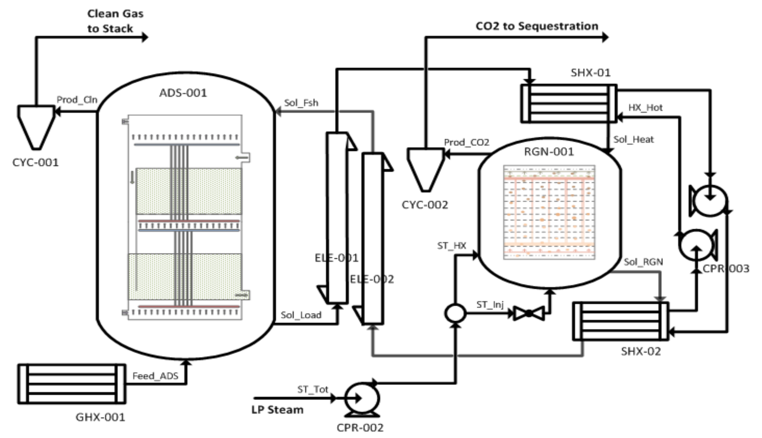
Solid Sorbent Simulation: Early Development and UQ Evaluation Tools

CCSI™ Carbon Capture Simulation Initiative

Guang Lin, Bledar A. Konomi , Avik Sarkar, Xin Sun, Jie Bao, Charles Tong, Joanne Wendelberger, K. Sham Bhat, Leslie Moore, Brenda Ng, David Miller, Moe Khaleel

- **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 and to the need to understand and manage economic impact of incorporation of carbon capture systems in current industry operations.
- **This poster** illustrates the use of a few UQ concepts in early stage development and evaluation of requirements for developing a full scale simulation for solid sorbent absorber and regulator.



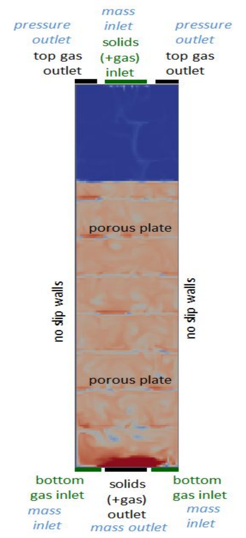
Immediate objectives:

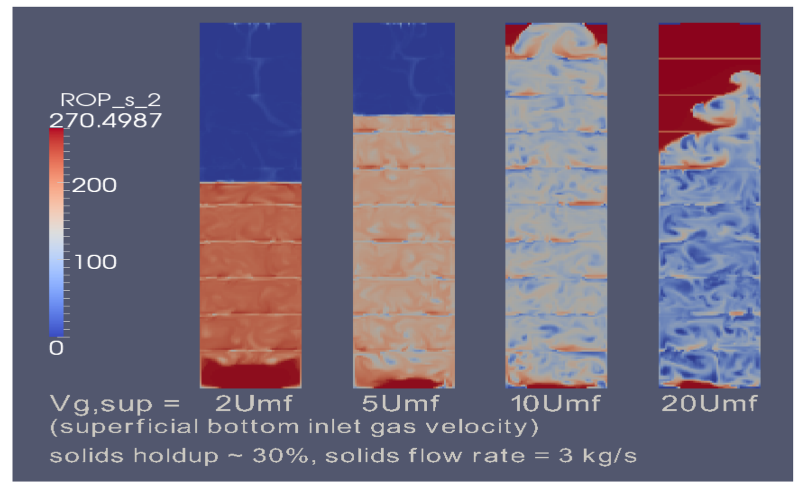
- Input sensitivity and uncertainty: identify appropriate input ranges and impacts on simulation code results;
- Input calibration: estimate ‘best’ simulation input or parameters that determine equilibrium constants consistent with physical experimental results;
- Quantify the uncertainty by the posterior distribution of the model distribution of the parameters

