NATIONAL ENERGY TECHNOLOGY LABORATORY

Applications of Multiphase Flow in DOE's Energy Portfolio

Geo Richards

Focus Area Leader, Energy System Dynamics

NETL 2011 Workshop on Multiphase Flow Science

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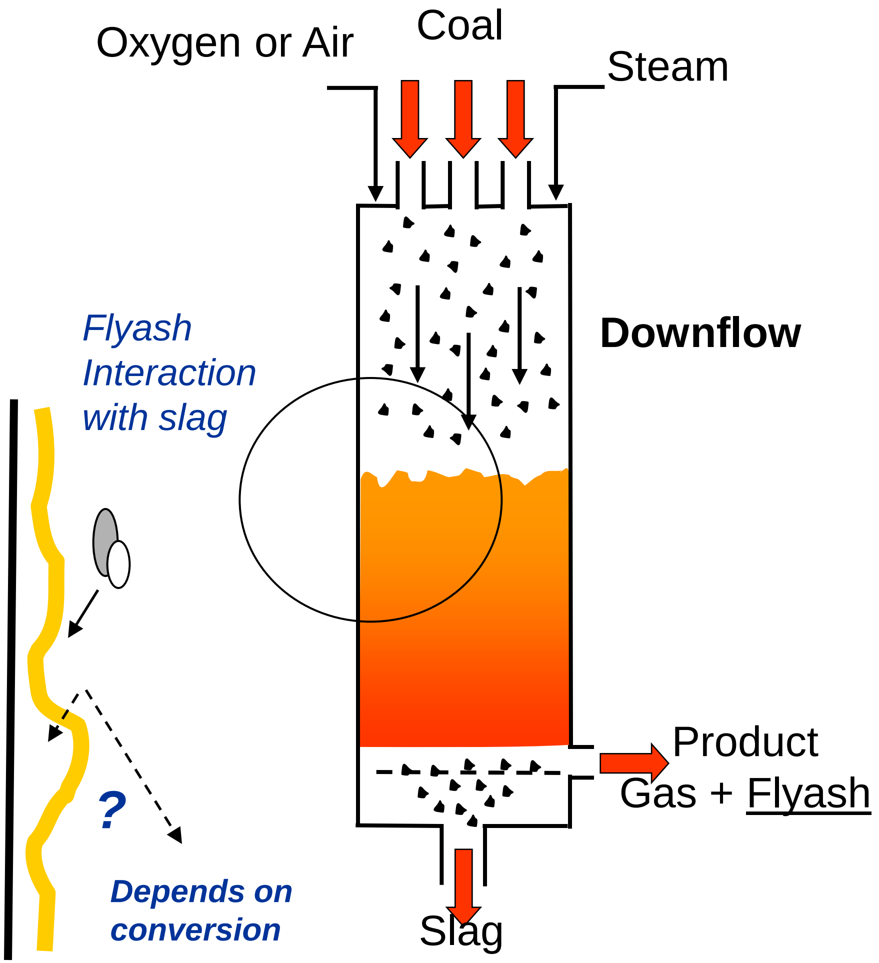
Multi-phase flow in existing and emerging energy technologies

- **Gasifiers**
  - Entrained flow ash/slag
  - Feed systems
  - Low-rank coals
- **Sorbent systems for CO2 capture**
  - Hydrodynamics
  - Heat exchanger
  - Attrition
- **Chemical Looping**
  - Conversion
  - Ash separation
  - Attrition

Entrained flow gasifiers

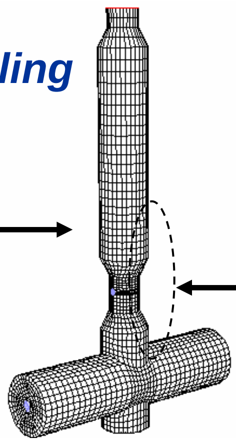
- **Calculating the coal conversion and flyash carryover.**
  - An important issue to reduce syngas cooler fouling, particle recycle.
- **Need to know the carbon conversion (even approximate) along the reactor**
  - Little data for any fuel!
  - Very practical issue: affects the downstream ash deposition, etc.



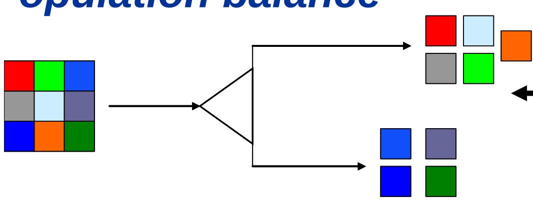
Example of Research Activity – Materials Thrust / Flexible Feedstock

Multi-scale modeling – NETL (Morgantown)

