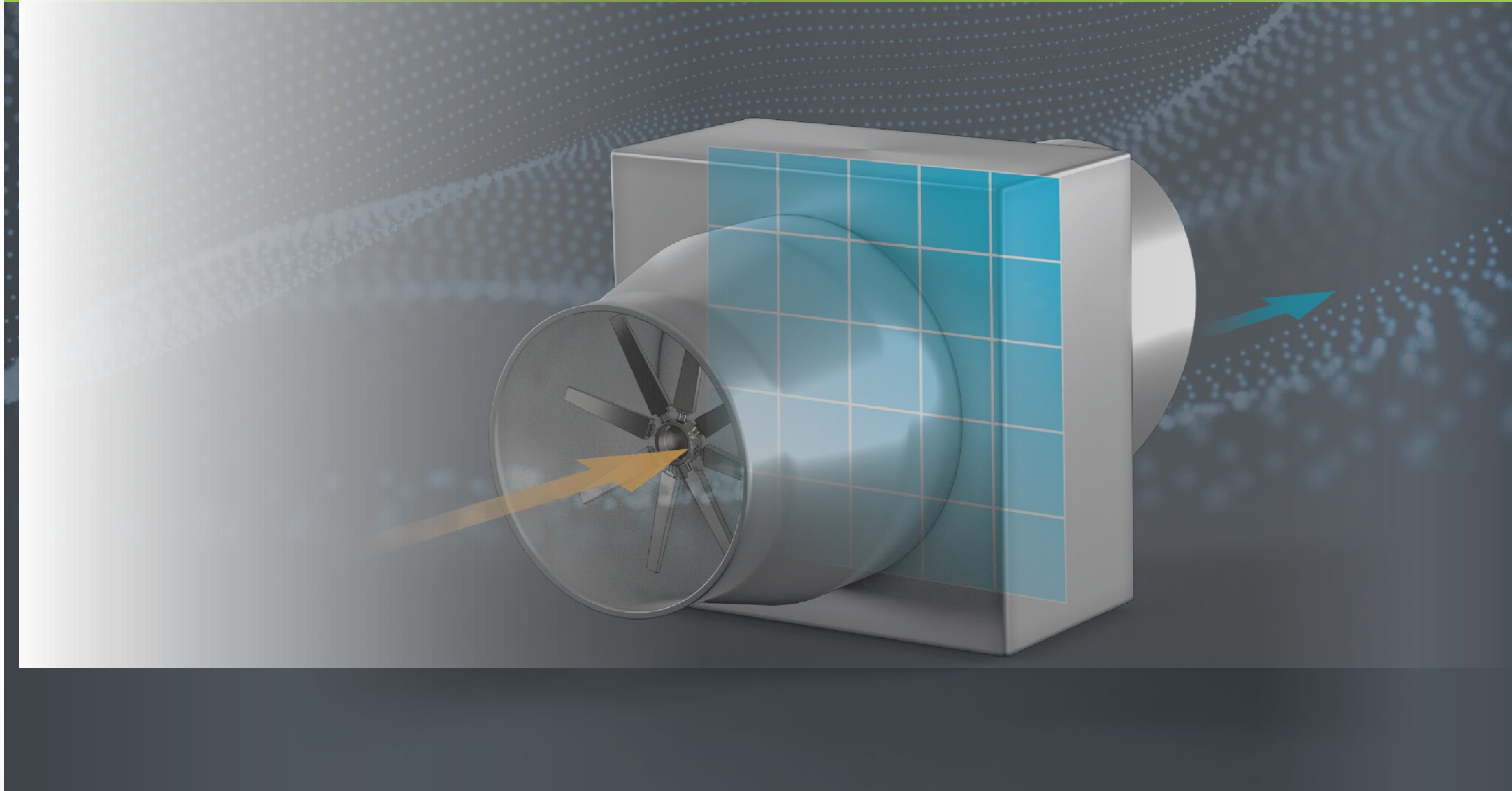
Forming the Future of Direct Air Capture

CFD for Direct Air Capture

David Huckaby



CFD Resources

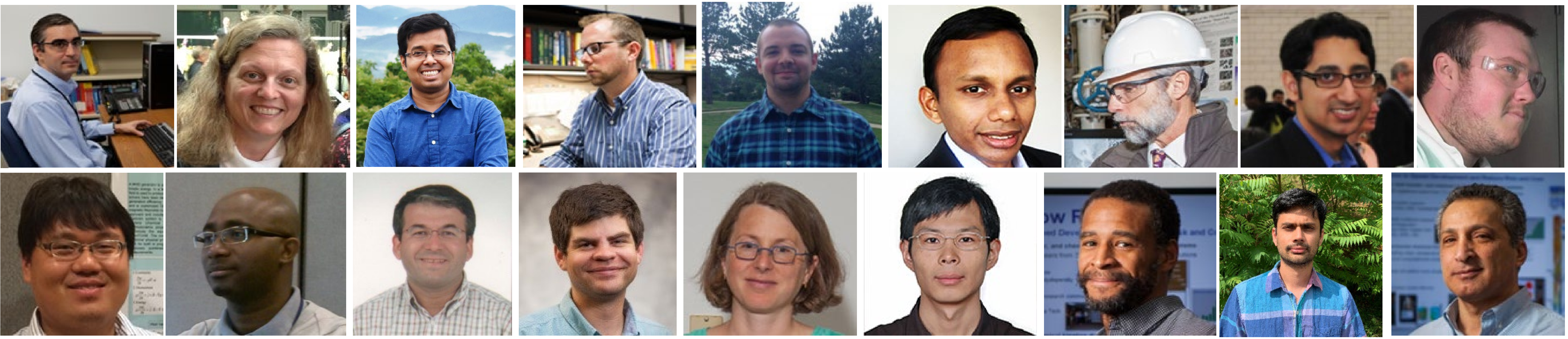
- People
- Computational Tools – Software and Hardware
- Experimental Facilities

NETL CFD and Multiphase Flow Science Team

NATIONAL ENERGY TECHNOLOGY LABORATORY

18 Researchers

applying modeling, simulation and laboratory testing



Project Portfolio

NATIONAL ENERGY TECHNOLOGY LABORATORY

across a wide range of DOE projects …

- Biomass Pyrolysis
- Biomass Gasification
- Microwave Catalyst Bed Heating
- Point Source Capture
- MHD Power Gen.
- H2 Storage
- MFIX
- Direct Air Capture
- Acoustic Sensing for Drilling
- O2 Separation
- MFIX-EXA
- DAC Center

Modeling Toolset

Tools are adapted to resources, capabilities and project objectives …

MFiX
Multiphase Flow with Interphase eXchanges

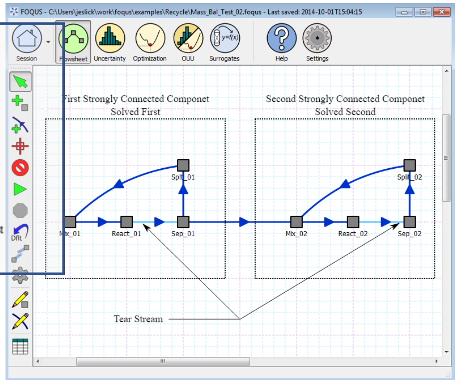
Nodeworks

Ansys

COMSOL

FOQUS

CCSI[2]
Carbon Capture Simulation for Industry Impact



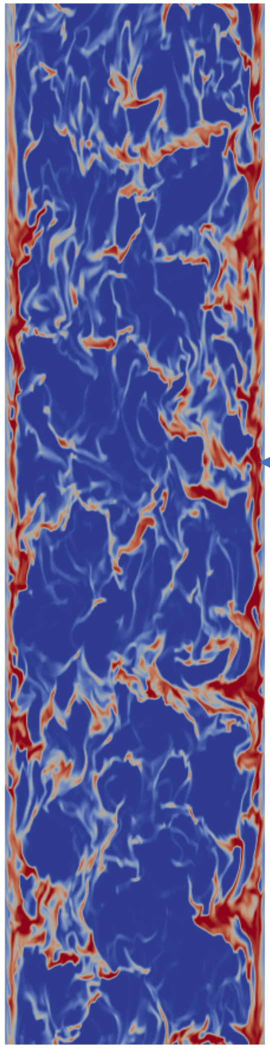
OpenFOAM®

DAKOTA
Explore and predict with confidence.

