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Multiphase CFD Modeling in the CCSI – Flow Dynamics of Sorbents in the Regenerator of a Carbon-Capture Unit

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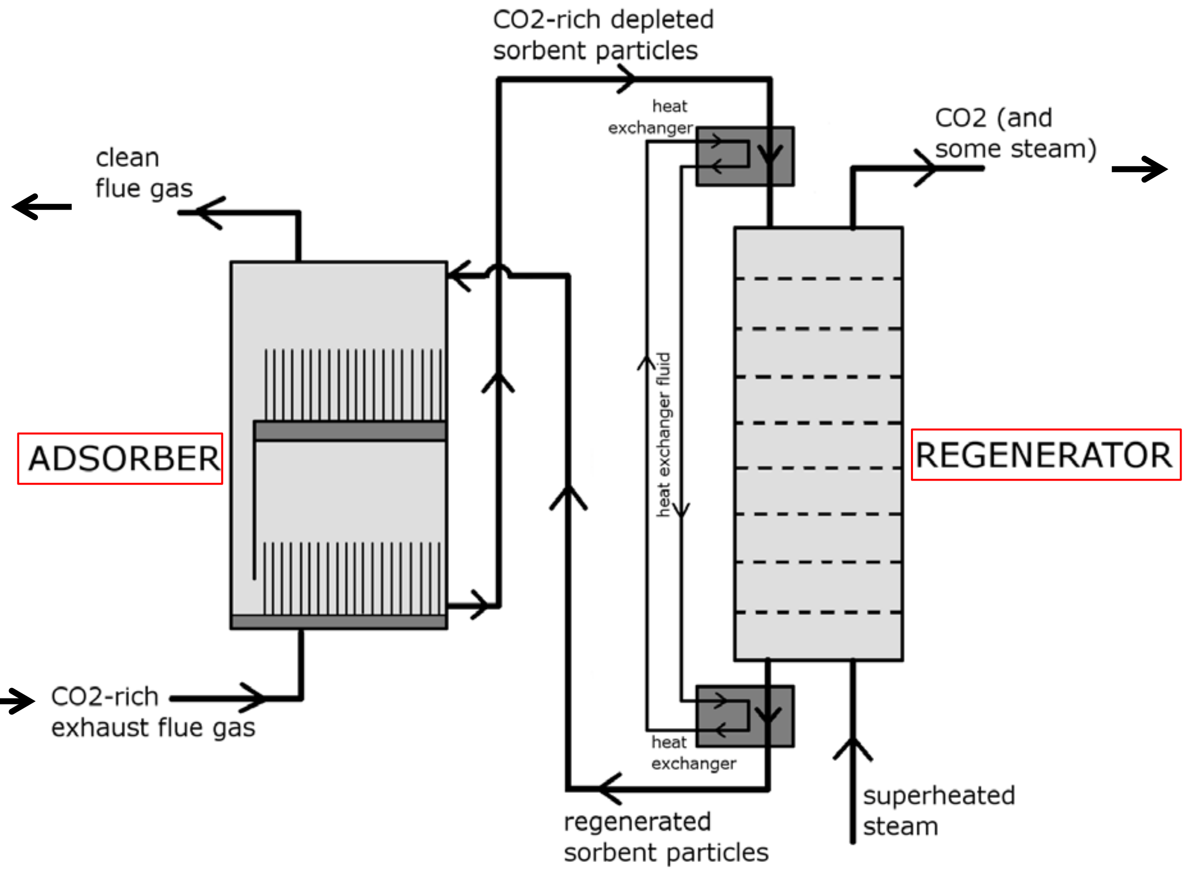
Outline

- The Carbon-Capture Unit
- Regenerator Modeling
  - Effect of sorbent holdup
  - Effect of gas velocity
  - Effect of particle size
- Adsorber Modeling
- Summary and Future Work

