Full-loop Particle-Fluid Simulation of Carbon Capture Unit with Thermal and Chemistry

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Introduction

- This study presents results from a Barracuda numerical simulation of a full-loop CO_2 capture system.

- Outline:

  – Overview of the modeled NETL C2U experiment, presenting a full-loop, cold-flow simulation to study particle-gas flow

  – Discussion of modeling CO_2 capture chemistry with the R&D version of Barracuda

- This work is part of a joint-effort project between NETL and CPFD.

  – CPFD Team Members: Sam Clark, James Parker, Dale Snider

  – NETL Team Members: E. David Huckaby, Esmail Monazam, Kringan Saha, Lawrence Shadle, James Spenik

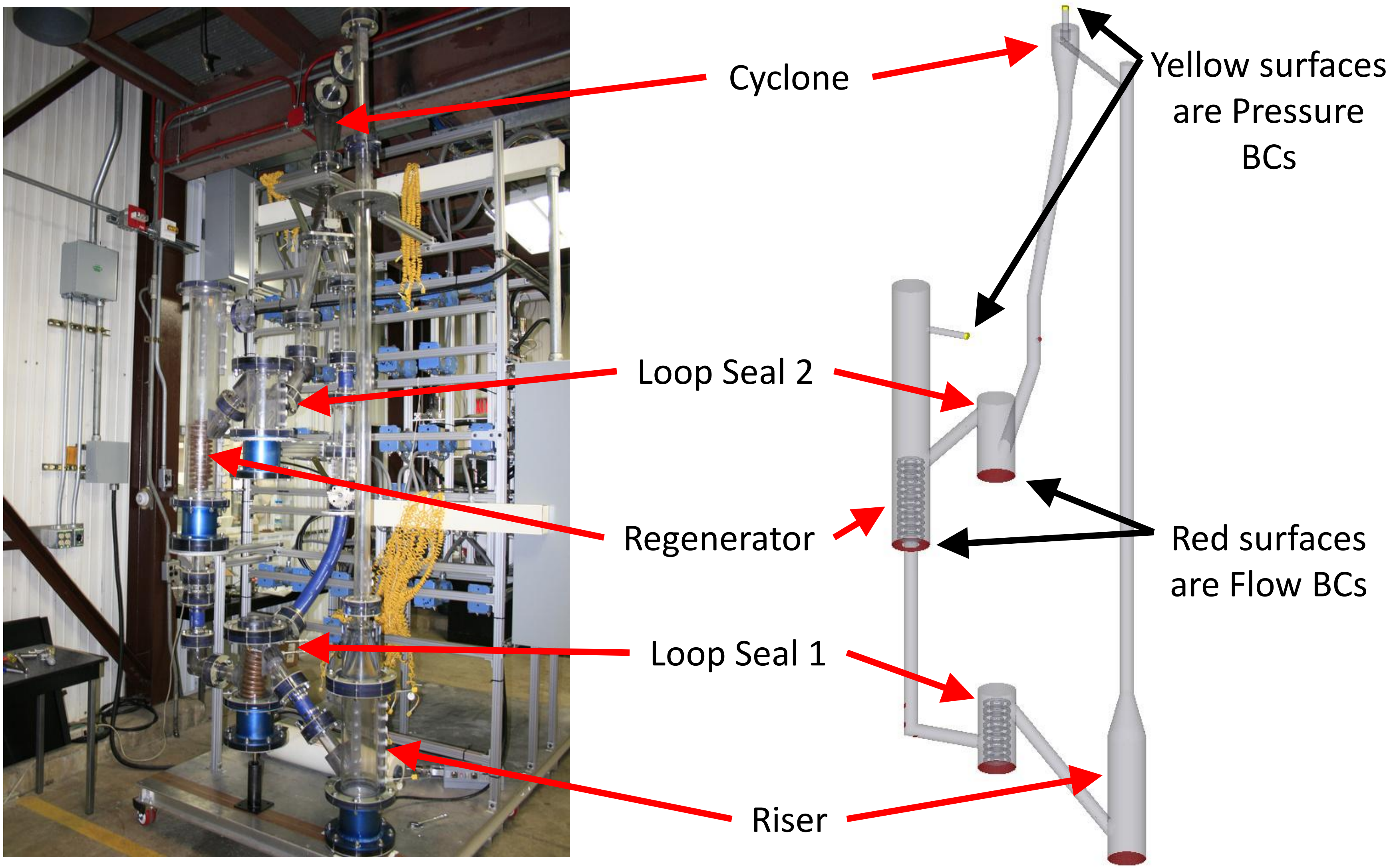
Motivation for Numerical Simulations of CO_2 Capture Systems