PSUADE

MFiX Suite of Multiphase CFD Software

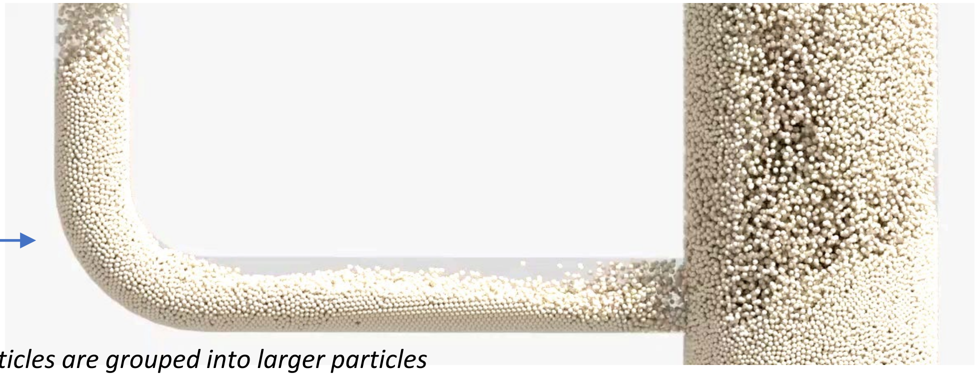
Managing the tradeoff between accuracy and time to solution



DNS

Direct Numerical Simulation: fine scale, accurate simulations for limited size domain

MFiX DEM — *Discrete Element Method: Track individual particles and resolve collisions*

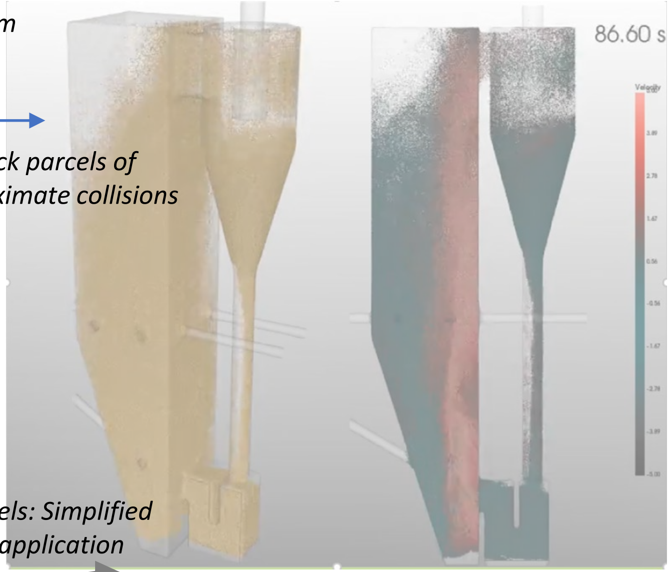


MFiX CGP — *Coarse Grain DEM: particles are grouped into larger particles (CGP). CGP are individually tracked, resolving collisions*

MFiX TFM — *Two-Fluid Model: Gas and solids form an interpenetrating continuum*

MFiX PIC — *Particle-in-Cell : Track parcels of particles and approximate collisions*

classic



MFiX Exa — *Exascale: New code for new generation of computers*

ROM

Reduced Order Models: Simplified models with limited application

Time to Solution

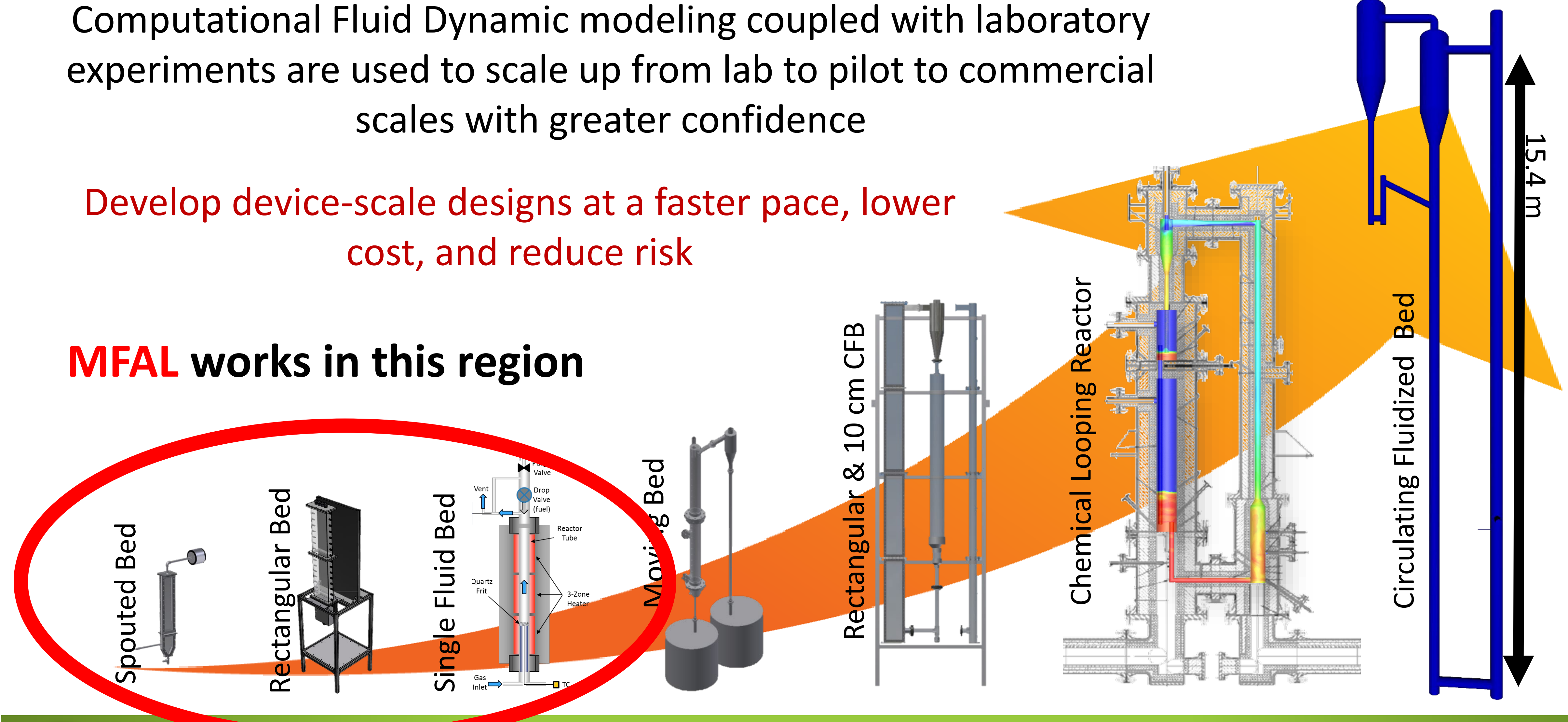
Model Uncertainty

Multiphase Flow Analysis Laboratory (MFAL)

Computational Fluid Dynamic modeling coupled with laboratory experiments are used to scale up from lab to pilot to commercial scales with greater confidence