The CCSI Carbon-Capture Unit

CCSI : Carbon Capture Simulation Initiative

underground sequestration of CO_2



Modeling the Regenerator

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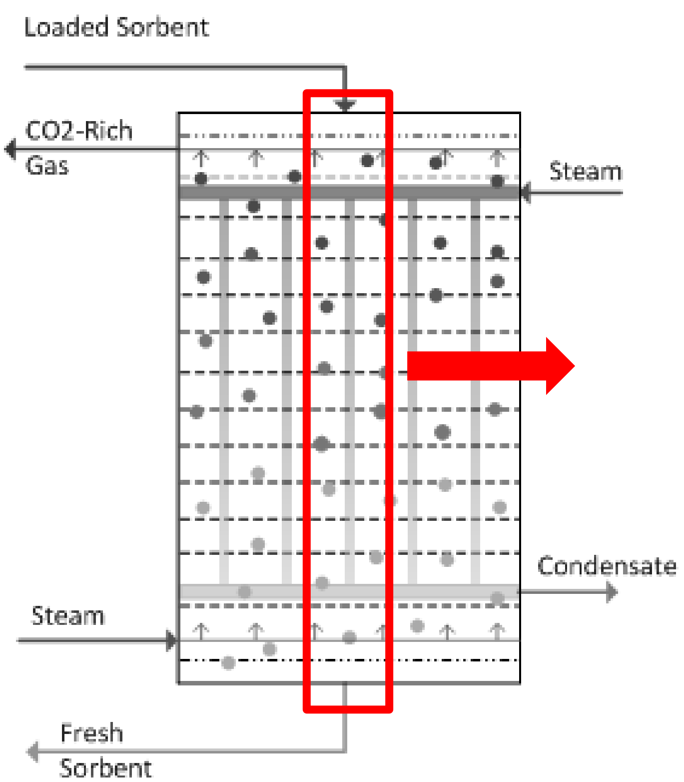
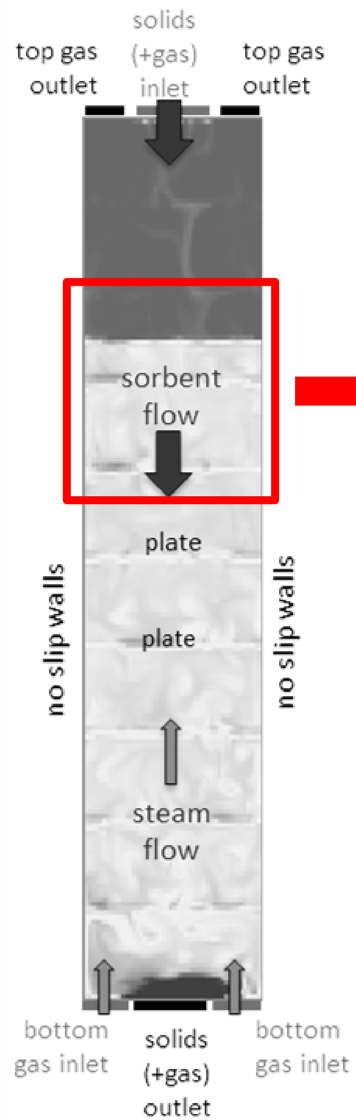
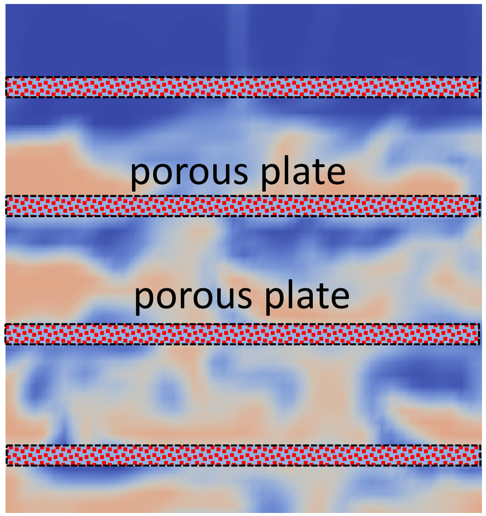
Full-scale regenerator design (10 m × 10 m)



Regenerator model (2 m × 10 m)