- Faster and less expensive deployment of new hardware for industrial systems
- Reliable math-based software is a key player in reducing costs for both design and operation
- CO_2 capture is a new technology which has limited commercial experience -- math-based tools can help this new technology to be effectively implemented commercially
- Numerical simulations can provide insights into fundamental system behaviors that are impossible to measure experimentally

Specific Goals of Present Barracuda Simulations

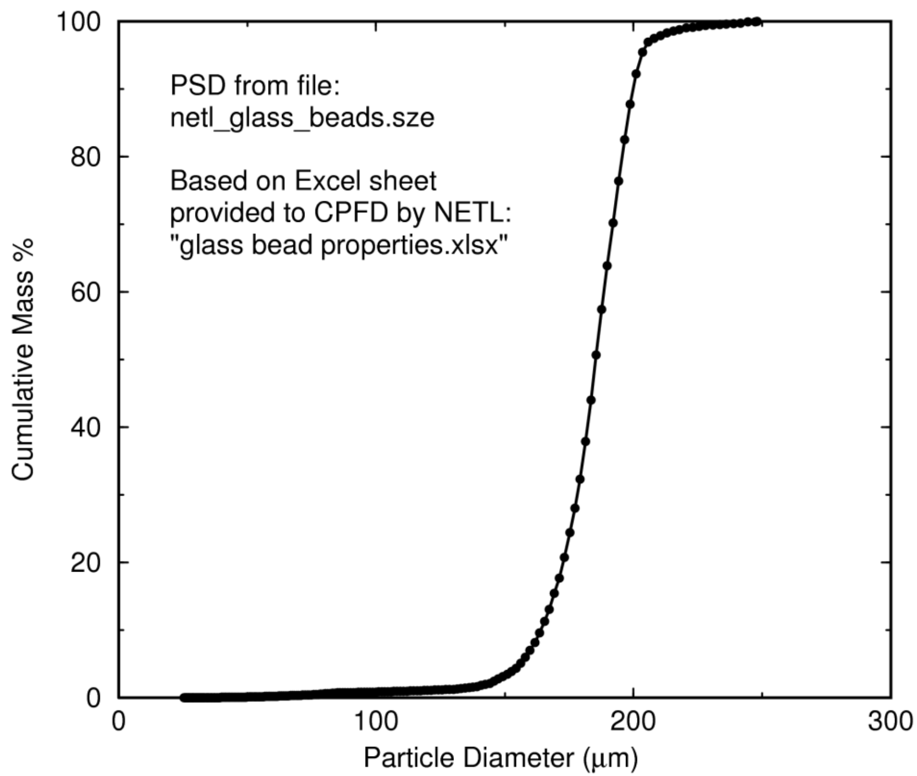
- Augment NETL Carbon Capture Unit (C2U) experimental work by providing insights unique to numerical simulations
  - Determine solids mass circulation rates throughout system
- Assist NETL in the analysis and operation of the C2U experiment
  - Identify regions where fluidization behavior could be improved
- Validate Barracuda for predicting the performance of this particular CO_2 capture system, giving confidence in its usefulness as a math-based tool for designing future commercial CO_2 capture systems.
  - Compare with data from the C2U experiment
- Assess the strengths and weaknesses of the numerical solution methods employed, providing guidance for future physics model development work