Develop device-scale designs at a faster pace, lower cost, and reduce risk

MFAL works in this region



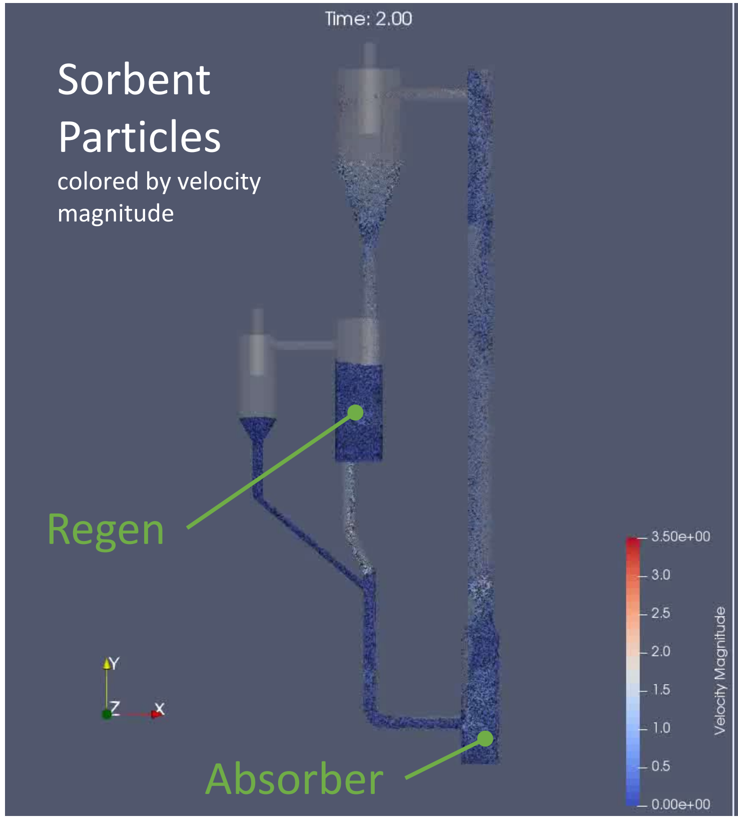
DAC Related Projects

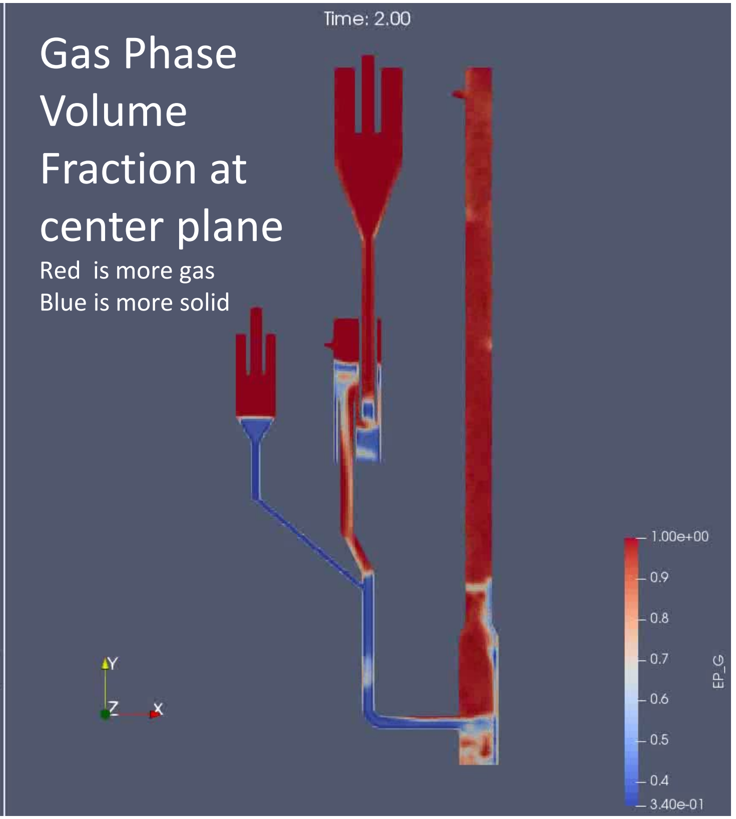
Biomass Pyrolysis	Biomass Gasification	Microwave Catalyst Bed Heating	Point Source Capture (Previous Projects)
MHD Power Gen.	H2 Storage	MFIX Development & Support	Direct Air Capture (New)
Acoustic Sensing for Drilling	O2 Separation	MFIX-EXA Development	DAC Center (New)

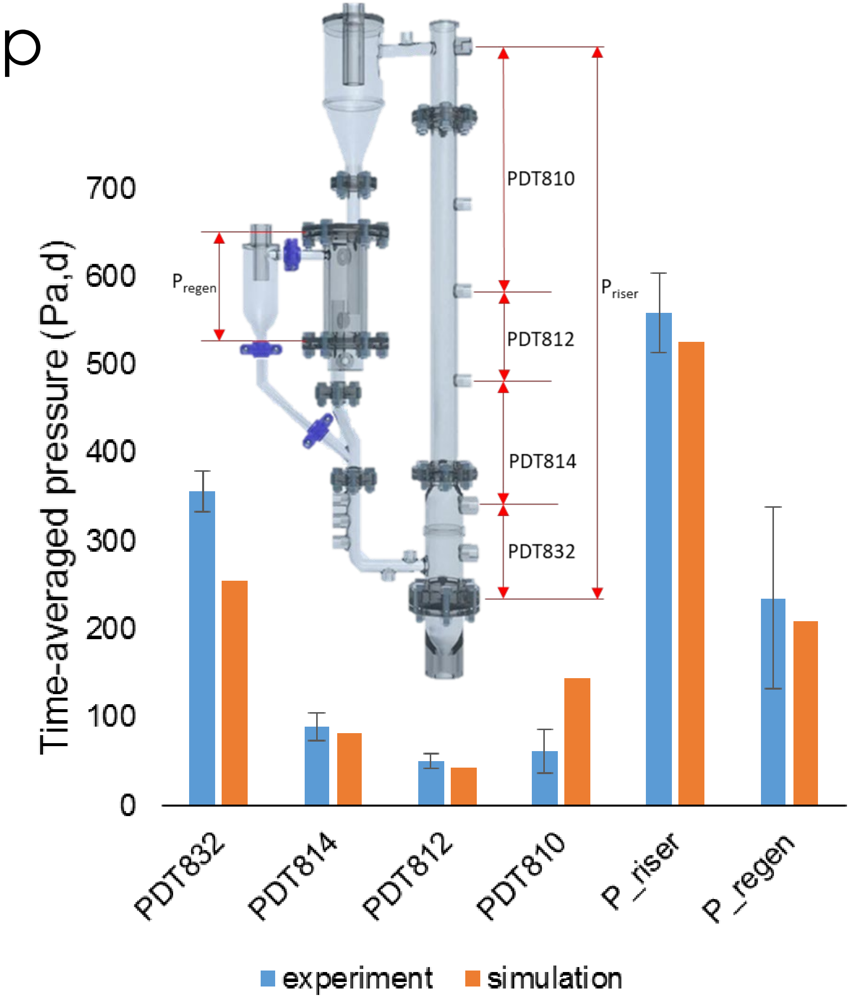
Circulating Dual Fluid Bed

Cold Flow Hydrodynamics

Excellent comparison between modeled and measured solids holdup(pressure drop values) around the flow loop

