CCSI™

Carbon Capture Simulation Initiative

# High Fidelity Models of Solid Sorbent Carbon Capture Systems

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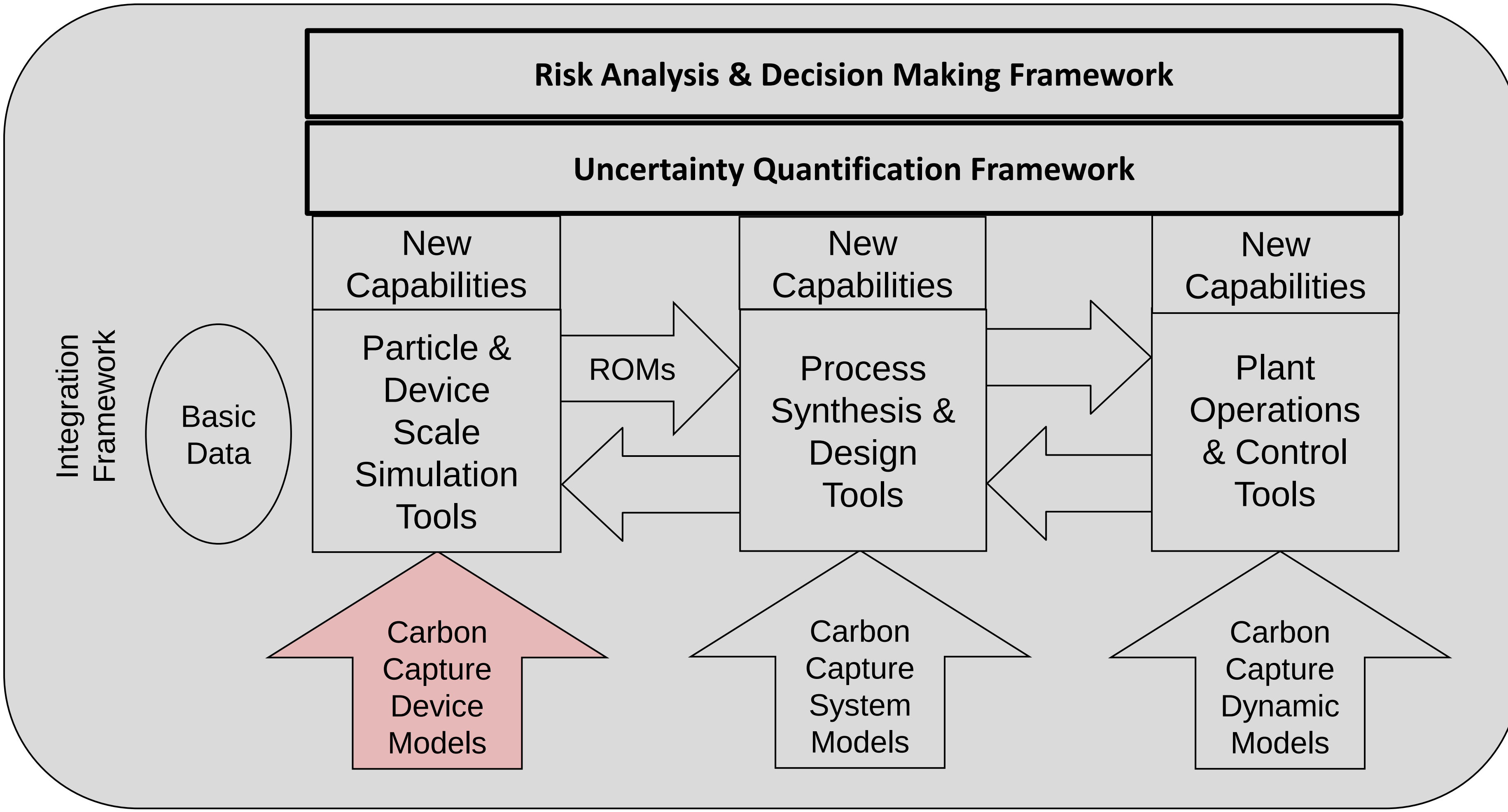
# High-fidelity models of solid sorbent carbon capture equipment