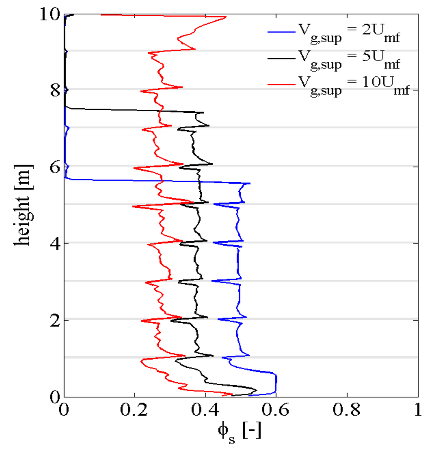
Full-scale Regenerator Model

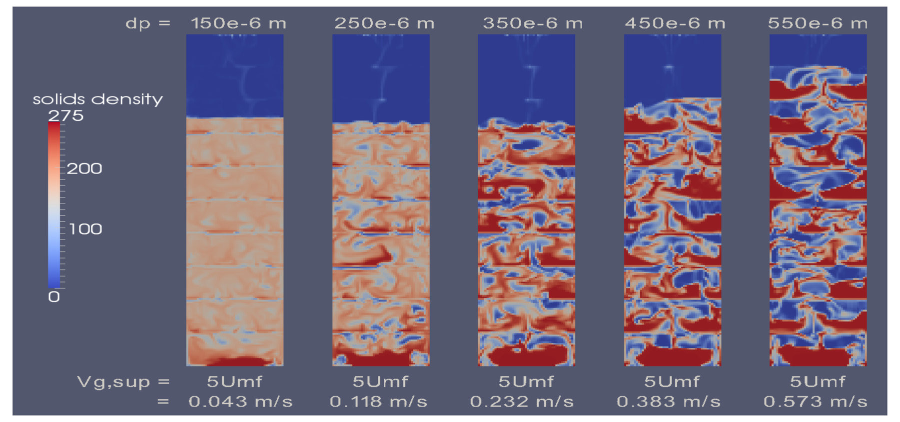
Solid fraction distribution for varying steam inlet superficial velocity, $V_{g,sup}$, expressed as a multiple of the minimum fluidization velocity, U_{mf}. The density of solids decreases at larger inlet steam velocities. At -$V_{g,sup}$ values larger than $10U_{mf}$, sorbent particles migrate to the top and accumulate as a packed bed, which is detrimental to device performance.

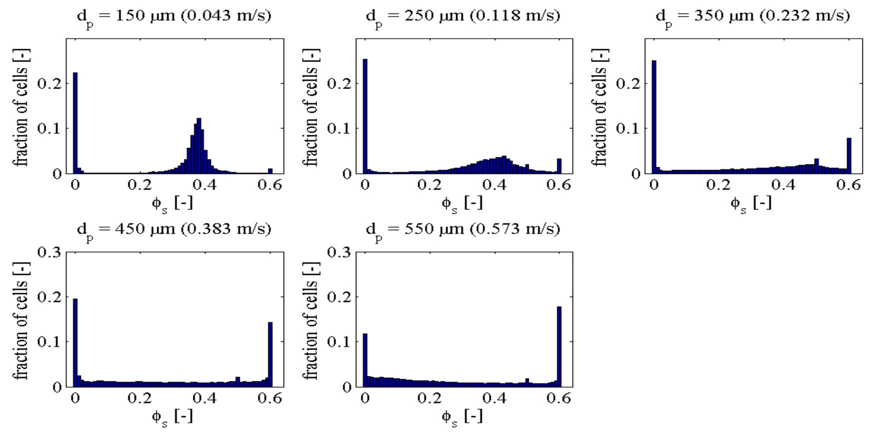
•Average solid fraction distribution in horizontal layers as a function of height. The steady solid fraction decreases with increasing inlet steam velocity along with a rise in the height of the free surface interface.











- The minimum fluidization velocity is given by:

$$U_{mf} = \frac{(\rho_s - \rho_g)\, g d_p^2}{150\,\mu_g} \cdot \frac{\phi_{s,mf}^3}{(1-\phi_{s,mf})}$$

ρ_s is the solids density, ρ_g is gas density, d_p is the particle diameter, μ_g is the gas viscosity.