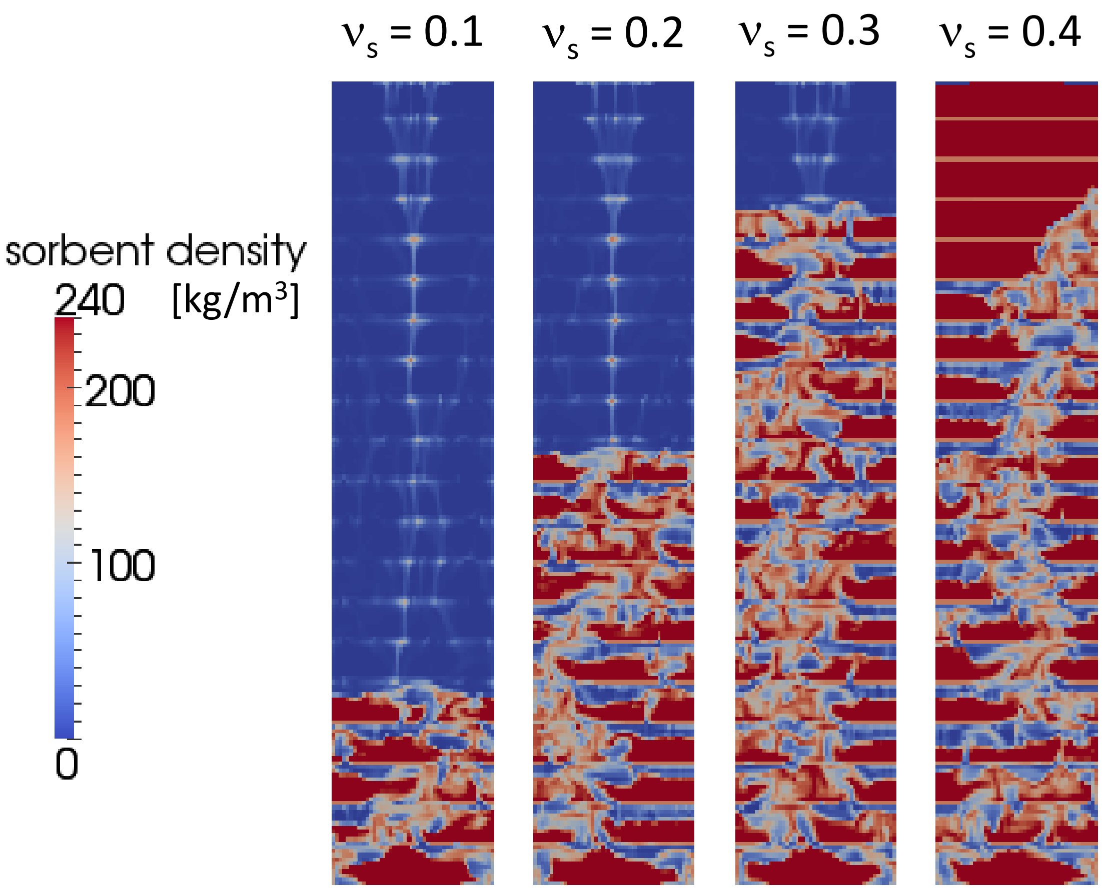
Perforated plates modeled as stationary, uniform porous media.



Porosity fixed at 80% for this work.