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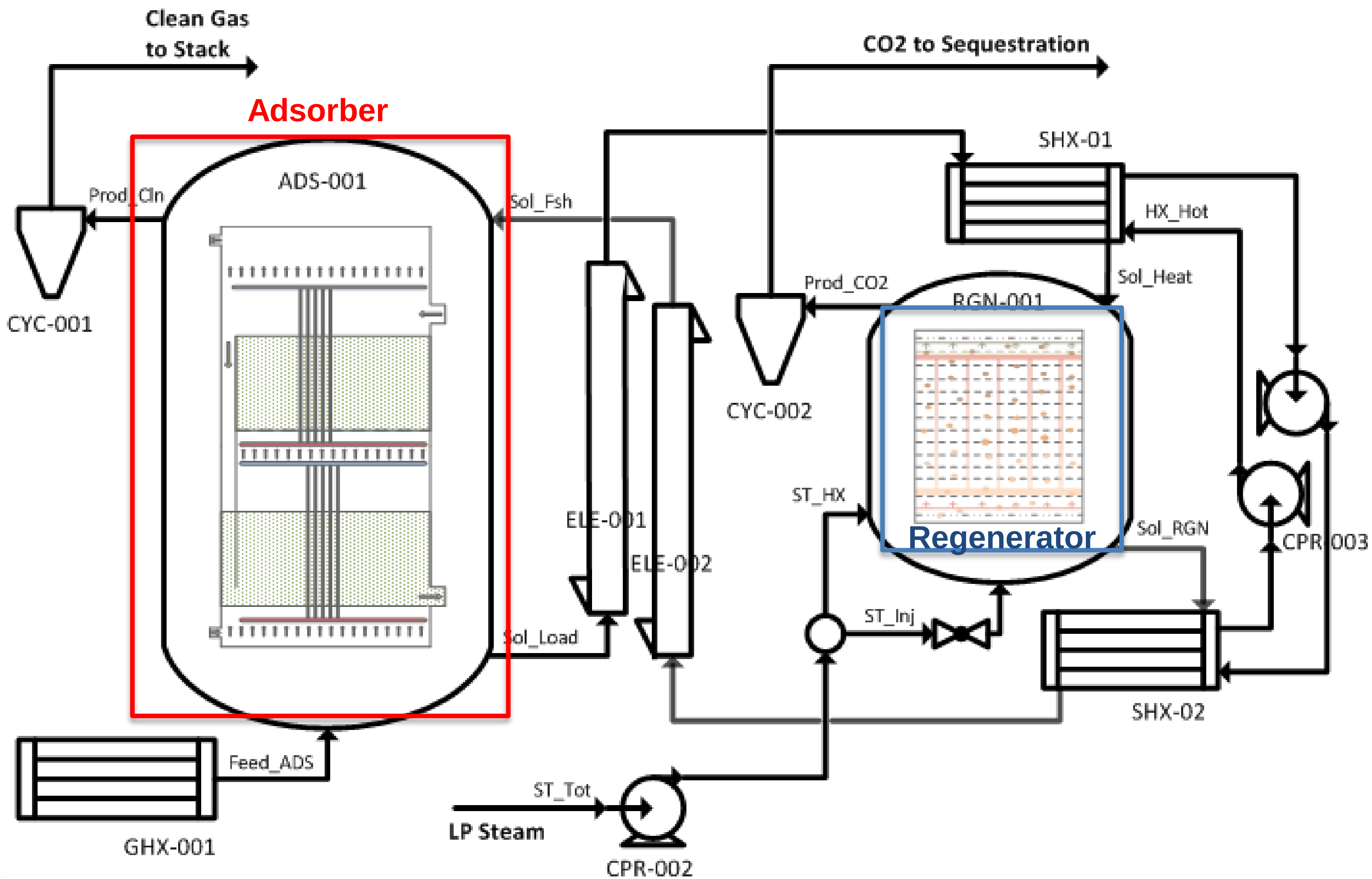
# Objectives

- Develop state-of-the-art device-scale simulation tools to accelerate the commercialization of carbon capture technologies.
  - Computational Fluid Dynamics (CFD) models of multi-phase bubbling, moving and fluidized beds
  - Includes hydrodynamics, reactions and heat transfer of solid sorbent systems.
  - Quantify the accuracy of the CFD models by validating them with experimental data.
- Collaborate with other teams in CCSI to improve the design and performance of carbon capture technologies.
- Cross country team of engineers:
  - Team lead: Xin Sun, PNNL
  - Team: D. DeCroix (LANL), E.D. Huckaby (NETL), W. Xu (PNNL), A. Sarkar (PNNL), W. Pan (PNNL), S. Dartevelle (LANL), S. Sundaresan (Princeton). C. Montgomery (NETL)