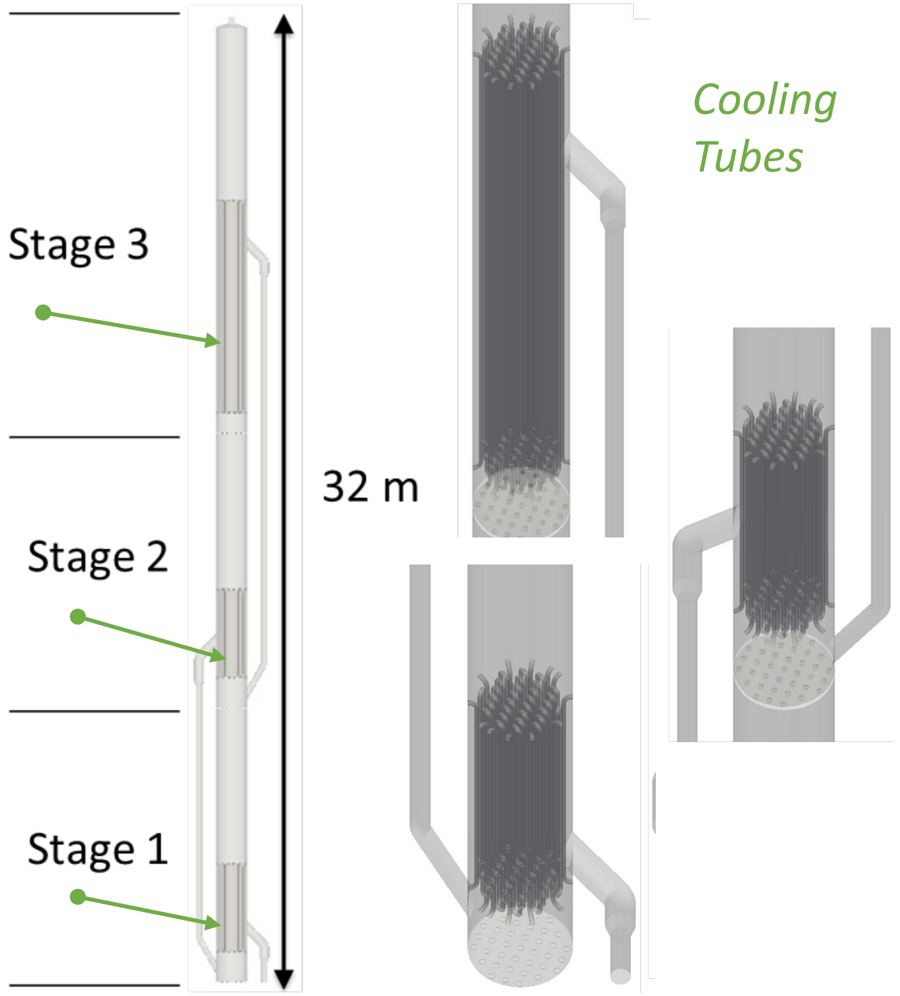


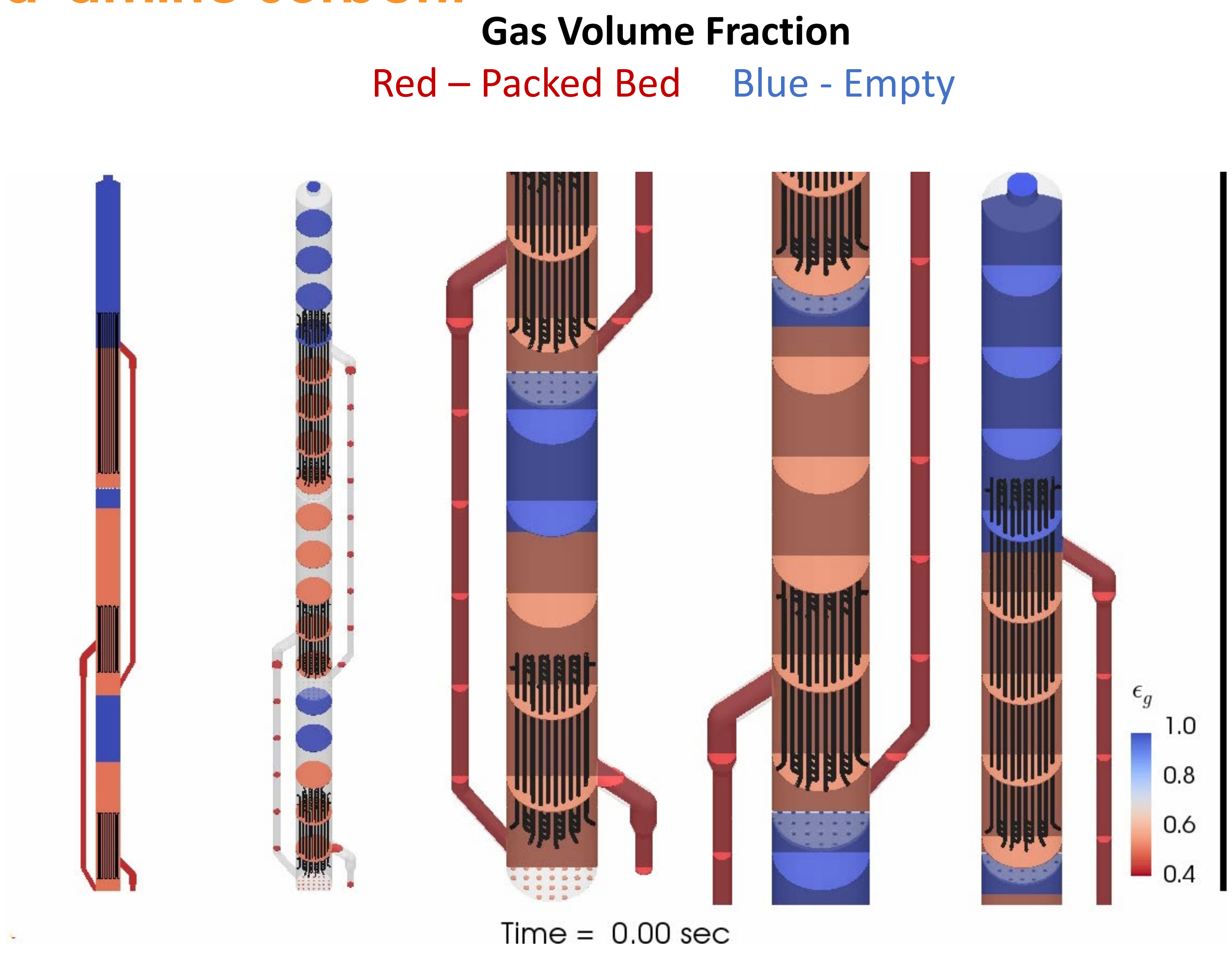




Three stage fluidized bed

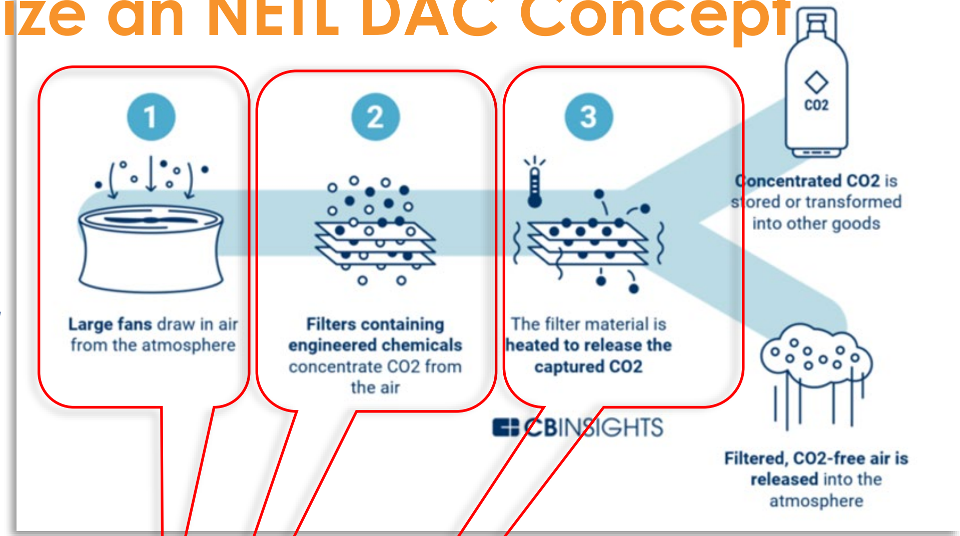
Flue Gas from 1 MW NGCC w/ fixed-amine sorbent

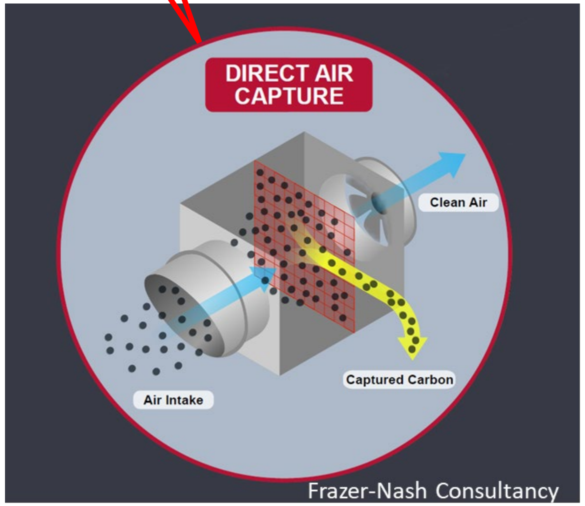




DAC – CFD for Design and Optimization

Use CFD Tools to Design and Optimize an NETL DAC Concept





Primary Tasks

- CFD Analyses of Inlet Fans and Ducting
  - Pressure Drop, Flow Distribution, Energy requirements
- Reacting CFD Analyses of Sorbent Beds
  - Pressure Drop, Flow Distribution, CO_2 Capture, Thermal behavior,
- Sorbent Bed Regeneration
  - Thermal swing, pressure swing, transient bed behavior during regeneration