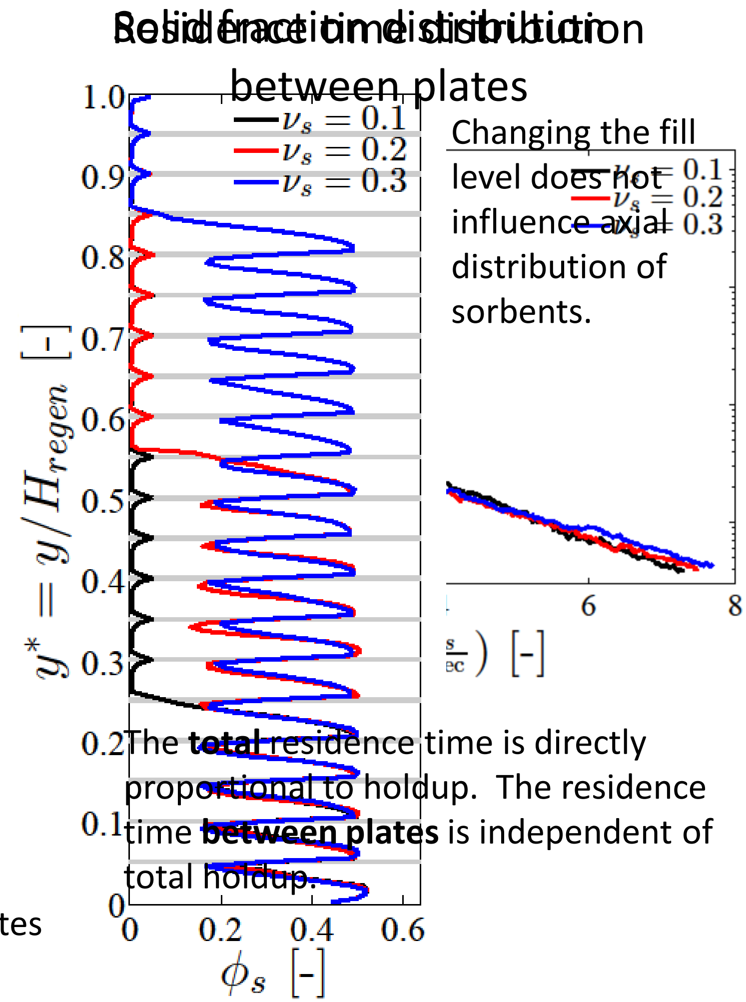
Effect of Sorbent Holdup

Volume fill fraction



d_p = 350 μm, $V_{g,sup}$ = 5U_{mf}

Overfilling creates a dense packed bed at the roof.



Changing the fill level does not influence axial distribution of sorbents.

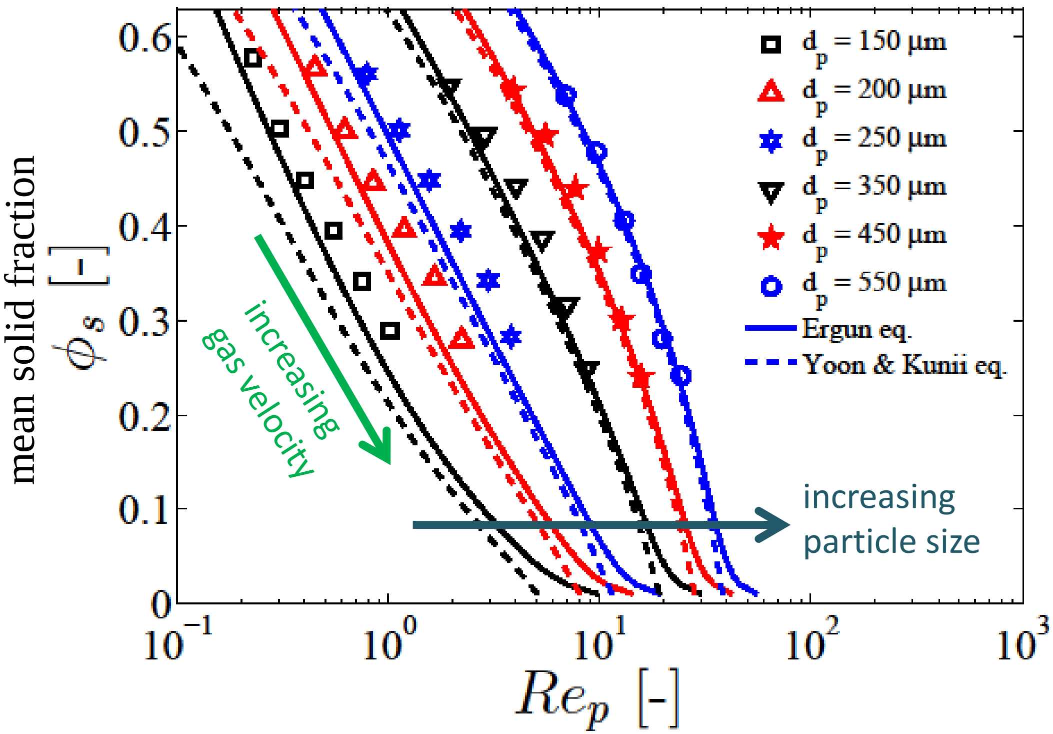
The **total** residence time is directly proportional to holdup. The residence time **between plates** is independent of total holdup.