Barracuda Model of C2U Experiment



C2U Cold-flow Simulation Conditions

- Isothermal at T = 80 °C = 353 K
- Compressible gas flow with air as the only fluid species
- Pressure boundary conditions (BCs) set to 1 atm = 100 kPa
- Flow BCs set as specified by NETL experimentalists
- Particle properties:
  - Glass beads
  - Density = 2250 kg/m^3
  - d_{50} particle size ≈185 microns
  - Full particle size distribution (shown in plot) used in Barracuda simulation



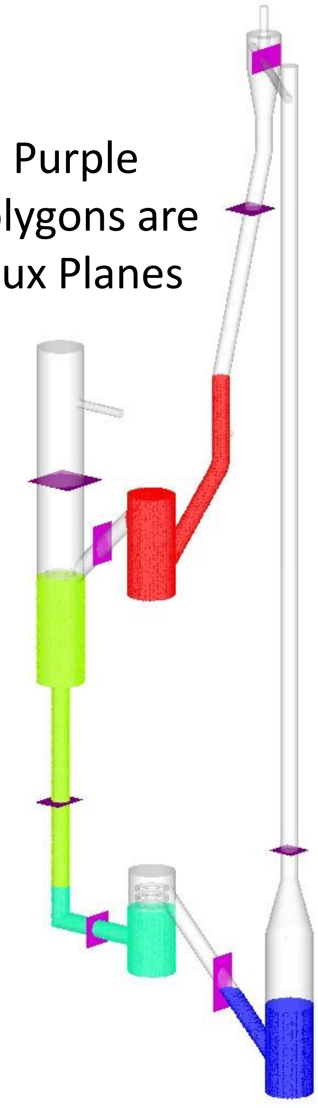
Features of Barracuda Model

- Particles initialized in system as shown at right
  - Different "particle species" were defined to give visual indications of particle mixing.
  - All particle species have the same physical properties.
  - Particles were initialized at rest in the different vessels of the C2U loop.