CFD-modeling

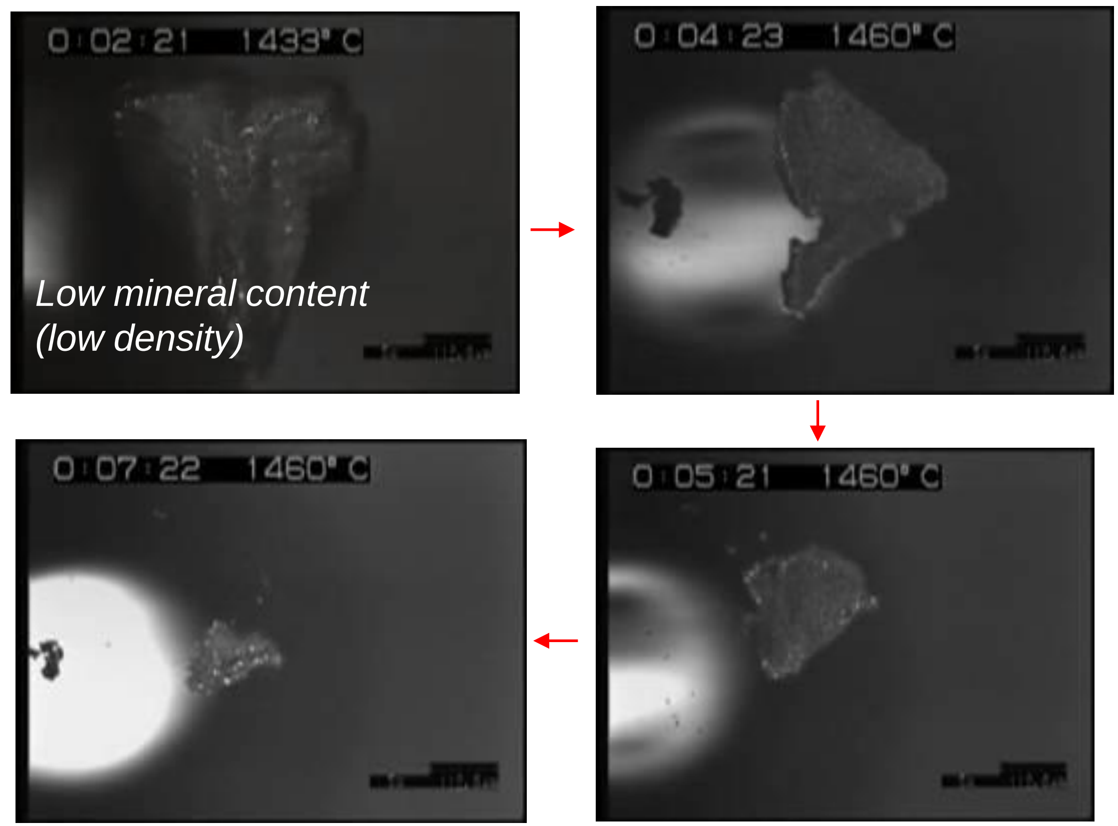


Population balance



Feedstock/slag interactions- Pittsburgh Coal

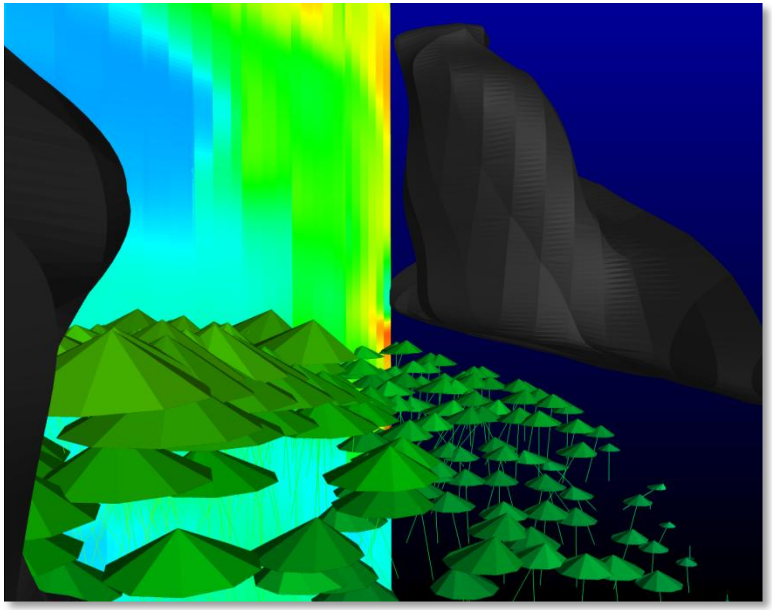
$$C + CO_2 = 2CO$$



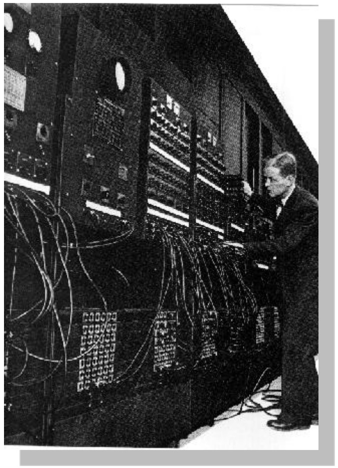
Sridhar Seetharaman (CMU), Pete Rozelle (DOE-HQ), Larry Shadle (NETL)

Design prediction versus insight?