Effect of Steam Velocity and Particle Size

- Expressed in terms of dimensionless quantities:
  - **Particle Reynold's number** , $Re_p = \frac{\rho_g d_p |\vec{v}_g - \vec{v}_s|}{\mu_g}$
  - **Stoke's number**, $St = \frac{(\rho_s - \rho_g)\, d_p^2 g}{18\mu_g |\vec{v}_g - \vec{v}_s|}$

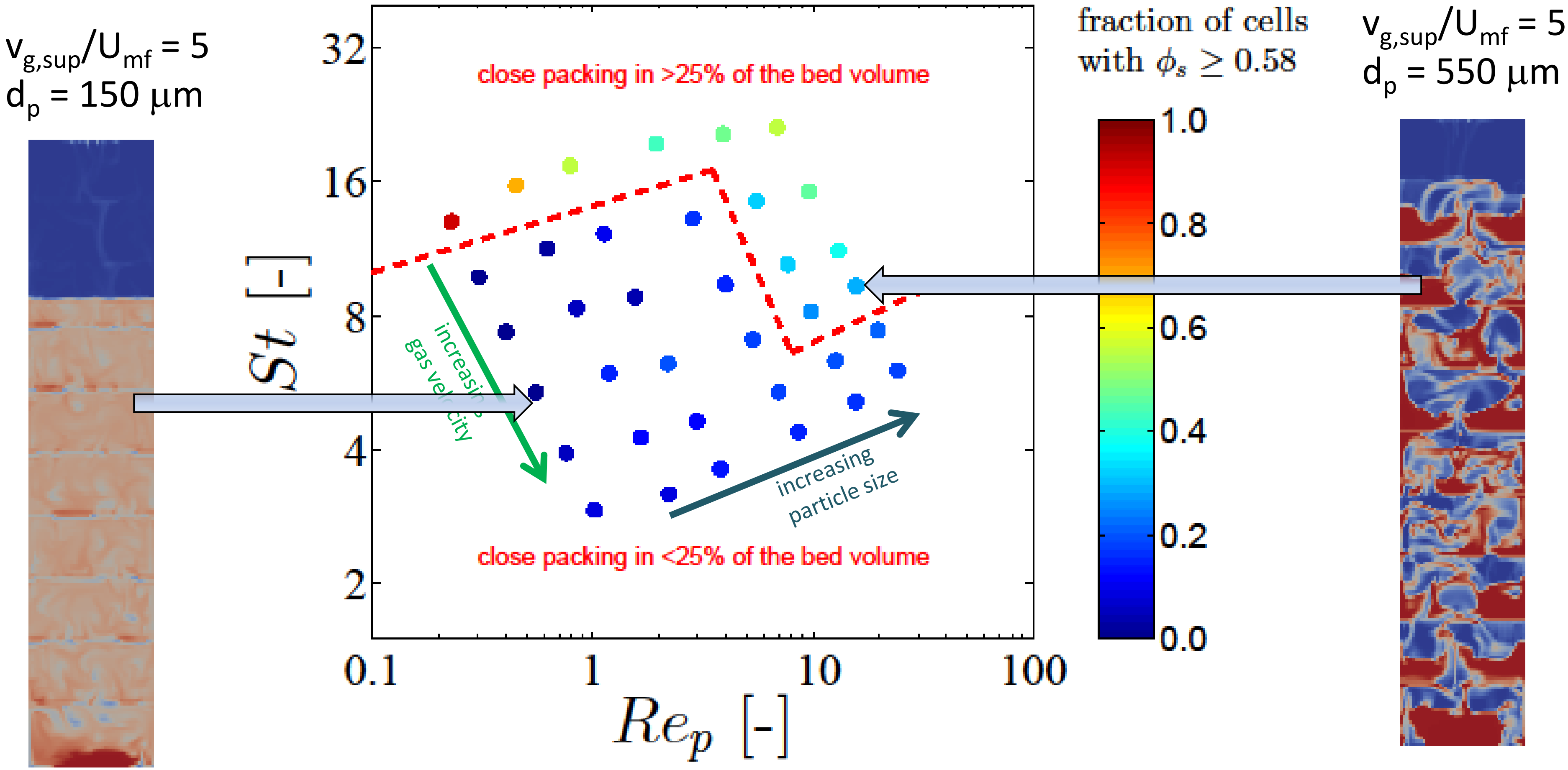
<u>Effect on mean solid fraction</u>

- Similar to fluidized beds.
- Compared with Ergun's eq.[1]
  - For stationary beds.
- Compared with Yoon & Kunii eq.[2]
  - For moving beds.



[1]S. Ergun. Chemical Engineering Progress, 48:89-94, 1952.
[2]S. Yoon and D. Kunii. Industrial & Engineering Chemistry Process Design and Development, 9(4):559-565, 1970.