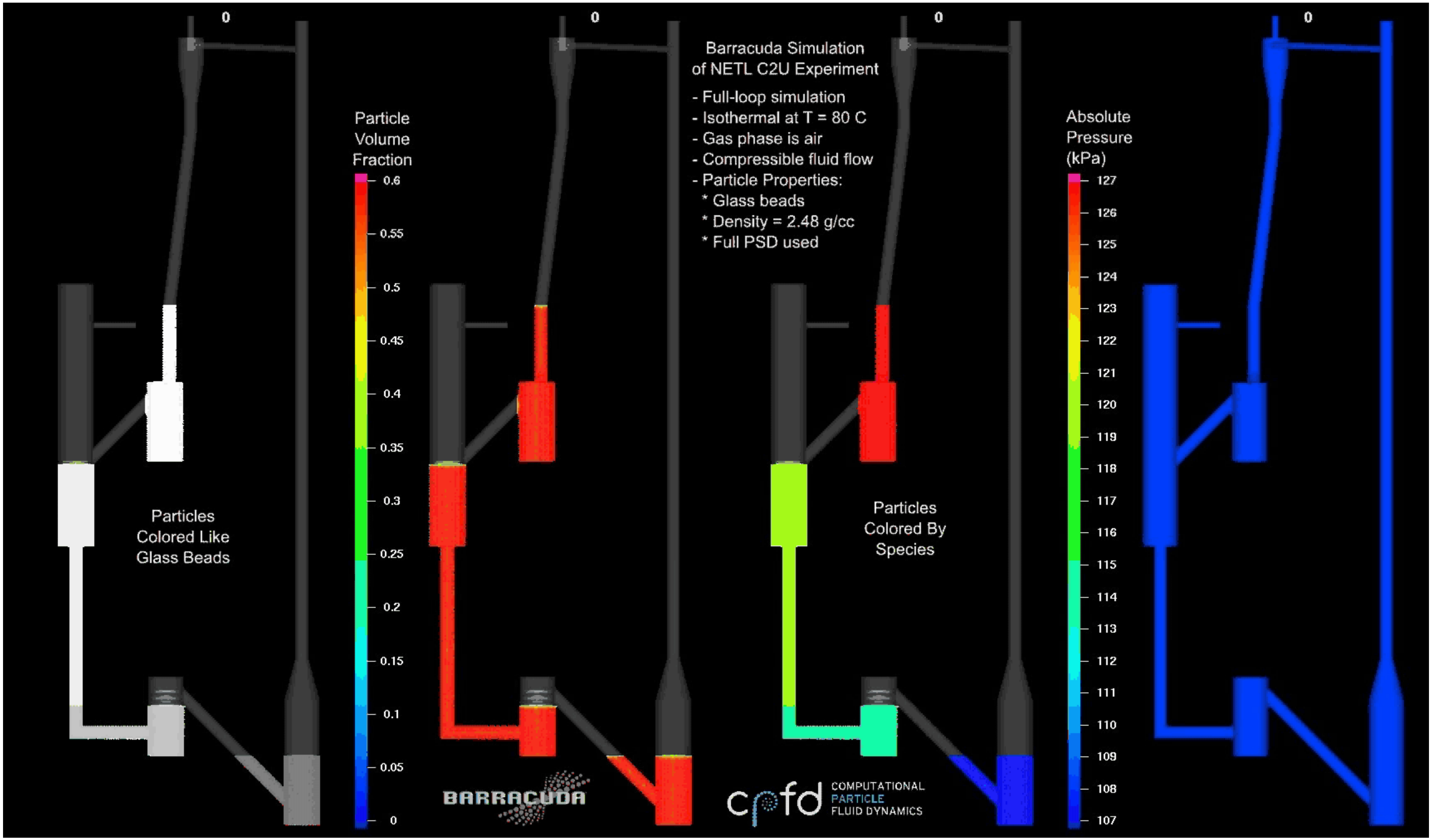
- Full 3-D computational model of the full-loop C2U system
  - Barracuda predicts full range of lean to dense particle concentrations.
  - No prior knowledge of where the lean or dense regions will be located.

- All Barracuda models are transient
  - A start-up period is simulated while the particles and fluid go from their initial conditions to some "quasi-steady state”
  - A strict "steady state" is never achieved, because the motion of the particles is always dynamic.
  - Engineering decisions are best made based on time-average data obtained once a "quasi-steady state" has been reached.