Climeworks.com
theengineer.co.uk/direct-air-capture-net-zero/
cbinsights.com/research/direct-air-capture-corporate-carbon-reduction/

DAC – CFD for Design and Optimization

Big Picture

Start with NETL Sorbent Defined by the FWP Team

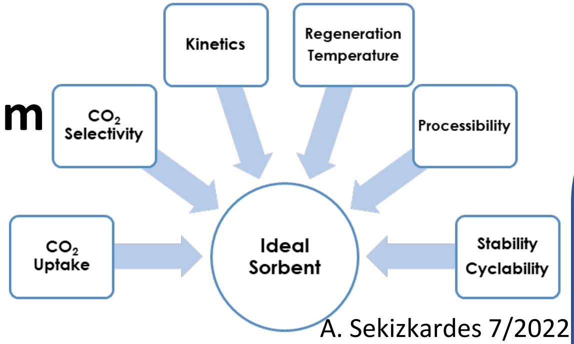
- Microporous Polymer – particle and/or fiber

Assume a Fixed Sorbent Bed to Start

- "Active" flow – flow is forced through the sorbent

Moving Sorbent Beds *could* be studied with CFD

- Moving, Fluidized, Circulating beds
- Not in the present scope



A. Sekizkardes 7/2022

Lab and Bench Scale CFD Models and Experiments studying NETL Sorbents

Validate the CFD modeling approach and model parameters

Use CFD Models to Scale Up DAC based on NETL Sorbents

Small Pilot Scale
Include ducting, fan, regeneration

Optimize performance

Use CFD Models to Scale Up DAC based on NETL Sorbents

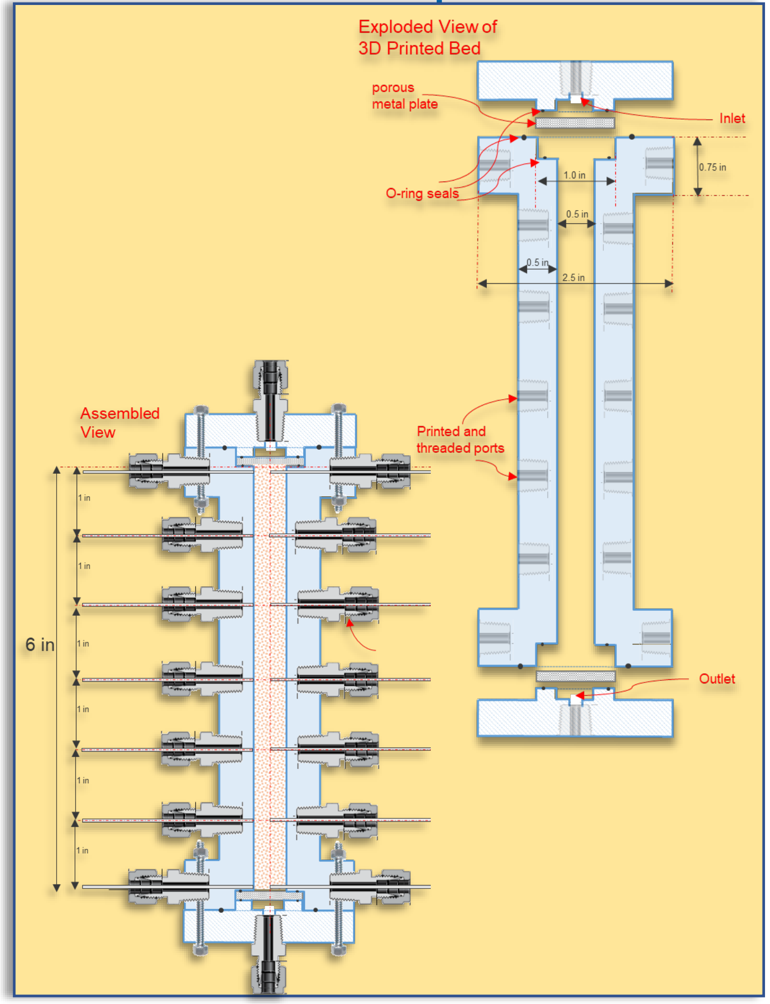
Small "Commercial" Scale
Include ducting, fan, regeneration

Optimize performance

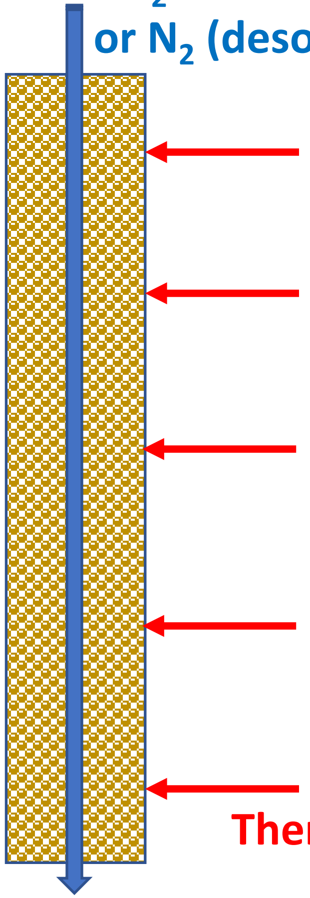
Lab Scale Fixed Bed Tests

Physical Models Provide CFD Model Validation Data

Concept



CO_2 and Air (adsorption) or N_2 (desorption)



Thermocouples

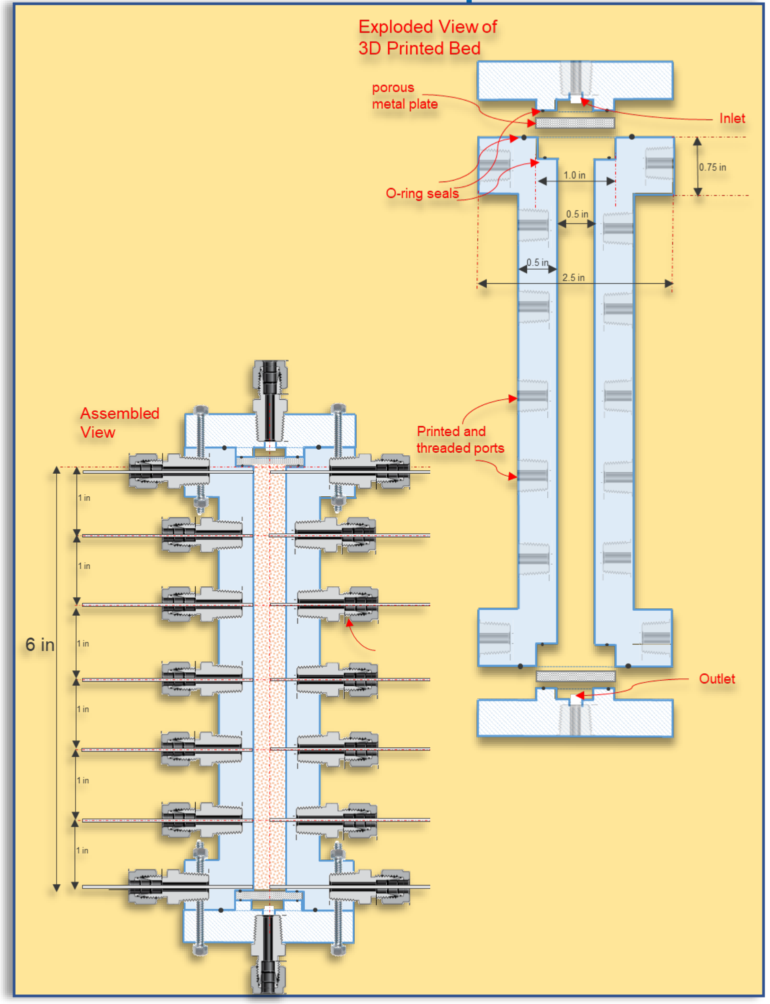
Measure CO_2 Concentration

First Step - Lab Scale Test – Fixed Bed

- Fluid flow, sorbent kinetics, gas and solid heat transfer models will be implemented
- Use data to validate the models
- NETL will use the validated lab-scale fixed bed model to support scale up to bench-scale DAC
- Goal is to measure temperature and concentration transients with quantified error