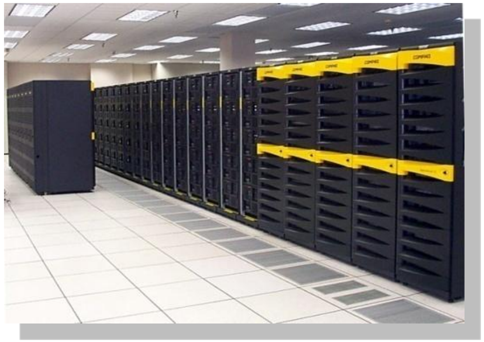
- **Reacting flow CFD has advanced significantly in the last three decades.**
- **CFD is an integral part of design of many practical devices *<u>because of fundamental insights</u>* embedded in simulations.**
- **Continued computation power will make large simulations practical in industry**



High Resolution (10M cells) simulation coal jet region.



Giant ENIAC (Electrical Numerical Integrator and Calculator) machine, University of Pennsylvania, circa ?

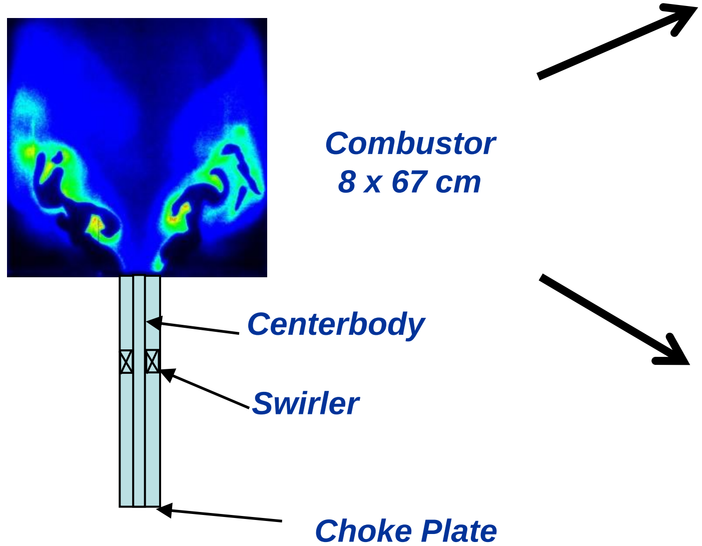


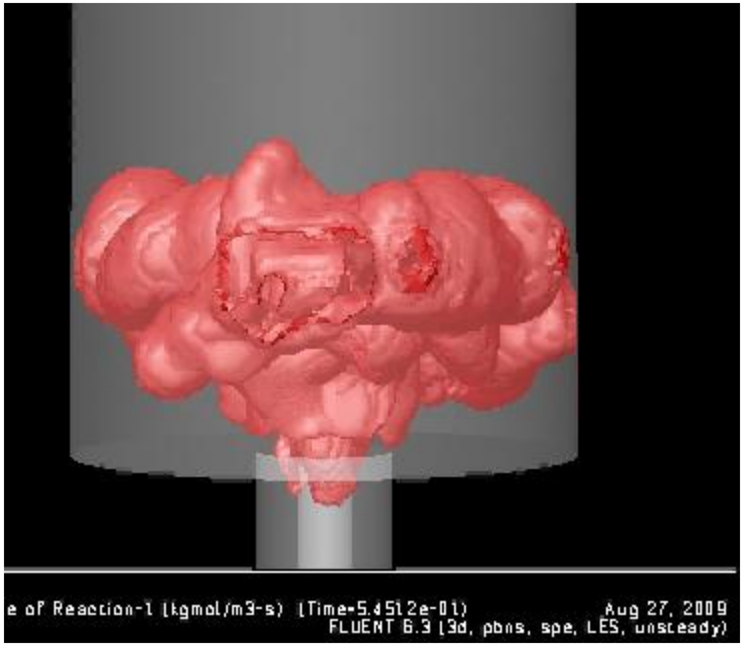
Computers at Pittsburgh Supercomputing Center

Progress in combustion simulation

- **Significant progress in combustion simulation**
  - Validating, time resolved experiments and models
- **Why is it different for gasification?**
  - The problem is harder
  - There has not been as much fundamental work