Purple polygons are Flux Planes

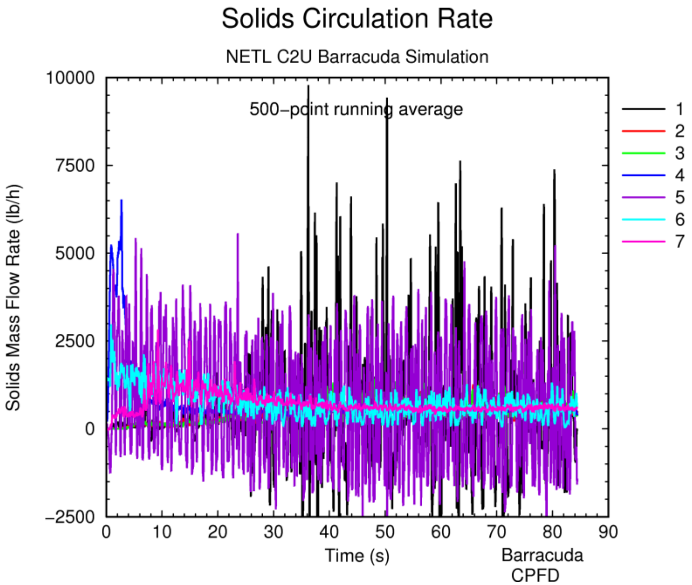


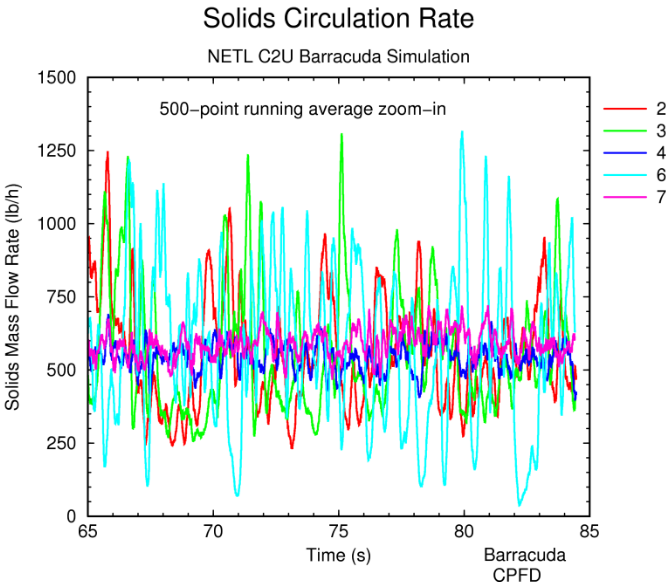
Animation of Full-Loop Simulation

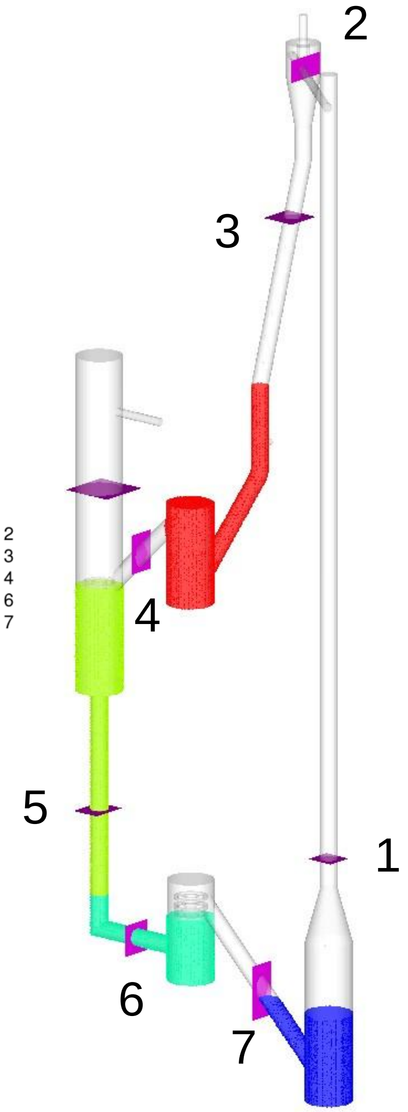


Solids Circulation Rate

- Barracuda can be used to predict the solids circulation rate at various locations around the loop of the C2U.
- The plots shown here are based on numerical results reported by Flux Planes defined in the simulation.