# Conceptual Full Scale CCSI Solid Sorbent Adsorber and Regenorator

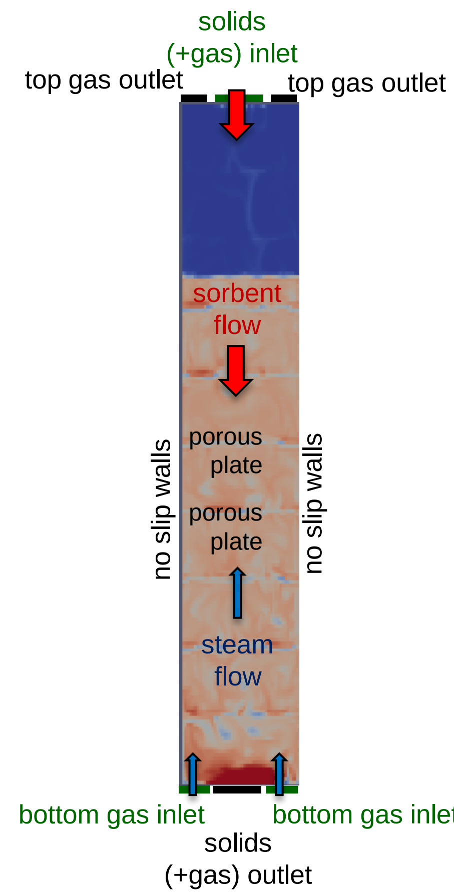


# Overview

- Model the multi-physics of the full scale CCSI carbon capture system
- Use appropriate state of the art simulations tools and sub-models
  - Based on open source CFD code MFIX
- Modeling approach: start with simpler unit problems and build up to complete multi-physics
  - Regenerator: multi-phase hydrodynamics
  - Adsorber: multi-phase hydrodynamics + dry reactions
  - Smaller scale system: multi-phase hydrodynamics + dry and wet reactions
- Validate models with experimental data

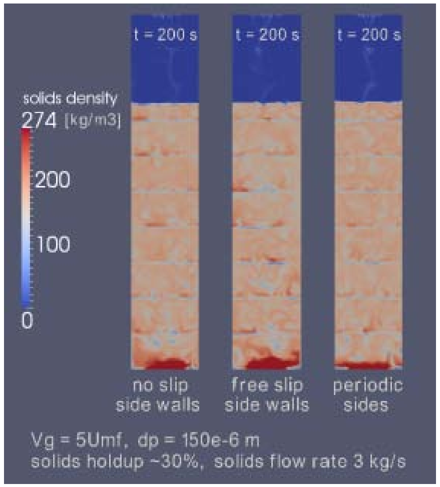
# Simulating Multi-Scale Hydrodynamics in the Regenerator

- Moving bed with perforated plates
- Model includes:
  - Gas flow
  - Solid sorbent particles
  - Isothermal, non-reacting flow
- Investigate the effects of boundary and operating conditions on the particle residence time