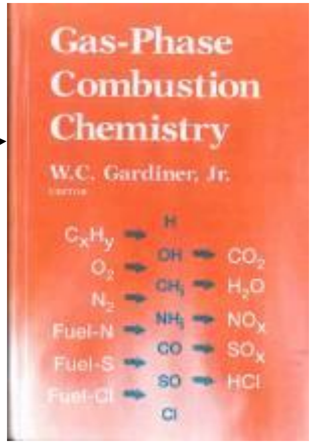
Experimental OH PLIF planar slice

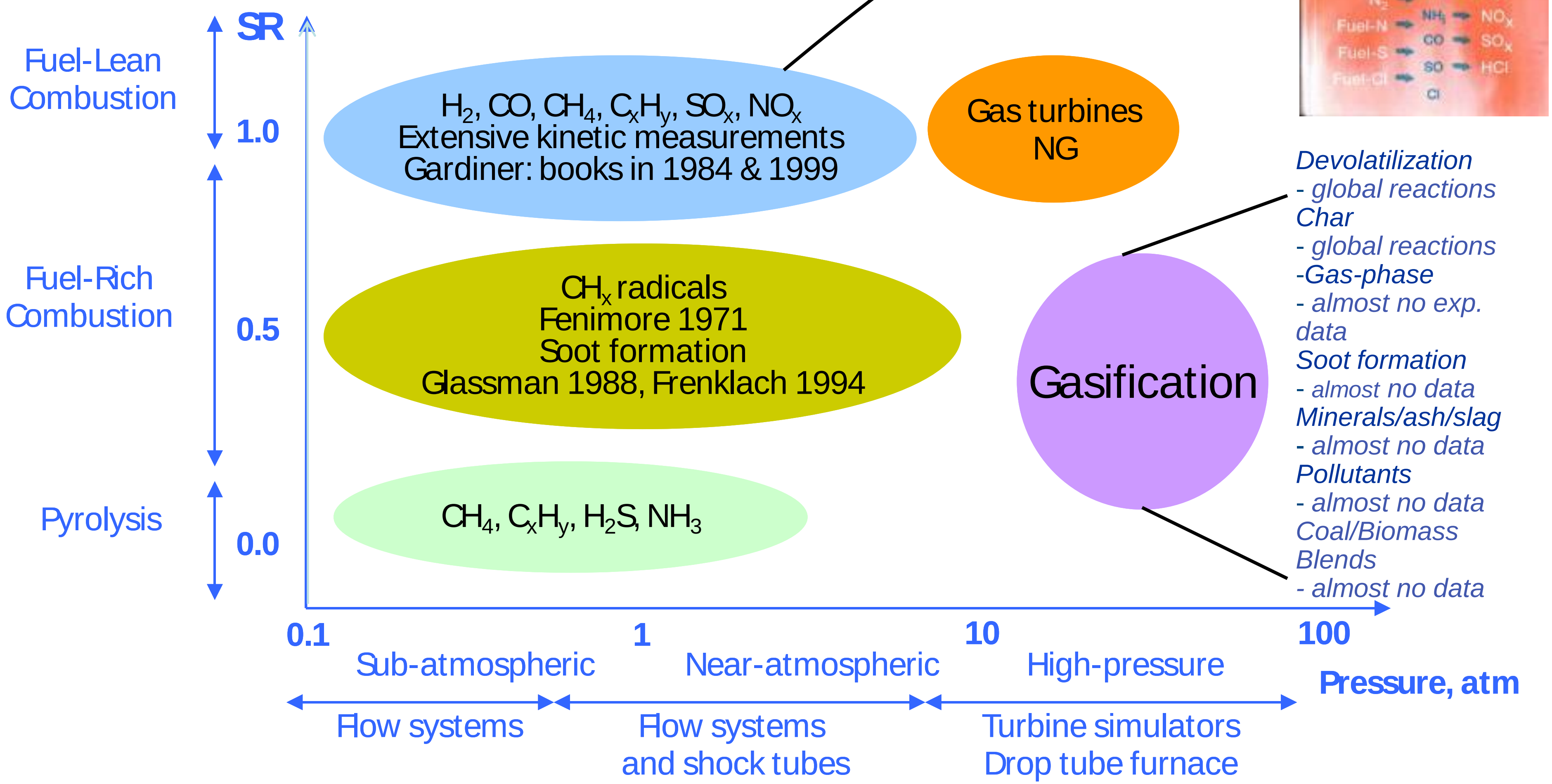




Gasification vs. Combustion

Courtesy V. Zamansky, GE





Fuel Conversion Modeling Capability

Courtesy V. Zamansky, GE

Combustion

- *Kinetics*
- *Reacting flow CFD*
- *Emissions modeling*
- *Fuel injection*
- *Fuel variability*
- *System cost*

- *Film / Impingement cooling*
- *Flame radiation*

Gasification

- *Kinetics*
- *Reacting flow CFD*
- *Emissions modeling*
- *Fuel injection*
- *Fuel variability*
- *System cost*

- *Fuel de-volatilization*
- *Char / soot formation*
- *Slagging characteristics*
- *Refractory modeling*
- *Syngas cooler deposition*

Well-validated models
Models w/ partial validation
Non-validated models

Design Effort

	Combustion	Gasification
Apply fundamental models	*80%*	*10%*
Experimental validation	*20%*	*90%*

Based upon 50 years of development

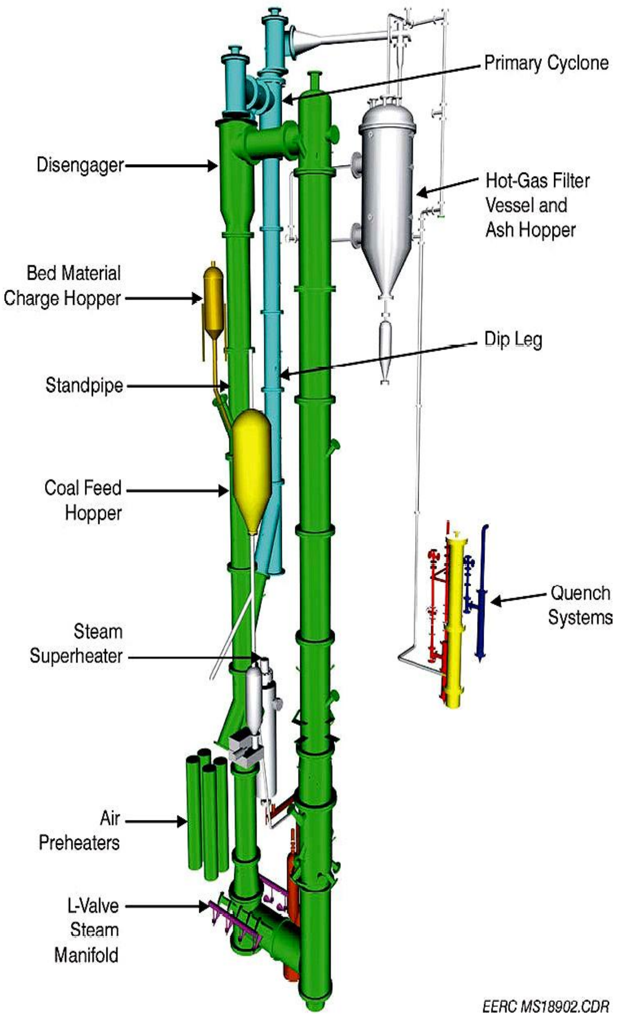
Demonstrated improvements:
- *Significant cost reduction*
- *High efficiency*
- *Low emissions*