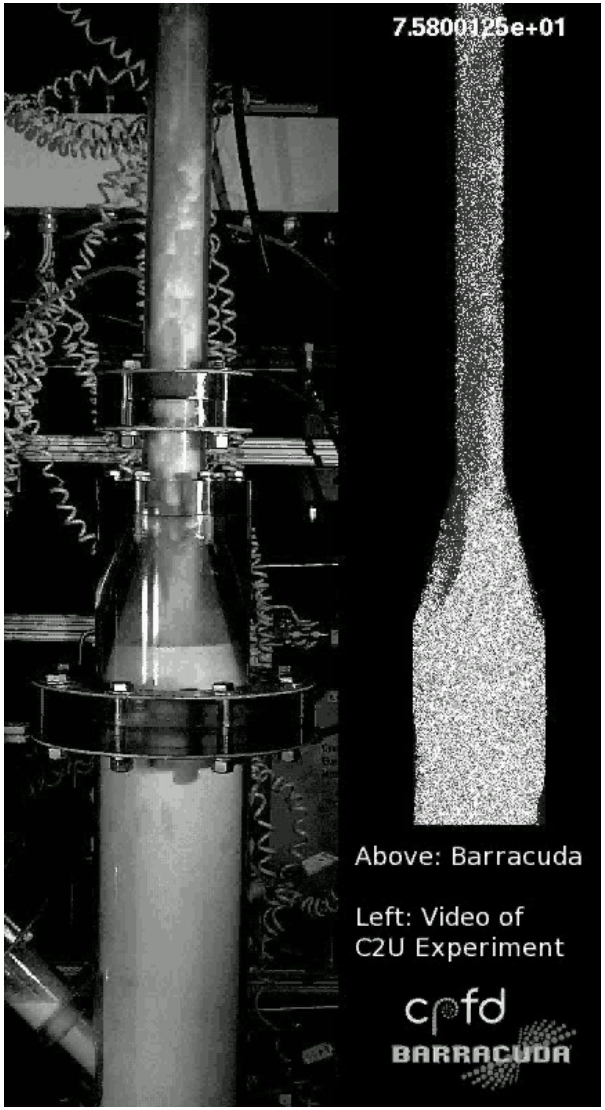




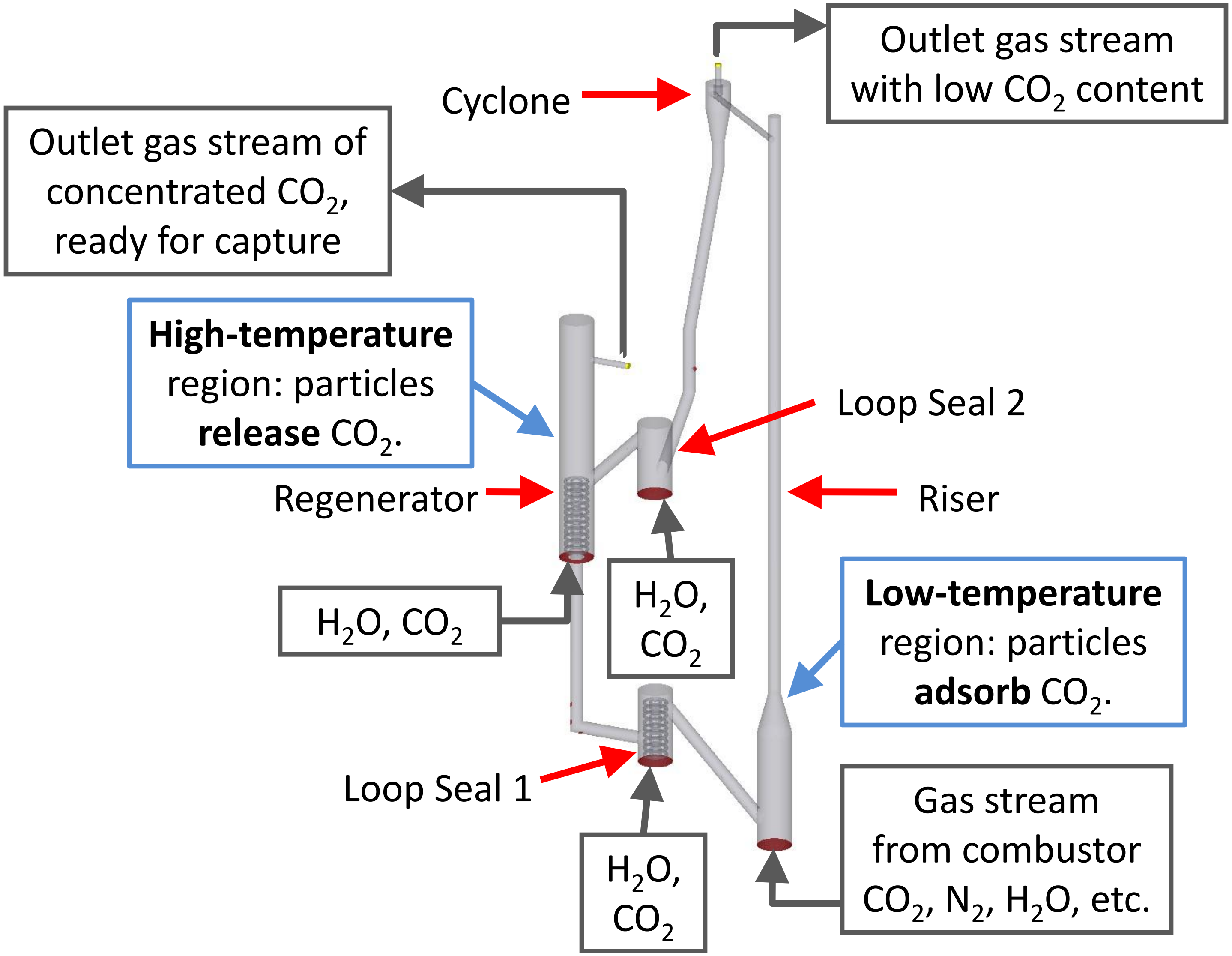
Validation Example 1: Riser "Slugging"