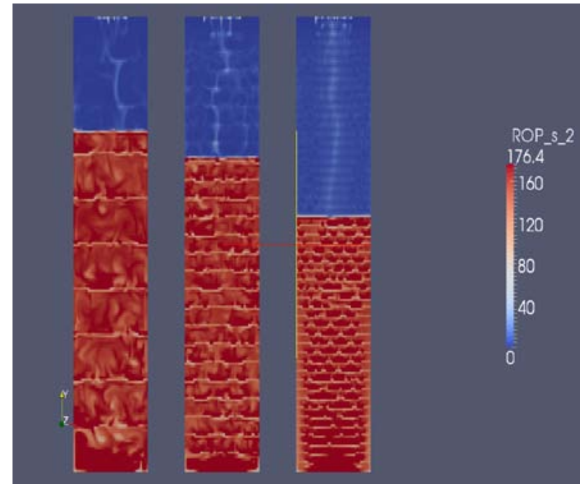


# Regenerator Simulations

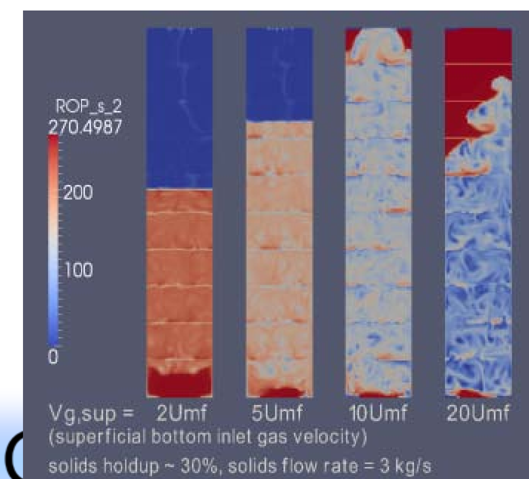
## Effects of Boundary Conditions



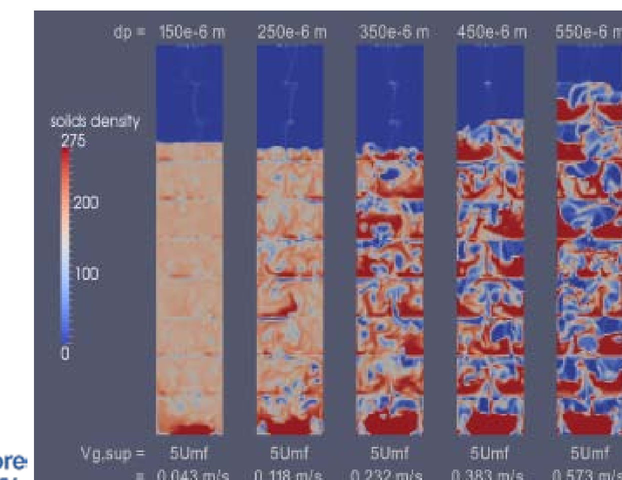

## Effect of Perforated Plate Spacing




## Effects of Steam Inlet Velocity

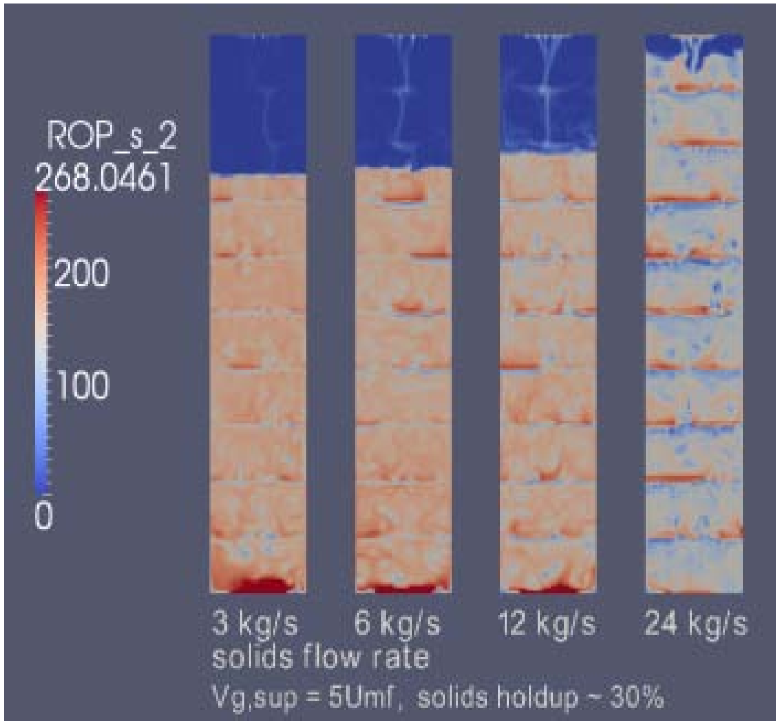



## Effect of Particle Size



# Regenerator Simulations

Effect of Sorbent Flow Rate



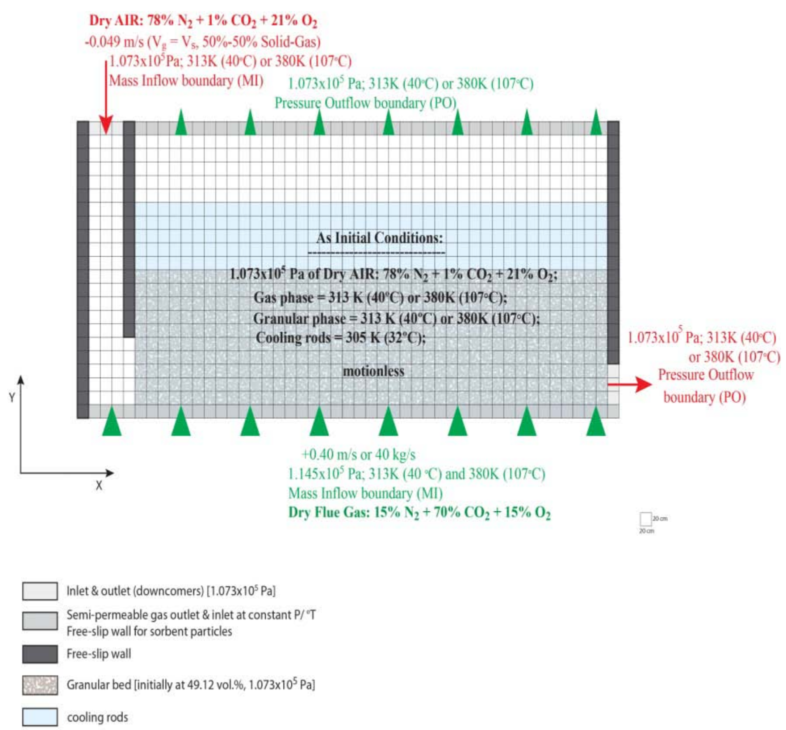

- Effects of initial particle loading (holdup) and sorbent velocity have greatest affect on residence time
  - Although residence time may be the same in some cases it does not necessarily produce the same particle distribution.