Influence on Density Distribution of Sorbents



Residence Time Distribution and Axial Mixing

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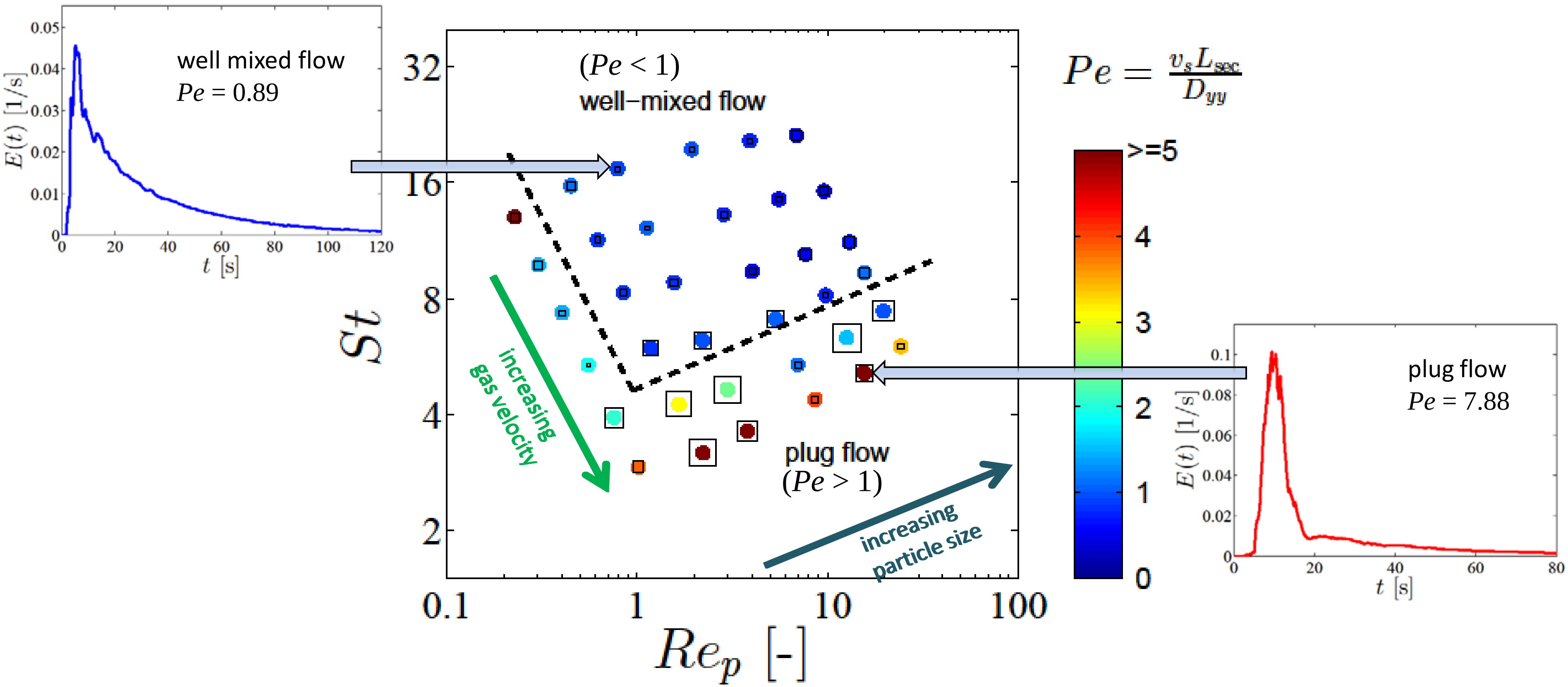
- Tracer injection used to determine the residence time distribution between two plates.
- RTD fit using the equation[1,2]: $E(t) = \frac{L}{\sqrt{4\pi D_{yy} t^3}} \exp\left[\frac{-(L - v_s t)^2}{4 D_{yy} t}\right]$



[1]O. Levenspiel. *Chemical Reaction Engineering*. John Wiley & Sons, 3rd ed., 1999.
[2]L.G. Gibilaro. Chemical Engineering Science, 33, 487-491, 1978.