Lab Scale Fixed Bed Tests

Concept → Design → 3D Printed

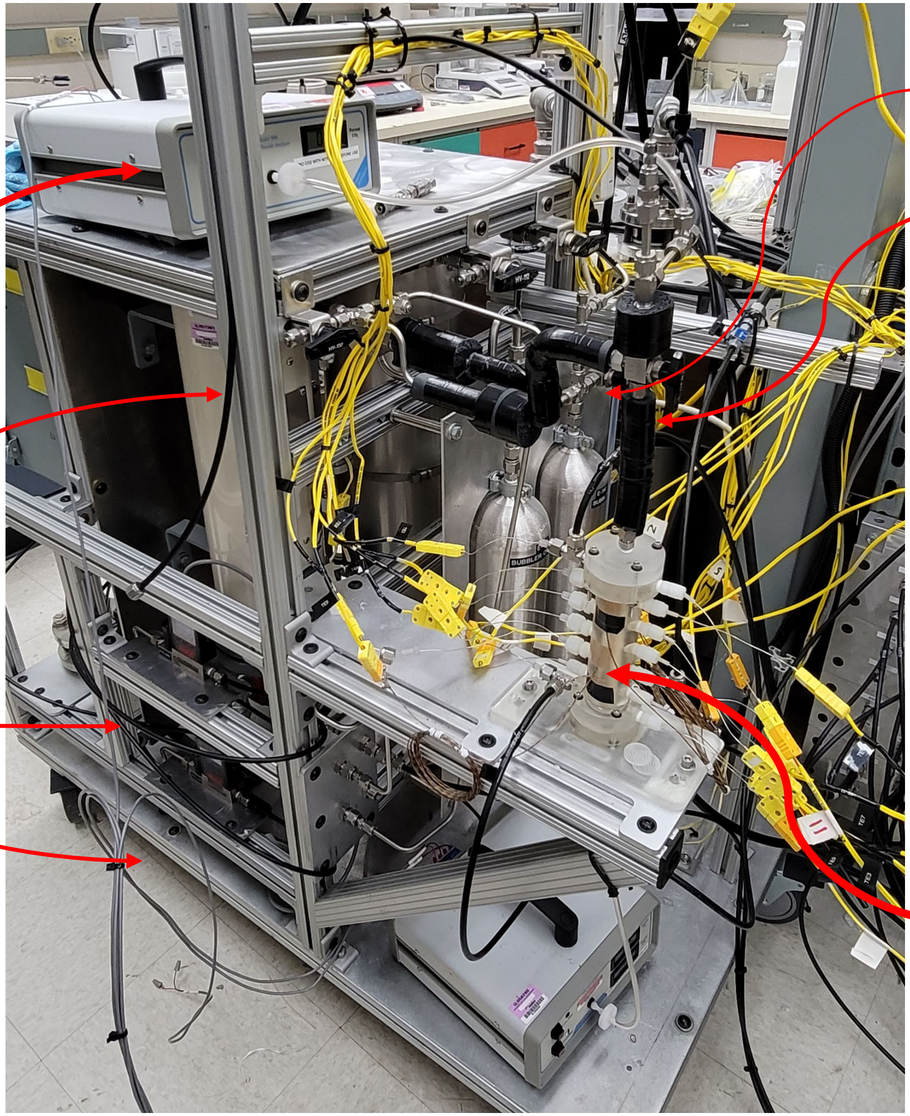


Lab Scale Fixed Bed Tests

NATIONAL ENERGY TECHNOLOGY LABORATORY

Small Scale Test Rig

3-D print bed for rapid prototyping



CO$_2$ Analyzers

2 Flow Heaters

Flow Control
Air, N$_2$ and CO$_2$

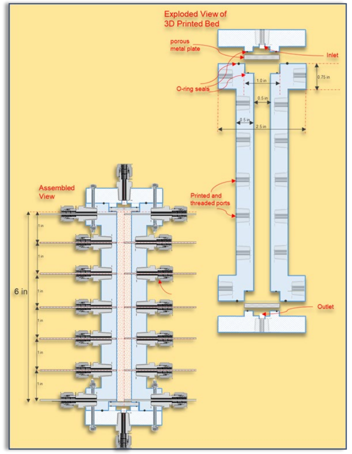
- LabVIEW Software
- Pressure transducers available

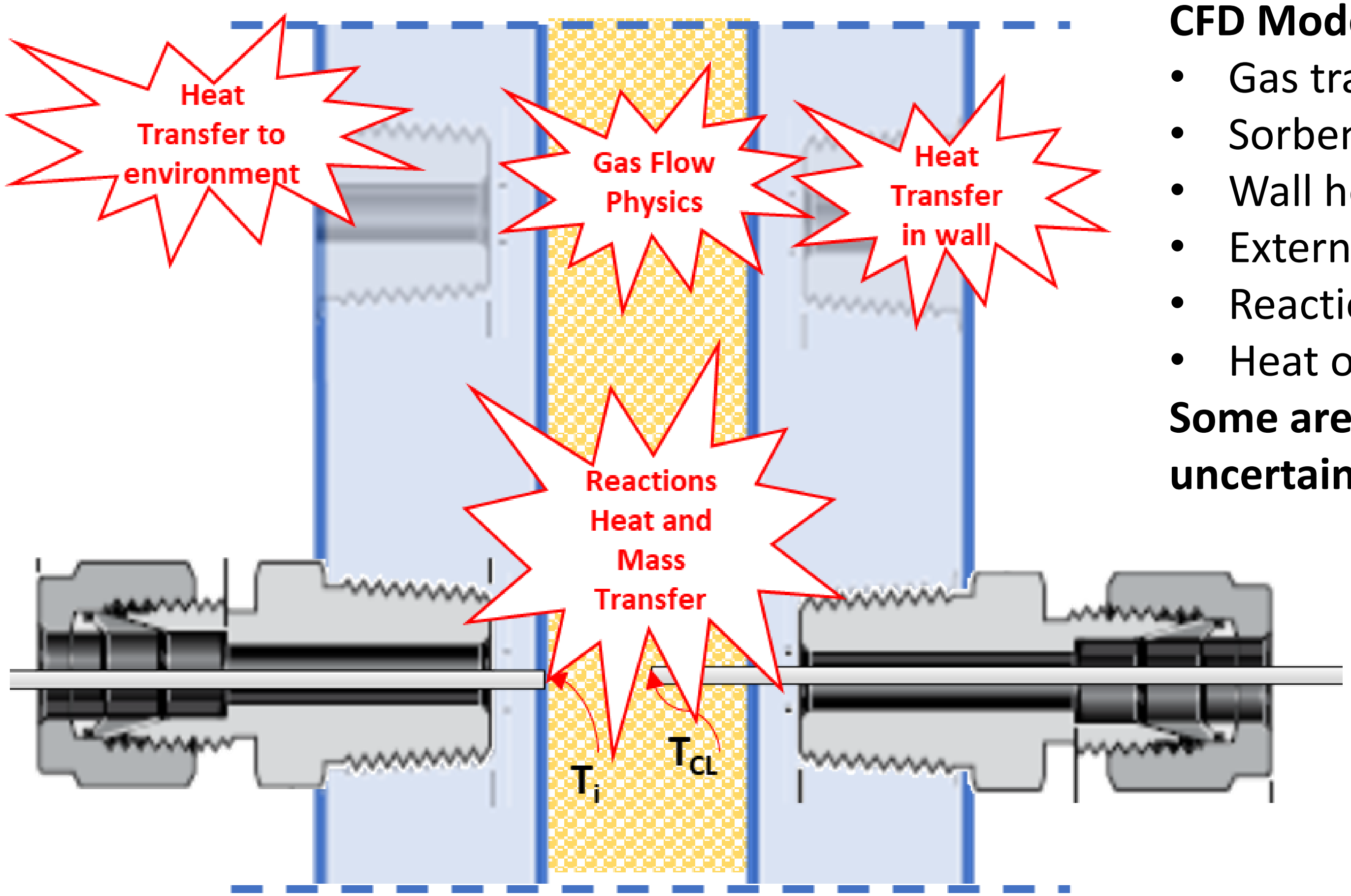
Bubblers for humidity – we can measure, not really control

Plumbing for fast switching of flow conditions

Lab Scale Fixed Bed Tests

Of course, in research nothing is ever simple…..