- Next step will be to add in the dry reactions of $CO_2$

| | 20% holdup | 30% holdup | 40% holdup | 50% holdup |
|---|---|---|---|---|
| **Mean residence time** | 588 s, or 9.8 min | 882 s, or 14.7 min | 1176 s, or 19.6 min | 1470 s, or 24.5 min |

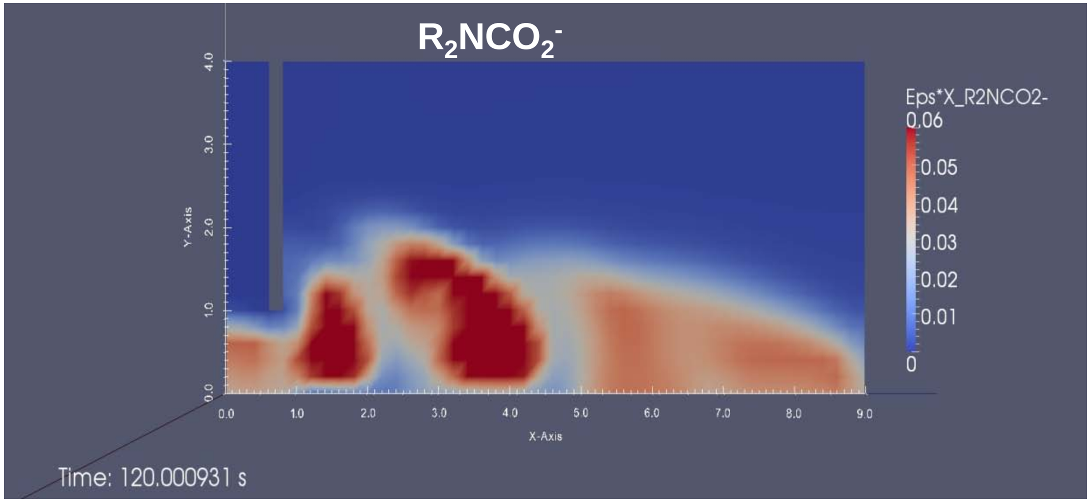
# Simulating Reactive Transport in the Adsorber

- Multi-stage moving bed with heat exchanger tubes
  - Model include one stage
  - Porous media model for HX tubes
- Implementation of a dry, isothermal adsorption-desorption model in MFIX
  - $2\ R_2NH + CO_2(g) \leftrightarrow R_2NCO_2^- + R_2H_2^+$
- Simulating transient startup from fresh adsorbent
  - Looking at 2 operating temperature to investigate changes in $CO_2$ adsorption