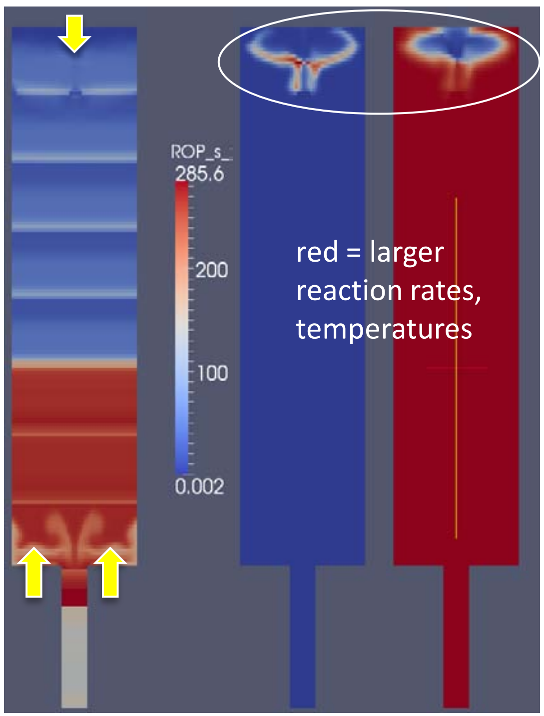
Sorbent Regeneration Chemical Kinetics

- Currently under development.
- Implementing the chemical kinetics in a smaller, simpler system.

Sorbent density

Reaction rate & temperature

sorbent inlet



gas inlet

Regenerator reacting flow simulations

- Multi-step chemical kinetics[1].

$$2R_2NH + CO_2\ (gas) \rightarrow R_2NCO_2^- + R_2NH_2^+$$
$$R_2NH + H_2O\ (phys) + CO_2\ (gas) \rightarrow HCO_3^- + R_2NH_2^+$$
$$H_2O\ (gas) \rightarrow H_2O\ (phys)$$

- Currently, the chemical kinetics are being implemented in a larger system with realistic parameters.

Most of the sorbent regeneration occurs close to the solids inlet, for the set of simulation parameters used.

[1]D. Mebane, D. Fauth, A. Lee. First generation model for silica-supported amine sorbent NETL 196C. CCSI internal report, Sep 2011.