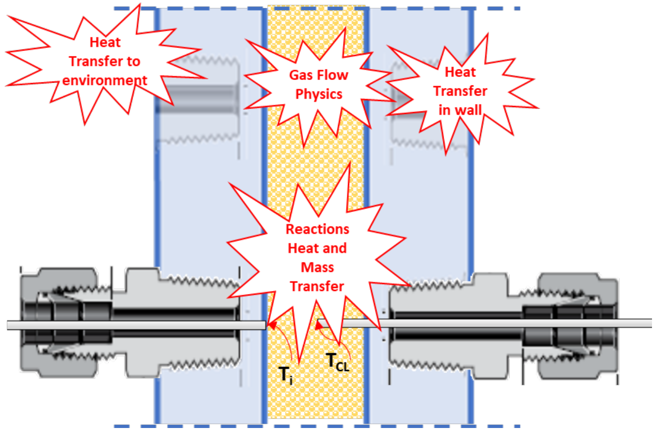
CFD Models Require

- Gas transport parameters, e.g., Cp_g, ρ_g, k_g, μ_g
- Sorbent phase properties, e.g., Cp_s, ρ_s, d_s, k_s
- Wall heat transfer parameters: Cp_w, ρ_w, k_w,
- External heat transfer parameters: $h_{O,w}$
- Reaction Rate Parameters
- Heat of adsorption

Some are well known; some are sources of uncertainty

Lab Scale Fixed Bed Tests

Lab Test Program is designed to minimize uncertainty



Flow and Heat Transfer without bed material

- Transient and Steady State
- Validates flow and heat transfer for gas and wall regions

Non-reacting Flow and Heat Transfer with bed material

- Transient and Steady State
- Validates effect of bed on flow and heat transfer

Reacting Flow and Heat Transfer with bed material

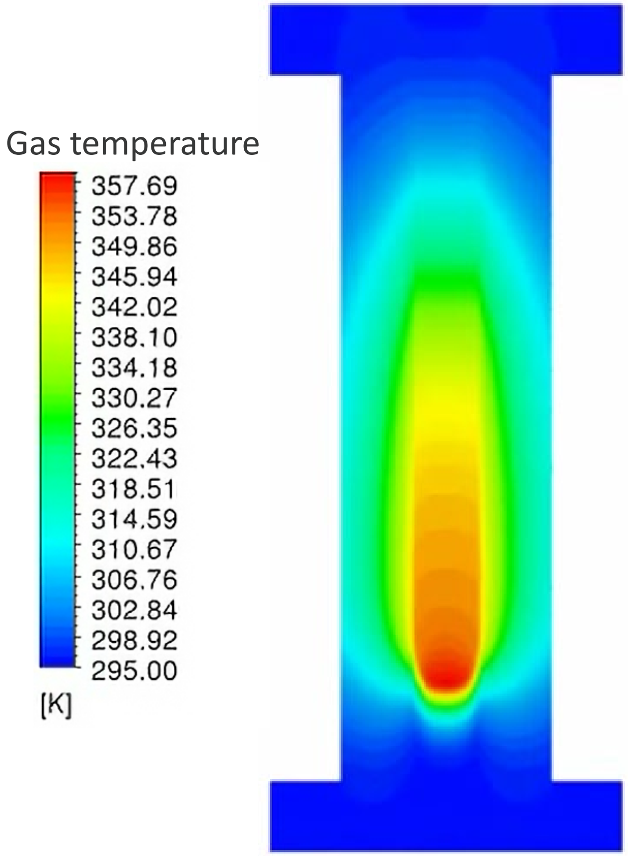
- Transient - Measure time to break through
- Vary inlet flow, inlet temperatures
- Validates reaction model parameters

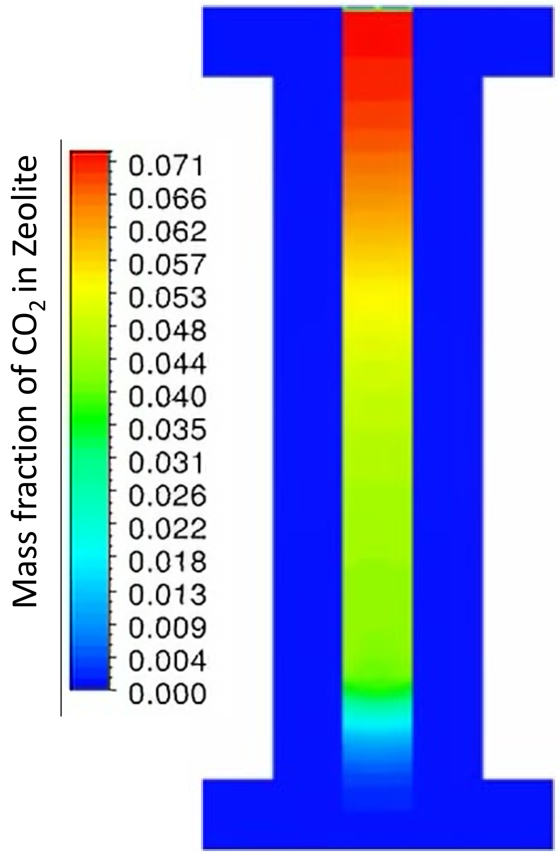
CFD Simulation Results for Fixed Bed – 13x