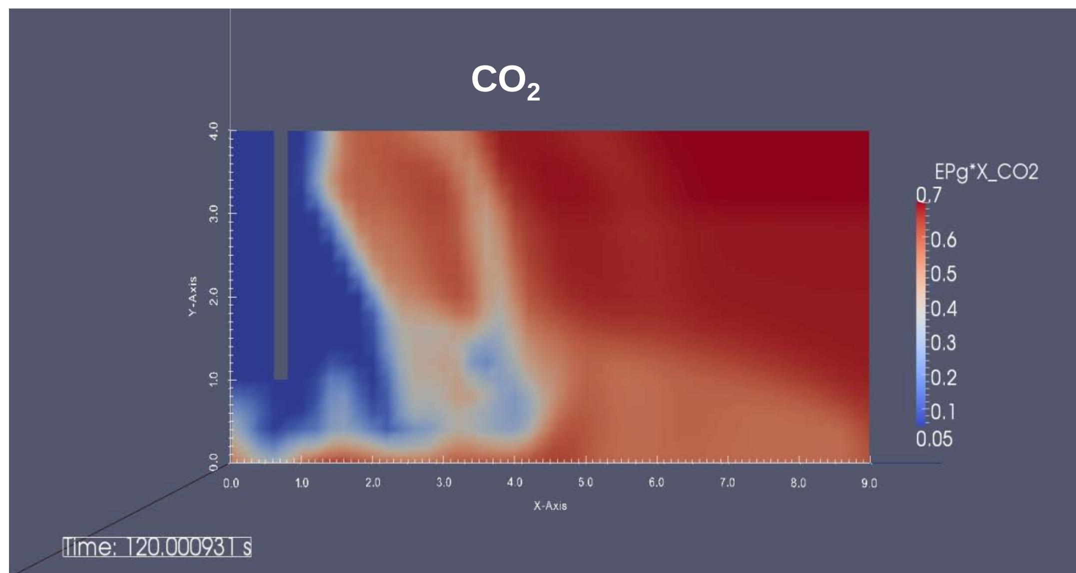
**Cross-sectional view: Initial and boundary conditions**



# Dry Reactions in the Adsorber




- Mass Fraction of Solid * Volumetric Fraction of $R_2NCO_2^-$ (adsorbed $CO_2$)




- Mass Fraction of Gas * Volumetric Fraction of gaseous CO2

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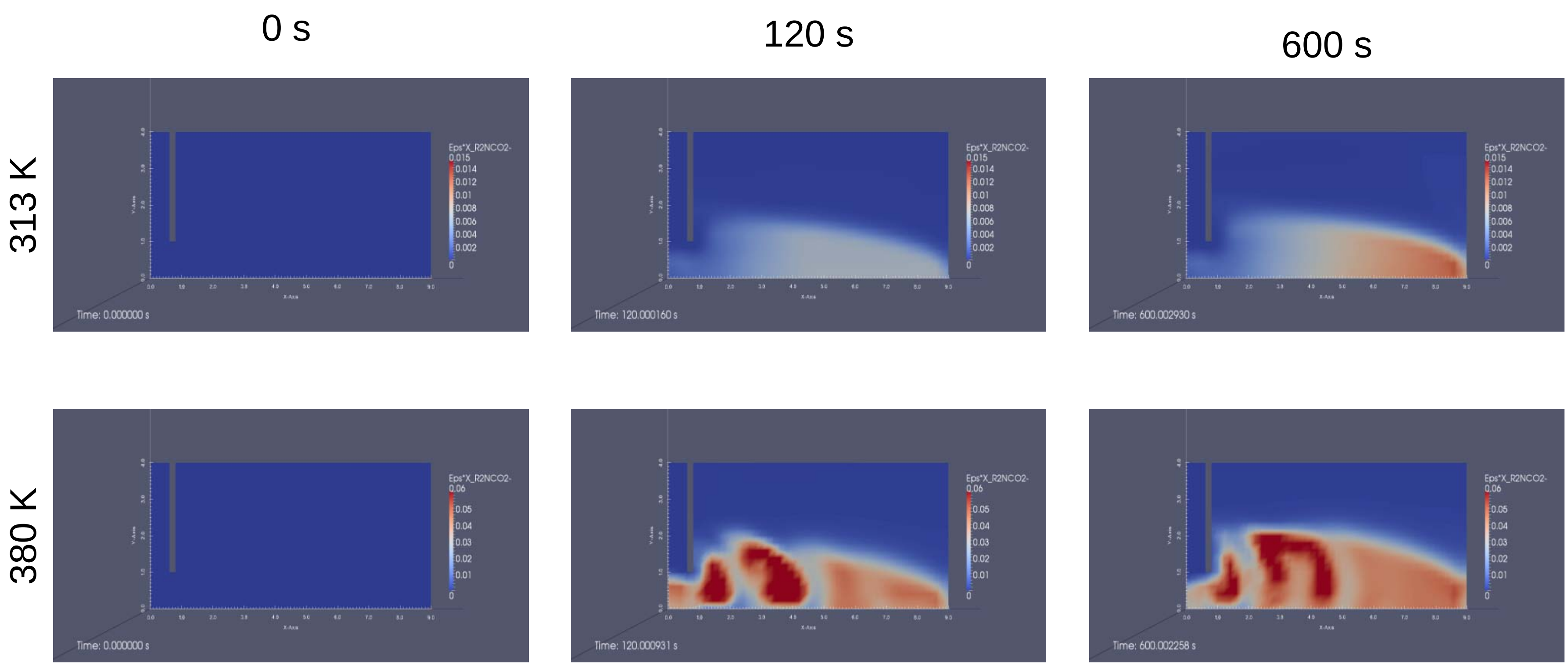
# Time and Temperature Dependence of CO2 Uptake