CO_2-Capture in the Adsorber

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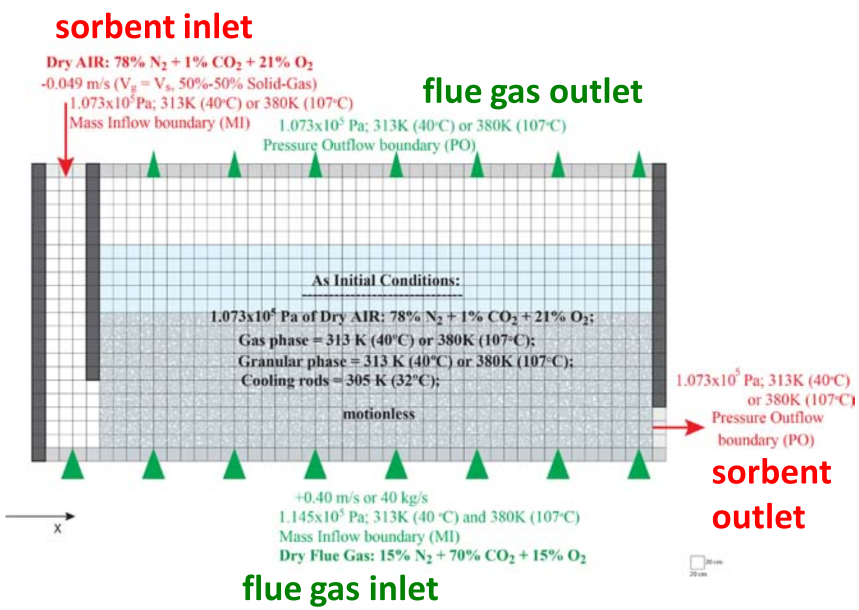
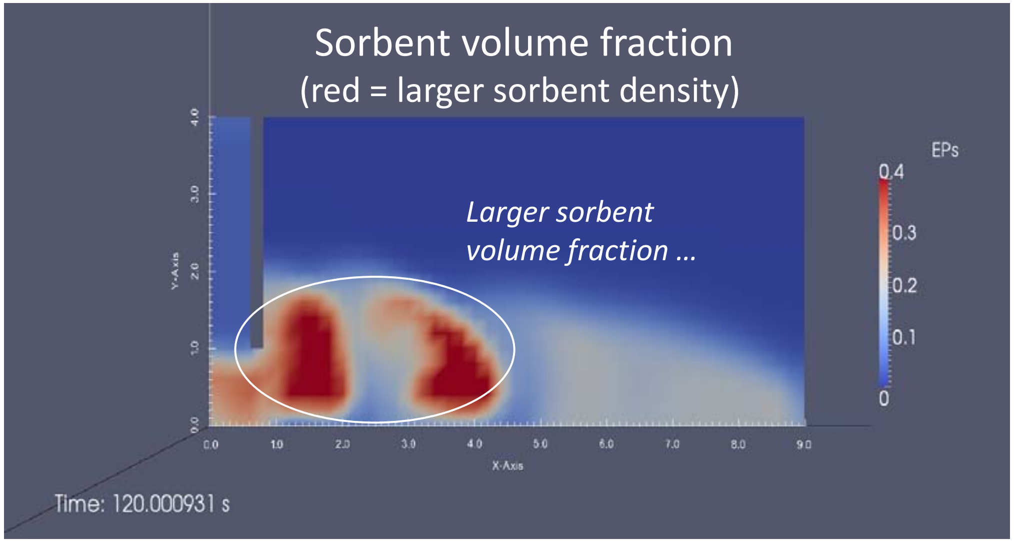
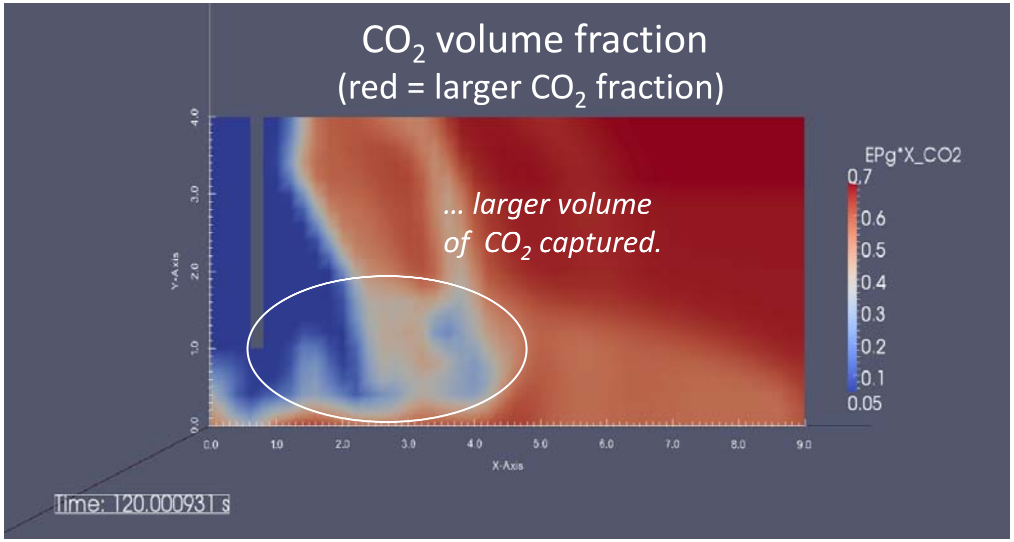
Adsorber Schematic







- Implemented a simpler, single step reaction.

$$2R_2NH + CO_2\ (\text{gas}) \square \quad R_2NCO_2^- + R_2NH_2^+$$

Summary and Future Work

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- Developed models for the regenerator and adsorber of a carbon-capture unit.
- Parametric studies of the regenerator:
  - Fill level affects the **total** residence time, but has negligible effect on solids distribution and RTD between plates.
  - Gas velocity and particle size have a significant effect.
  - Close packing, bubbling, and gas-solid segregation observed for,
    - larger particle sizes,
    - smaller gas velocities.
  - Both plug flow and well-mixed flow modes observed for varying operating conditions.
- Chemical kinetics implemented for the regenerator and the adsorber.
  - Currently under investigation in full-scale systems.

Future Work

- Incorporate chemical kinetics in full-scale system.
- Develop up-scaled ("filtered") relationships for,
  - Flow dynamics,
  - Internal structures (cooling rods in adsorber),
  - Reactions and heat transfer.
- Model sorbent attrition.

Acknowledgments

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