Example of Simulations for an Adsorption Cycle

Snapshot at 10sec. into the adsorption cycle

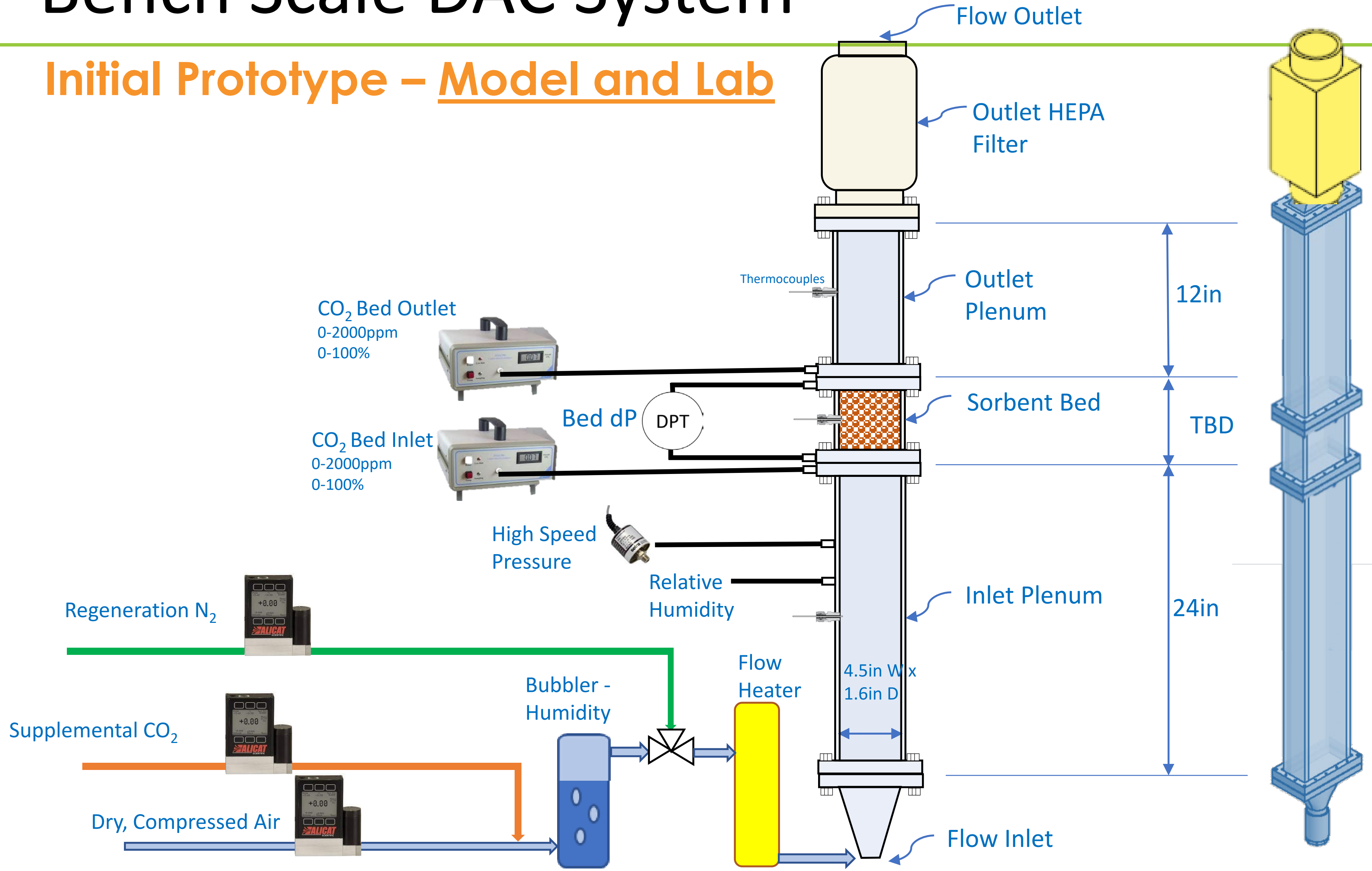
Downflow of N2 and CO2

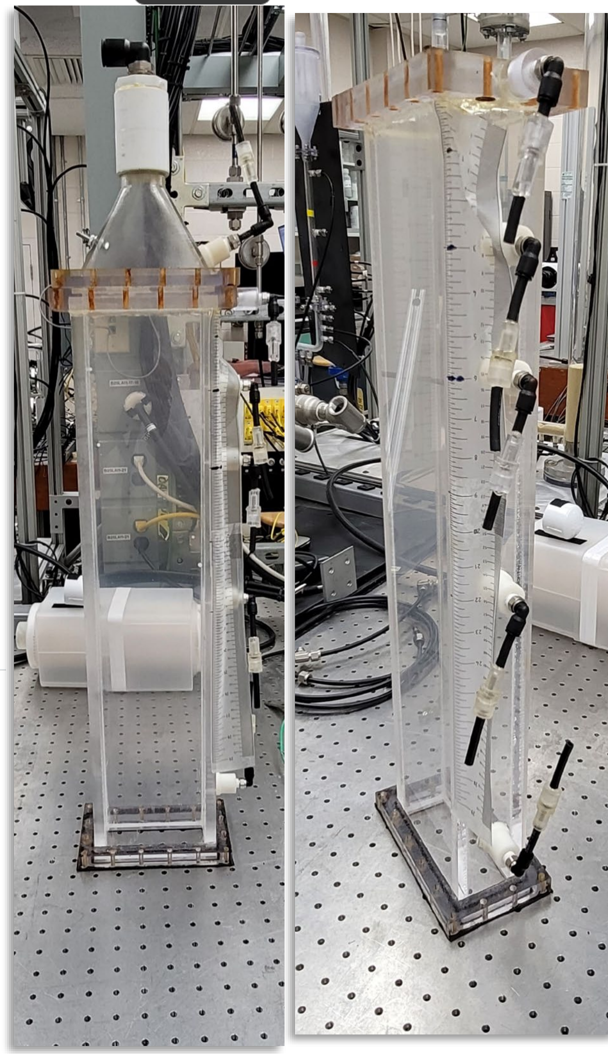




Bench Scale DAC System

Initial Prototype – Model and Lab



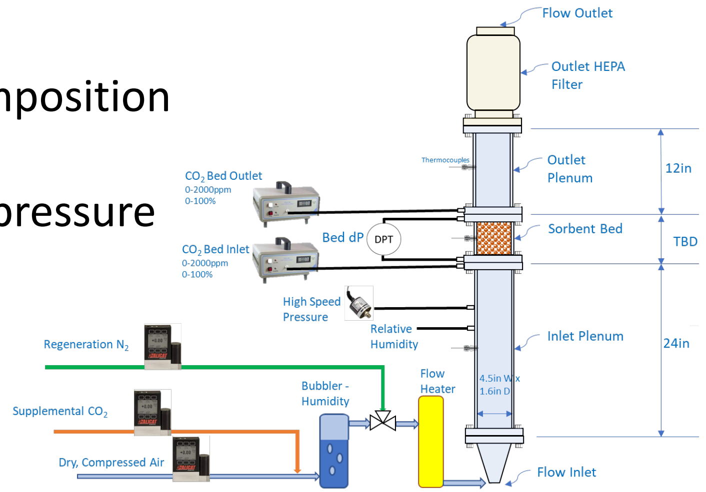


Bench Scale DAC System

Initial Lab Prototype Provides Validation Data

Measure and Control Flow Characteristics

- Control inlet flow rate, temperature, composition
- Measure:
  - Local flow velocities, temperature, pressure
  - Flow distribution across the bed
  - Flow instability
  - Local gas temperature
  - Humidity

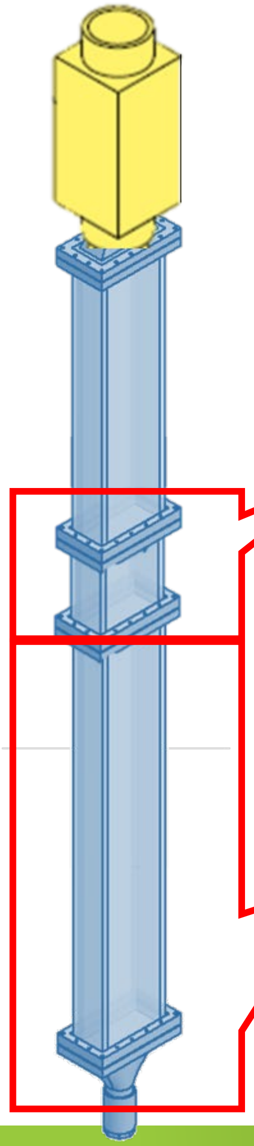


Measure Bed Performance –adsorption/desorption

- Bed Pressure Drop
- CO_2 In/Out of bed
- Temperature

Flexibility to Modify Design and Operating Conditions

- Pressure Drop
- Flow Distribution
- Duration of Adsorption/Desorption cycles



Flexible Bed Design, e.g.

- Vary Geometry
- Add heat exchanger
- Different sorbents
- Regeneration methods

Flexible Duct Design, e.g.

- Vary Geometry
- Allow for flow imaging
- Improve inlet flow distribution
- Fans, etc.

Bench Scale DAC System

Validation of the CFD Model

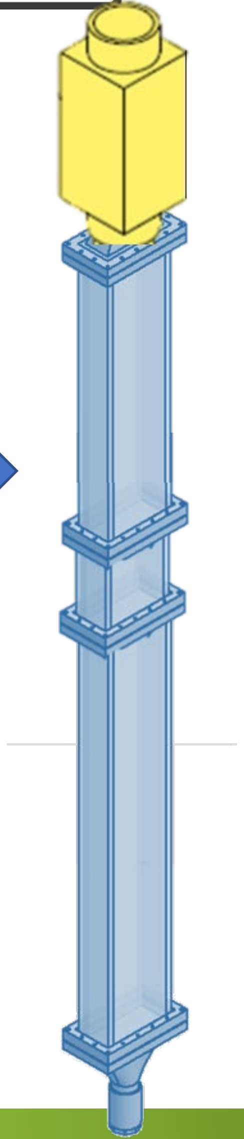
Measure and Control Flow Characteristics
- Control inlet flow rate, temperature, composition
- Measure:
  - Local flow velocities, temperature, pressure
  - Flow distribution across the bed
  - Flow instability
  - Local gas temperature
  - Humidity

Measure Bed Performance –adsorption/desorption
- Bed Pressure Drop
- CO_2 In/Out of bed
- Temperature

Flexibility to Modify Design and Operating Conditions
- Pressure Drop
- Flow Distribution
- Duration of Adsorption/Desorption cycles

Lab Data Used to Validate CFD Model

CFD Model Used to Guide Improvements to Bed Design



Summary of Team Capabilities

- Staff of computational researchers with experience covering..
  - A broad range of physical processes.
  - A wide-variety of open-source and commercial computational tools

- The MFiX Suite of Multiphase Computational Fluid Dynamics Software for Predicting Reactor Performance continues to advance.

- Experimental facilities to support simulation activities.
  - Particle characterization
  - Detailed Instrumentation
  - 3D Printing

- *Complimentary* project in optimization of a DAC system.