- Changes in mass fraction of solid * adsorbed CO2 at two different operating temperatures and various times during transient startup

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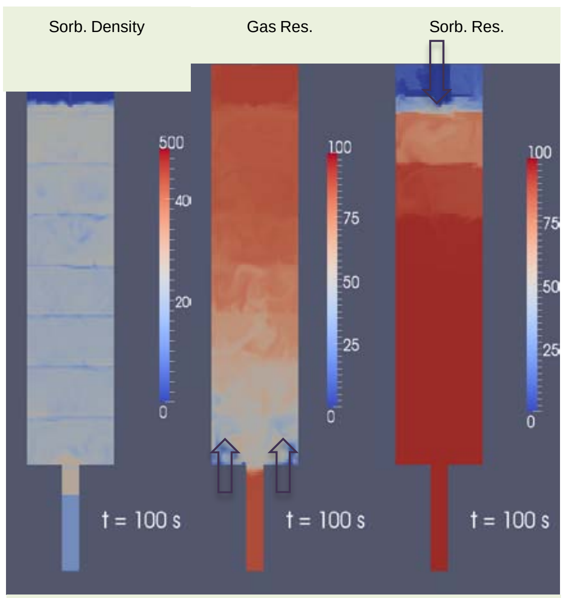
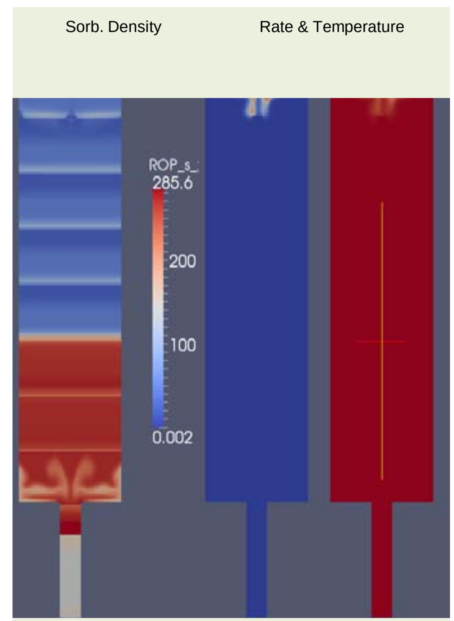
# Developing Reacting Flow Models

- Use simpler geometry and smaller systems to initially implement reactions
- We have implemented both dry and wet reactions in simplified full scale regenerator