- As the inlet gas velocity is increased, the bed of solids at the bottom experiences greater fluidization.
- The density of solids in the lower regions decreases with a corresponding increase in the height of the free surface.
- At larger inlet velocities $V_{g,sup} > 10U_{mf}$, material is found to accumulate at the top of the regenerator as a packed bed.
- For an even larger inlet velocity of $20U_{mf}$, a significant fraction of particles eventually accumulates at the top.

Frequency distribution of the solids fraction (ϕ_s) in all the cells, demonstrating segregation of steam and sorbents at larger particle diameters. 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.

The Statistical Model

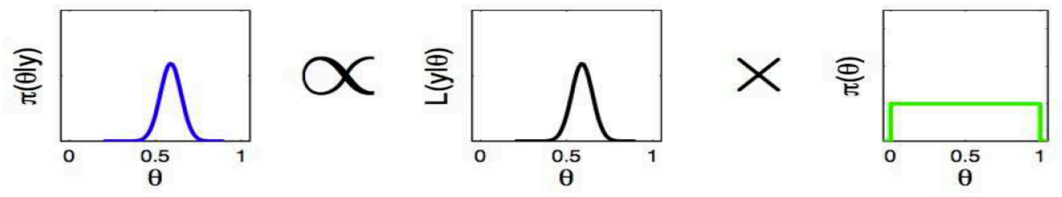
•Use Gaussian process (GP) to model for the pressure drop slope and the odds frequency distribution logarithm of the solid fraction.

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

where 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.

Bayesian Inference

•Use Bayesian statistics to combine what we already know and the model discrepancy with the data. Bayesian statistical approach quantifies uncertainty including model and observation error.



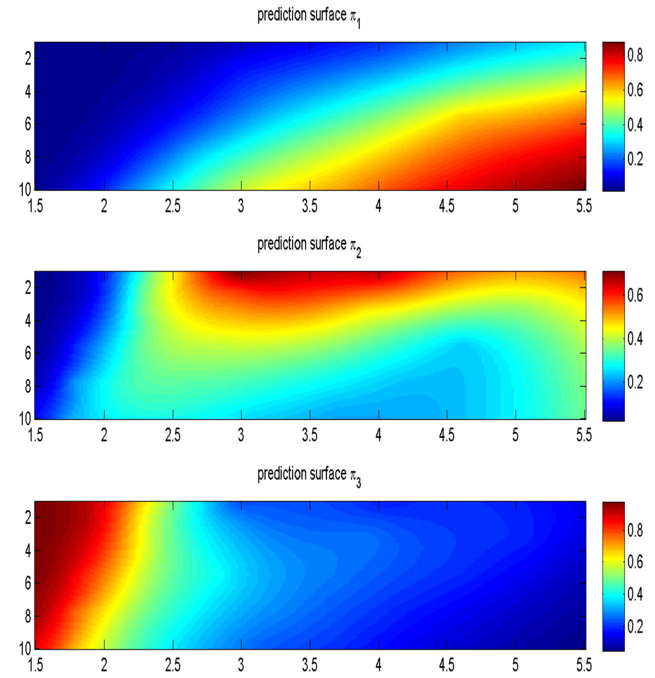
$$\pi(\theta|y) \propto L(y|\theta) \times \pi(\theta)$$

π(θ|y) is the posterior, L(y|θ) is the likelihood and π(θ) is the prior.

Goal:

•Find the posterior distribution of the parameters.

•Find the response surface and its uncertainty .