Today's models based on empirical relationships

What is the impact of empirical approach on:
- *Cost ?*
- *Efficiency ?*
- *Operating life, reliability ?*

Low Rank Coal Application

- **Lots of low-rank coal in the US!**
- **Allows lower temperature gasification technology.**
  - Dry ash, not slagging.
  - Bigger particles than entrained.
- **Conversion and hydrodynamics – can we predict?**



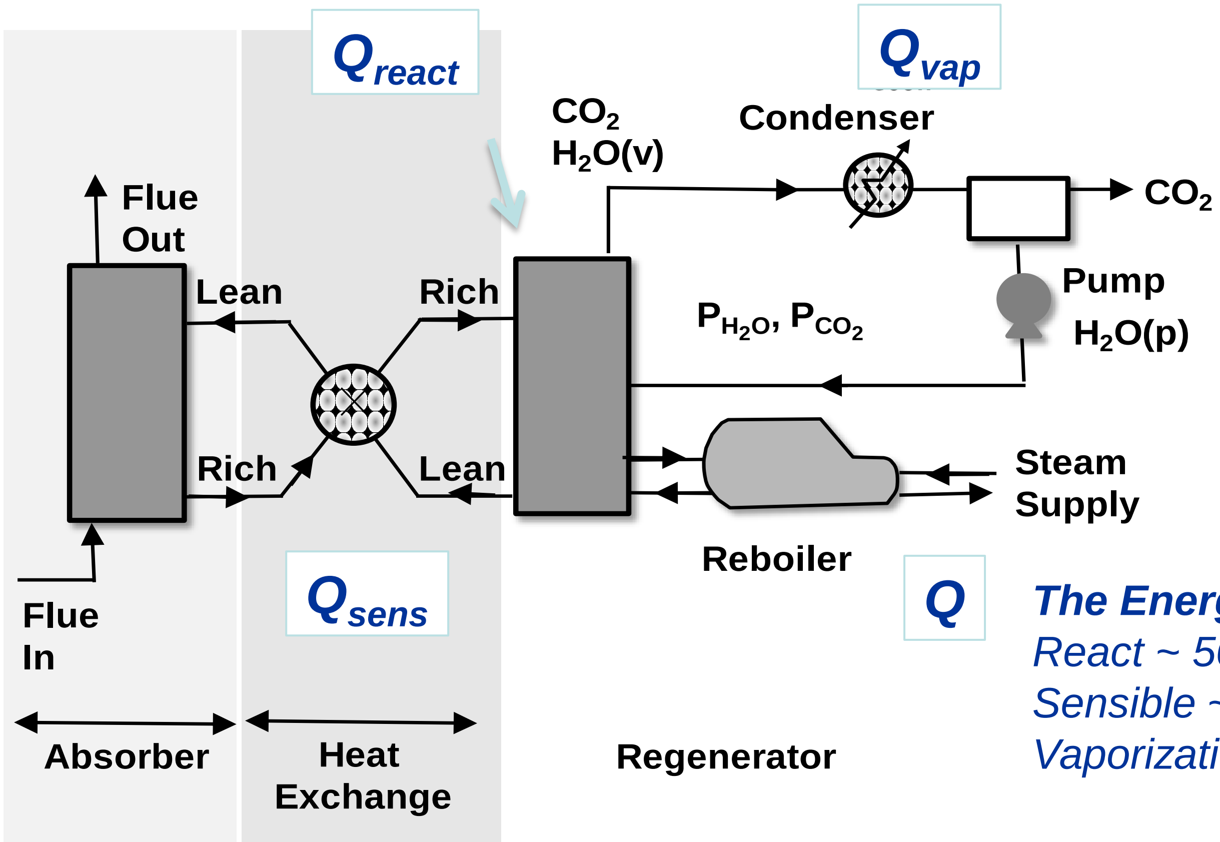
Solid Sorbents for CO_2 capture:

A proposed option for flue gas CO_2 capture.

A multi-phase flow funhouse.

The current capture technology

- Amine solvent scrubbing: familiar; widely used and studied.
- Approx, 20 – 30% of existing powerplant output needed to operate !
- Energy inputs: sensible, vaporization, reaction: $Q = Q_{sens} + Q_{vap} + Q_{react}$
- What can be done to reduce the energy penalty?



