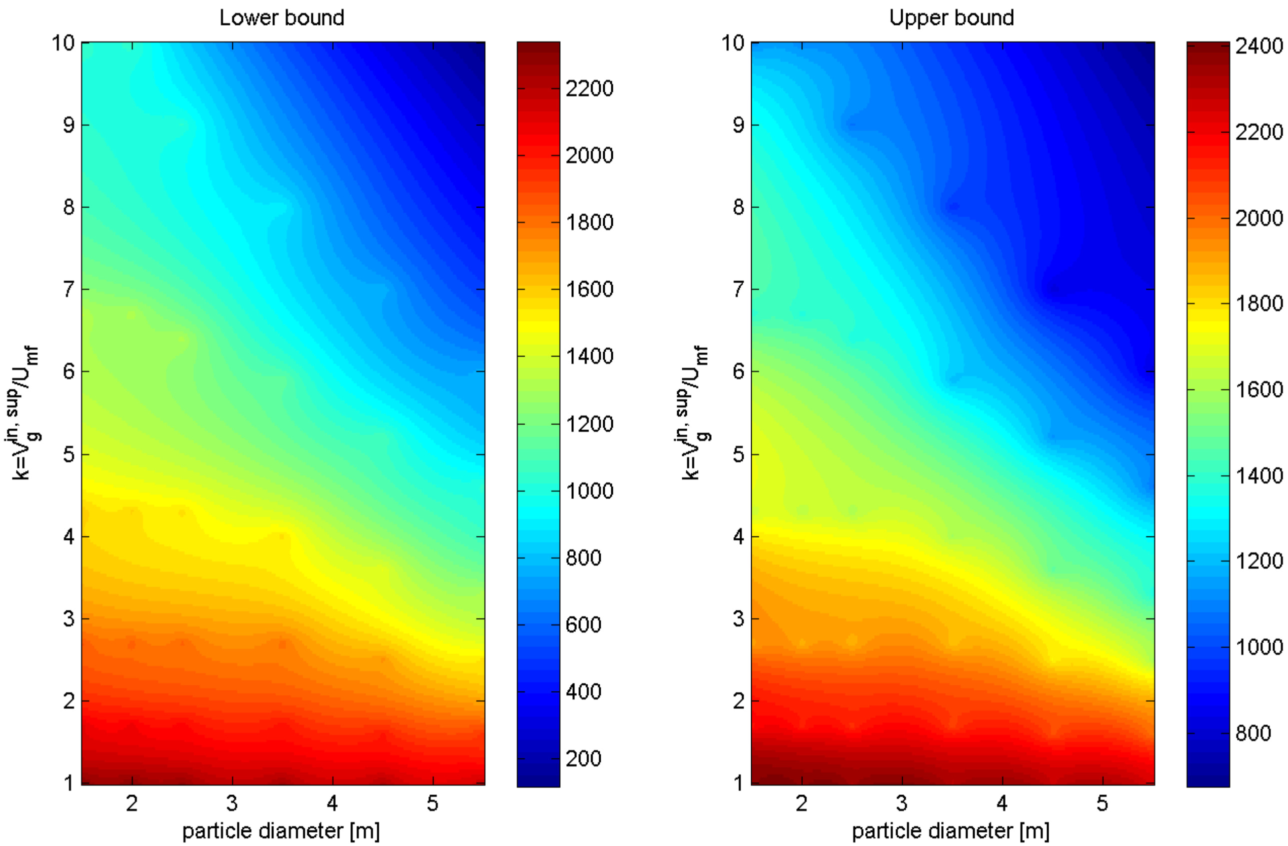
←Real observation of the pressure drop slope.

Prediction and variance → of the pressure drop slope Prediction surface matche well with left observed data.





Confident Interval: Lower and Upper Bound of the Predicted Pressure Drop



Summary

- Developed a CFD model for flow in the regenerator.
- Due to the computational cost, we only simulated 36 realizations in the input space.
- Developed a Gaussian process model for uncertainty analysis.
- Construct a response surface with error bars for the solid fraction distribution and the pressure drop gradient.
- Parametric uncertainty studies show:
  - Gas velocity and particle size more significant.
  - Smaller particles → uniform fluidization but allow small gas flow rates.
  - Larger particles → allow larger gas flow rates but tend to form dense clusters.

Questions?

Acknowledgements

- Fellow CCSI team members: G. Karagiannis, W. Pan, W. Xu, D. Suh, K. Saha, C. Montgomery, D. Miller, D. Mebane, J. Wendelberger, C. Tong.

Disclaimer