- The Barracuda model shows that particles cannot leave the lower vessel of the riser in a continuously smooth manner. Rather, there is a "slugging" nature to the flow.

- This type of behavior was also observed by NETL experimentalists when operating the C2U experiment at the flow conditions used in the Barracuda simulation.



CO_2 Capture Strategy of C2U



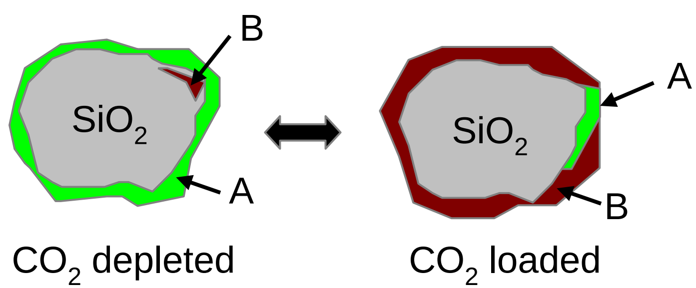
NETL CO_2 Capture Chemistry

- NETL scientists have investigated the kinetics of CO_2 adsorption with amine-based sorbents, specifically polyethyleneimene (PEI).
- Monazam, et al, fitted experimental data with a single chemical reaction, a rate equation, and an equilibrium equation, based on TGA experiments.
- Currently working with NETL in the process of formatting rate equations into a computationally fast format.
  - Monazam, Shadle, Fauth, Hoffman, Gray, and Pennline, "Kinetics Analysis of Carbon Dioxide Capture on Immobilized Amine on Meso-Porous Silica". Paper in review.

Modeling CO_2 Capture Chemistry with Barracuda Multi-Material Particles

- Chemical reaction: $\mathrm{A}(s) + \mathrm{CO}_2(g) \leftrightarrow \mathrm{B}(s)$

- Multi-material particles, available in the R&D version of Barracuda, are used to represent A(s), "CO_2 depleted", and B(s), "CO_2 loaded".