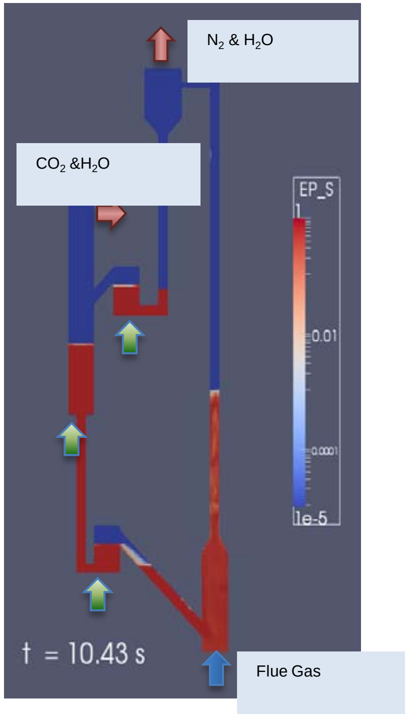

Residence time analysis
using convection-reaction equation




Reacting Flow Simulations

# 2D NETL $CO_2$ Capture Unit (C2U)

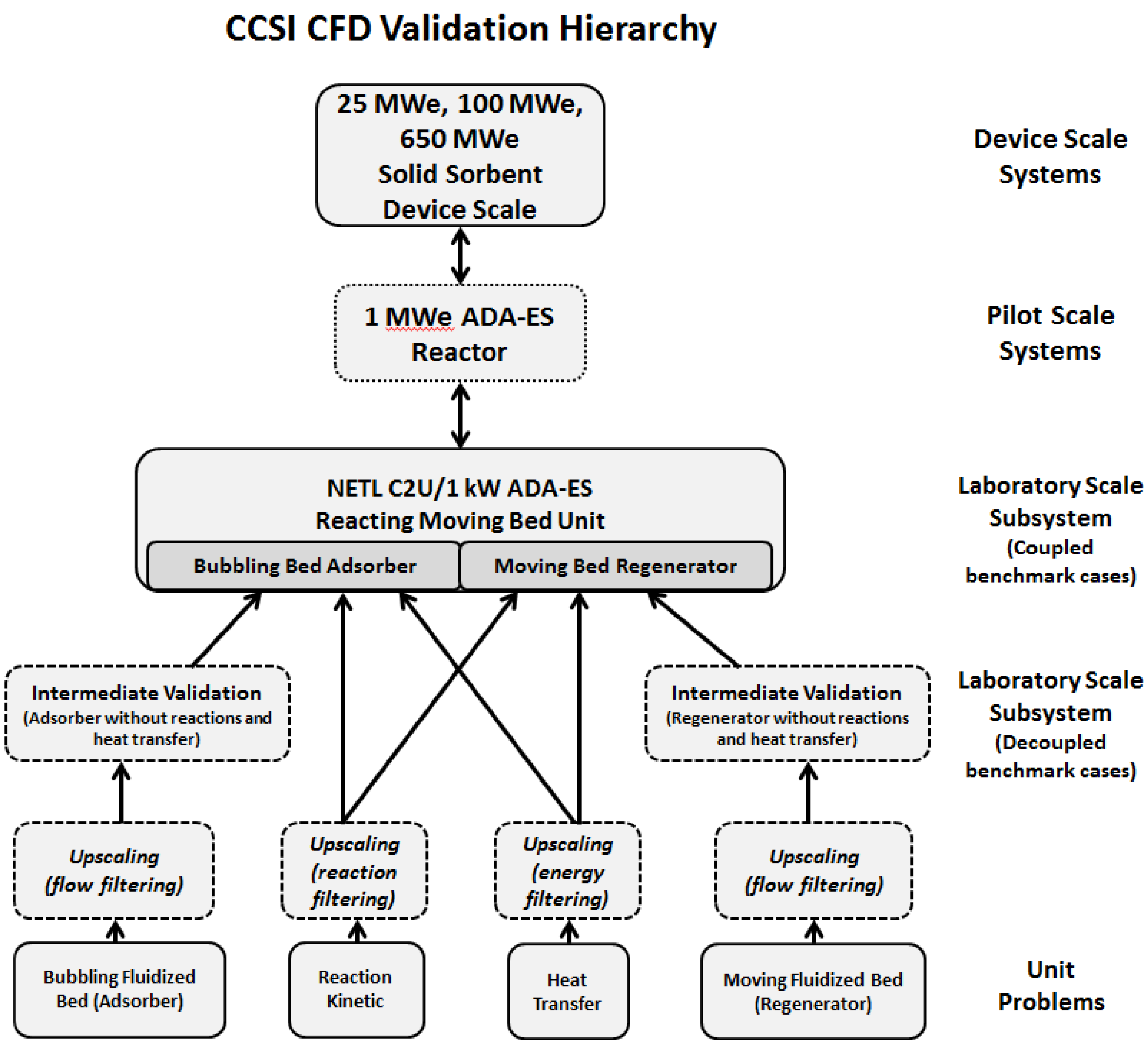
- 2D C2U reactor loop
  - Quick simulations of reactive transport
- Currently in development stage
- Will be used for validation studies of CCSI CFD models



# Validation and Uncertainty Analysis of CCSI CFD Models

- Developing a validation and UQ plan to assess confidence range for CFD models
- Hierarchical approach where complex multi-physics are broken down into simpler problems
- Considers coupling of physics and the upscaling of models to the device scale.
  - Upscaling methodologies are being developed to correctly include small scale features in the full scale models

# Validation Hierarchy



# Conclusions

- Working towards device-scale CFD models of the reactions, transport and heat transfer in CCSI solid sorbent systems
  - Building models up slowly to ensure correct implementation of physics
- Development of models includes the inclusion of solid sorbent reaction mechanisms and the development of upscaling methodologies.
- Validation of CFD models is an important aspect of the project and a plan is being developed to address the models' accuracy.

# Disclaimer