The Energy Budget:
React ~ 50%
Sensible ~ 25%
Vaporization ~ 25%

Reducing the energy penalty

Eliminate/reduce the vaporization and sensible heat

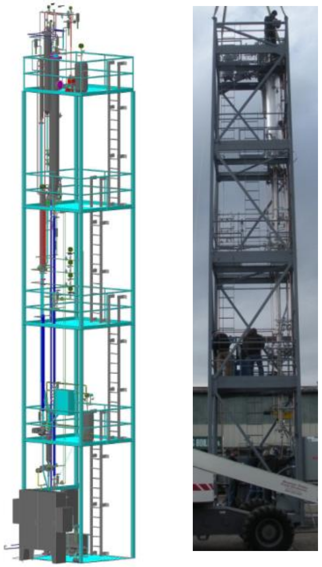
- **Aqueous solvents:**
  - Adding heat reverses the capture reaction.
  - Added penalties from water vaporization, sensible heating/cooling.
- **Dry Sorbent Alternative:**
  - New chemistry *possible* for lower reaction energy.
  - Avoid the vaporization term..with careful moisture management !
  - Still: heat and cooling sensible term.

The Energy Budget:
React ~ 50%
Sensible ~ 25%
Vaporization ~ 25%

Example of sorbents

- **Two different formulations studied at NETL:**
  - Clay substrate, amine impregnated.
  - Silica (catalyst support).
- **Both manufactured with commercial processes/partner.**

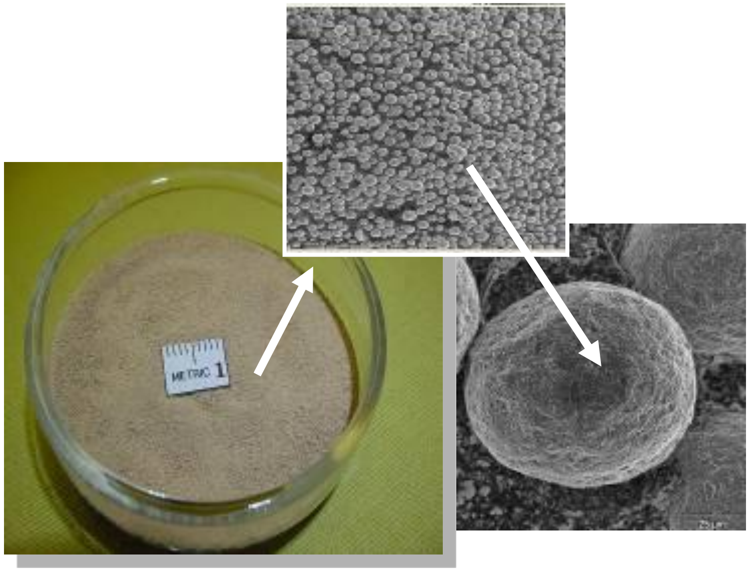
PEI on CARiACT Q10
(100 to 350 µm dia.)



Schematic and actual pilot unit with ADA.