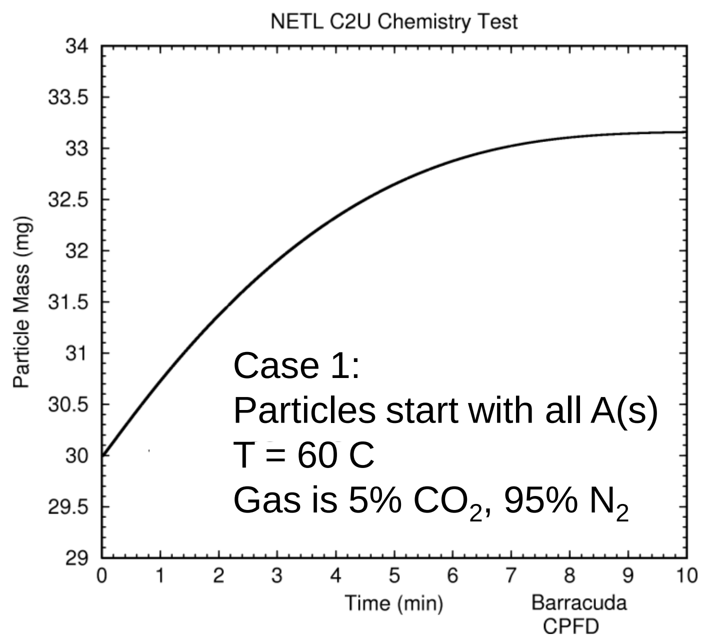


- Properties of multi-material particles:
  - Can contain any number of solid materials
  - Composition, size, and density change due to chemistry
  - Chemistry can involve any or all of the solid species – some species may be inert, others catalytic, and others reacting.

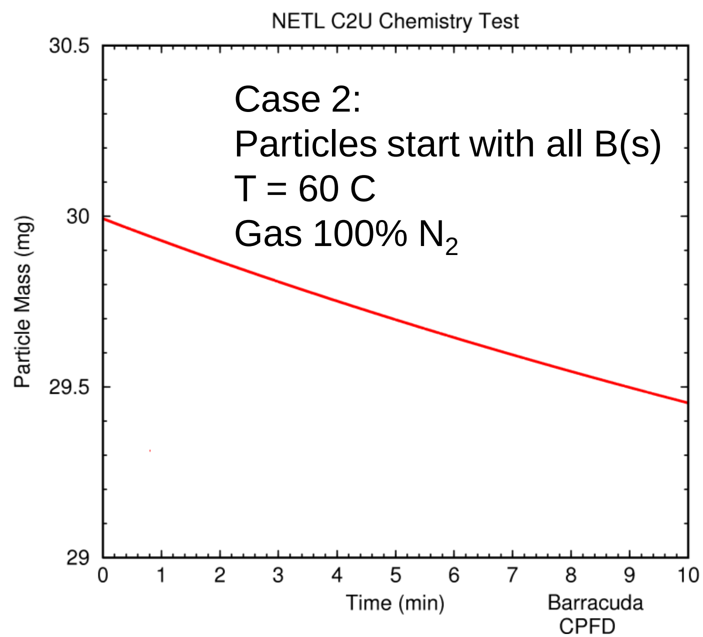
Demo CO_2 Capture Chemistry Simulation

- Chemistry based on Monazam, et al.
- Stoichiometric Reaction: $A(s)+CO_2(g)\leftrightarrow B(s)$
- Forward rate: $r_F = 120\cdot T^{0.55}\cdot p^{-1}\cdot e^{662/T}\cdot m_{s,A}^{0.5}\cdot [CO_2]^{1.057}$
- Reverse rate: $r_R = 6.5e-04\cdot T^{1.45}\cdot p^{-1}\cdot e^{662/T}\cdot m_{s,B}^{1.5}$

Transient Particle Mass – CO_2 Adsorption



Transient Particle Mass – CO_2 Release



Conclusion

- A full-scale 3-D, full-loop, cold-flow, simulation of the NETL C2U experimental unit was presented.
  - The calculation provided validation by exhibiting behavior encountered by experimentalists (i.e. riser "slugging").
  - Solids mass circulation rate was measured in the simulation.
  - Further quantitative validation will be based on pressure tap data from the experiment.

- Demonstrated chemistry
  - Multi-material particles, available in the R&D version of Barracuda, are being used to represent "CO_2-depleted" and "CO_2-loaded" PEI.
  - CO_2 adsorption chemistry is the current focus of modeling efforts for the CPFD/NETL C2U project.
  - Final goal: full-loop simulation of the C2U with chemical reactions and thermal calculations included.