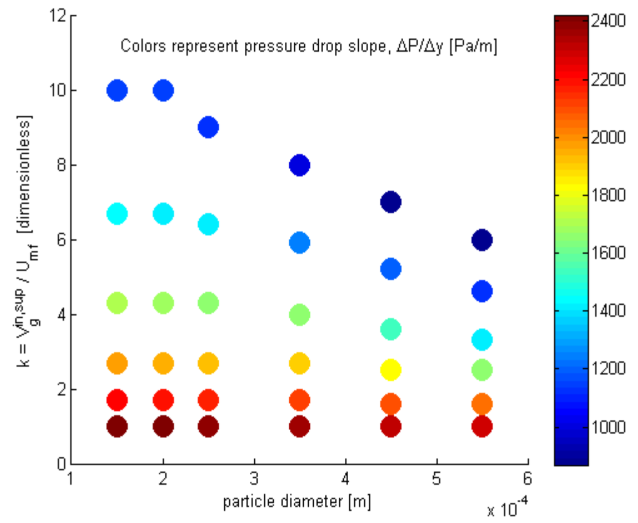


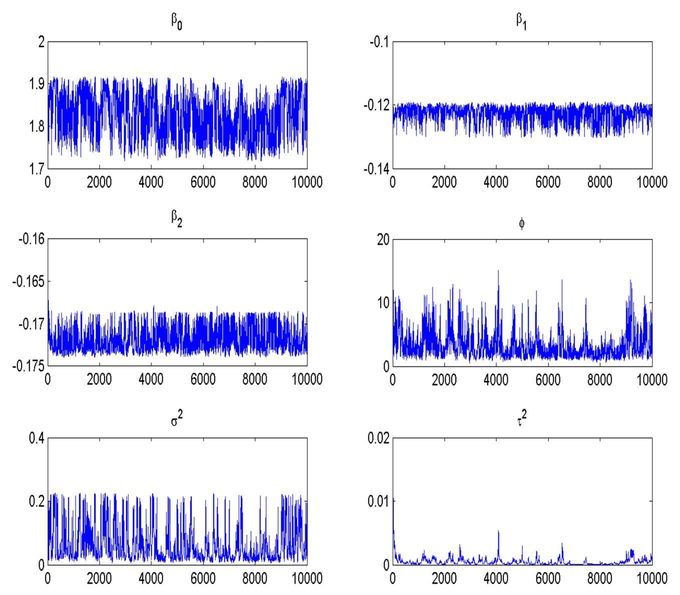
Statistical Inference

A parametric study → comprised of 36 simulations for varying particle diameter and gas velocity (input space).

← Proportion prediction

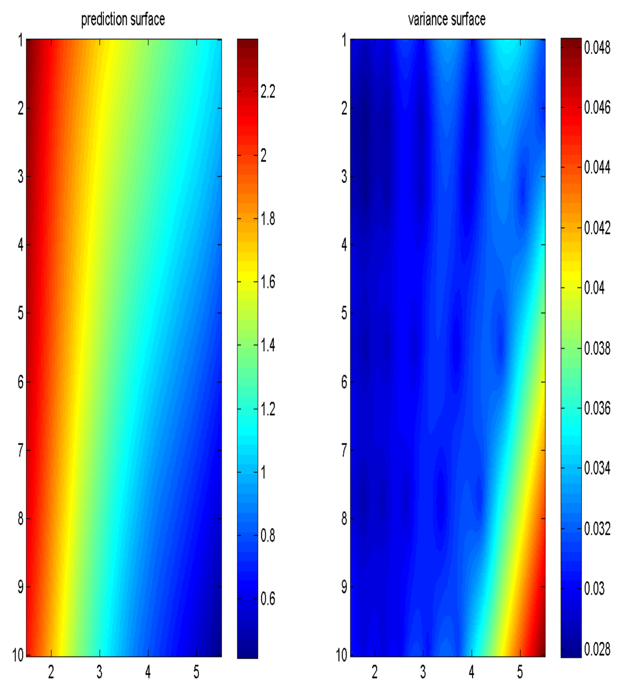
- π_1: proportionType equation here. of solid fraction < 0.25
- π_2: proportion of solid fraction > 0.25 & <0.45
- π_3: proportion of solid fraction <0.45





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

← Parameter uncertainty. MCMC of the posterior probability of the parameters of the Gaussian Process model. (the linear components of μ(s), the variance and covariance of w (s) and the variance of the nugget error ε(s))



Summary and Future work

- Full scale model of the CO_2 regenerator is developed and modeled using the open-source code MFIX.
- Gaussian process for the pressure drop slope and the log of the solid fraction odds is build.
- Study propagation of parameter uncertainty and response surface uncertainty.
- Determine important inputs and sample points where we obtain the most informative points.

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