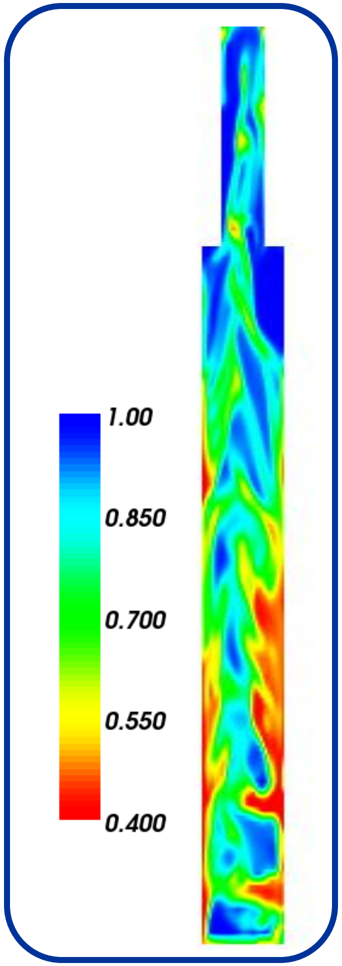
Lab-scale sorbent testing

Pressure Chemical Facility; production of 1200lb of sorbent



NETL CO_2 Sorbent , spray dried formula, 80μm

Process and Component Development for Solid Sorbents

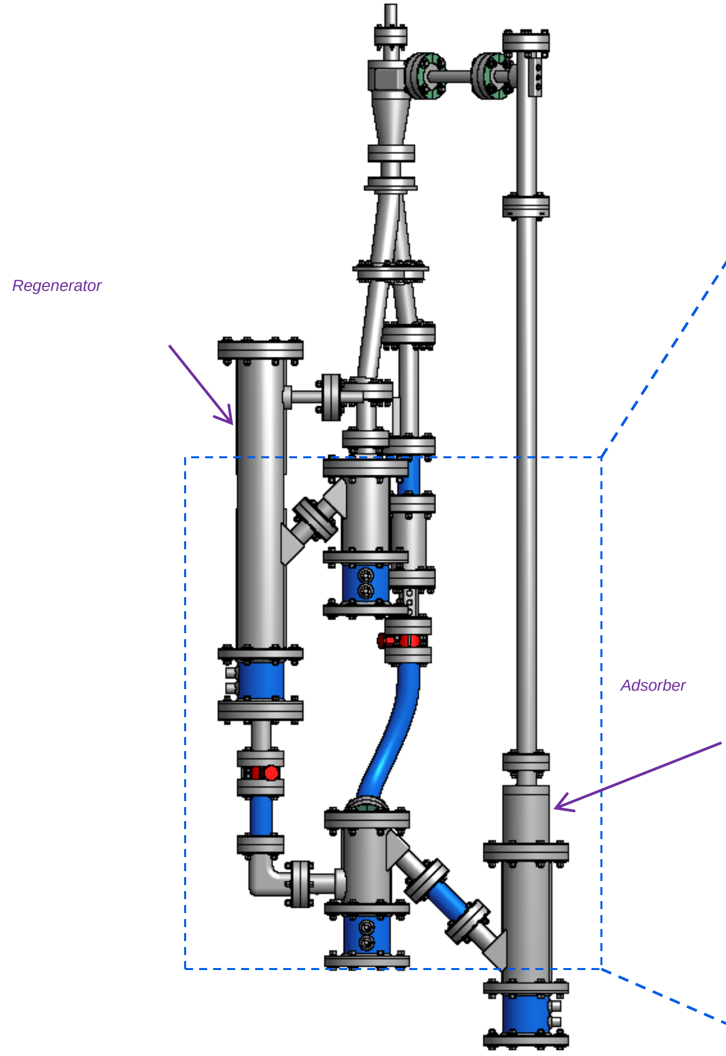


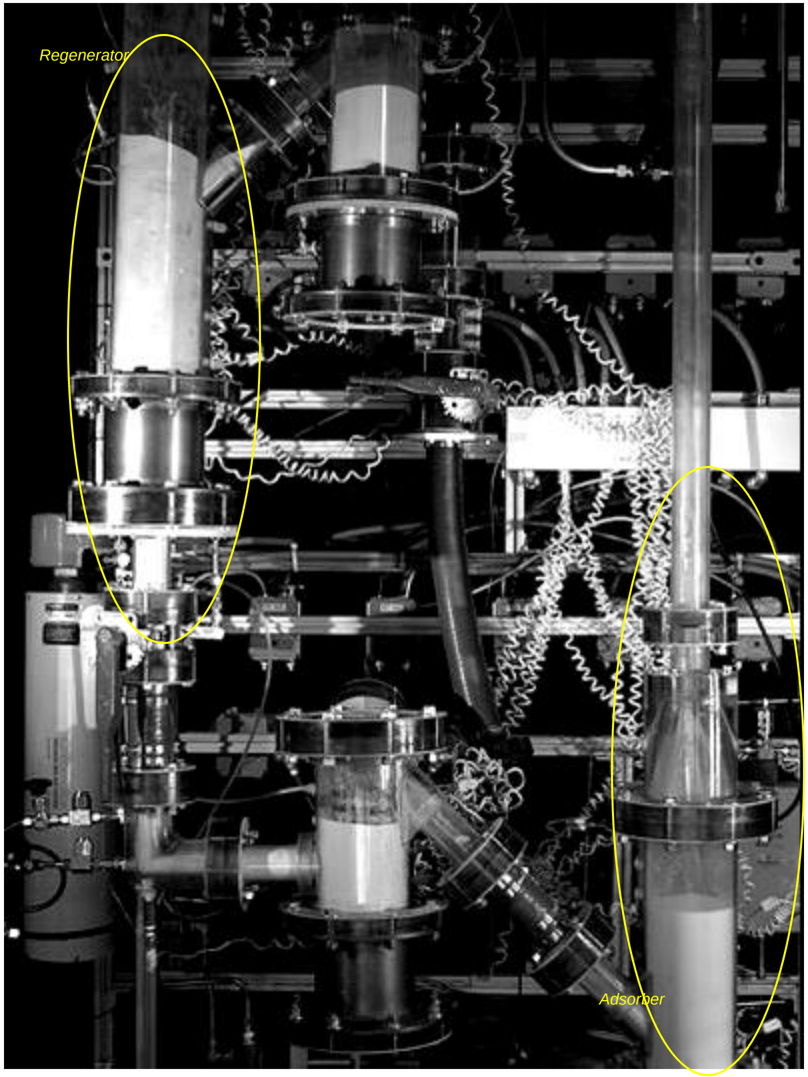
- **NETL experimental system.**
  - Lab size/scale allows rapid screening of component options.
  - circulating absorber & regenerator
  - validates thermal, hydrodynamic, transport, and kinetic performance
- **Validating data: enabling rapid numeric scale-up.**

*Predicted absorber gas fraction **

** Prediction from a different design than shown schematically*

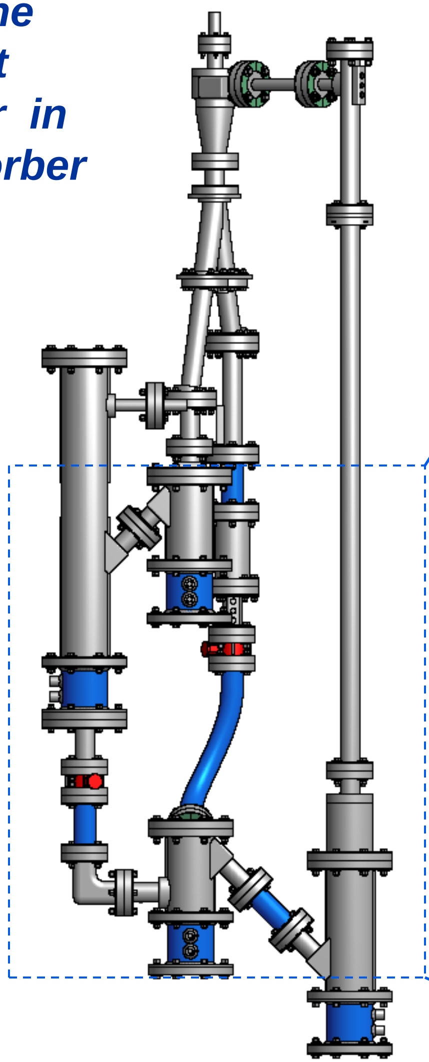
C2U video of design conditions

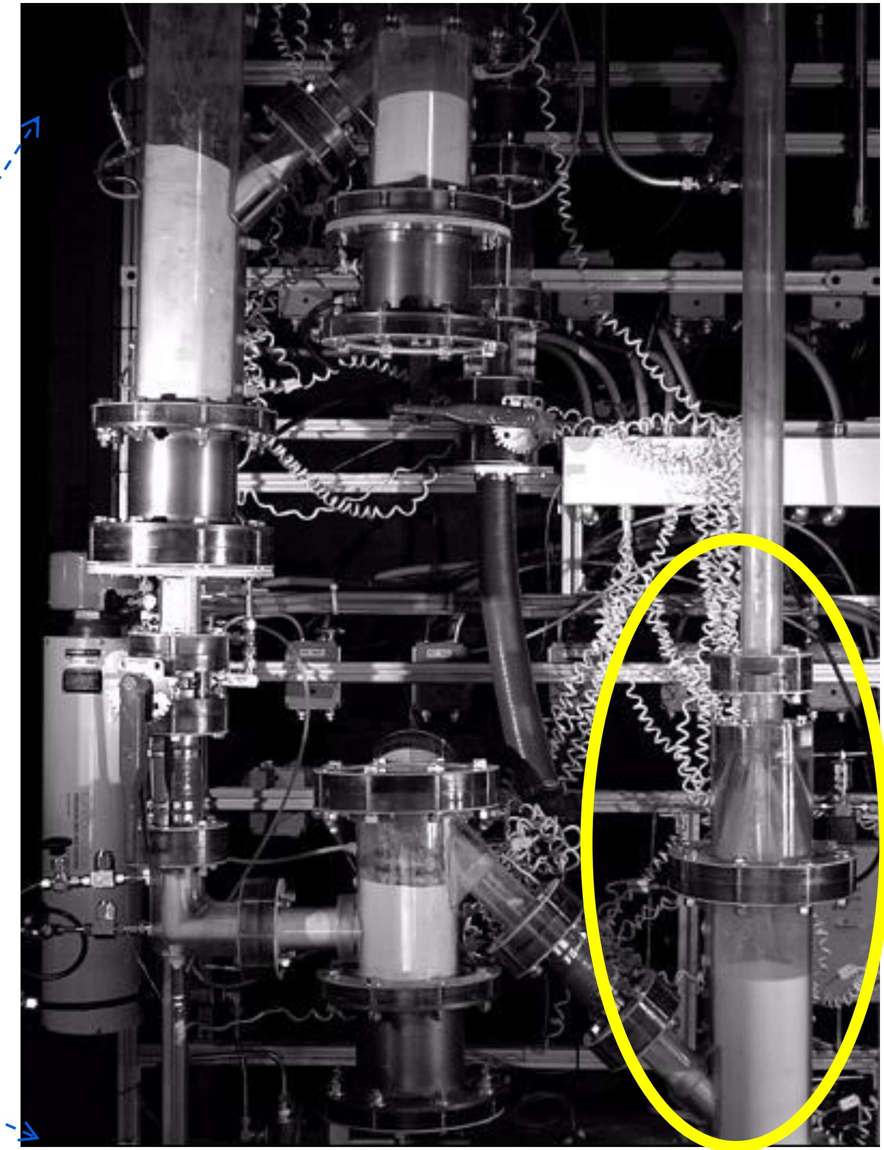




Riser operation

Notice the transient behavior in the absorber (yellow circle)





What key practical predictions (insight or design level) would we like from multi-phase flow simulations?

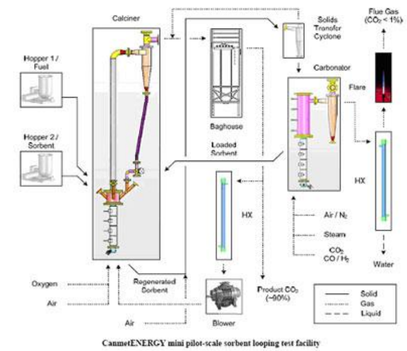
What key practical predictions (insight or design level) would we like from multi-phase flow simulations?

- **Attrition !**
- **Can multi-phase flow models be used to predict *<u>or prevent</u>* attrition in sorbent systems?**

Chemical Looping

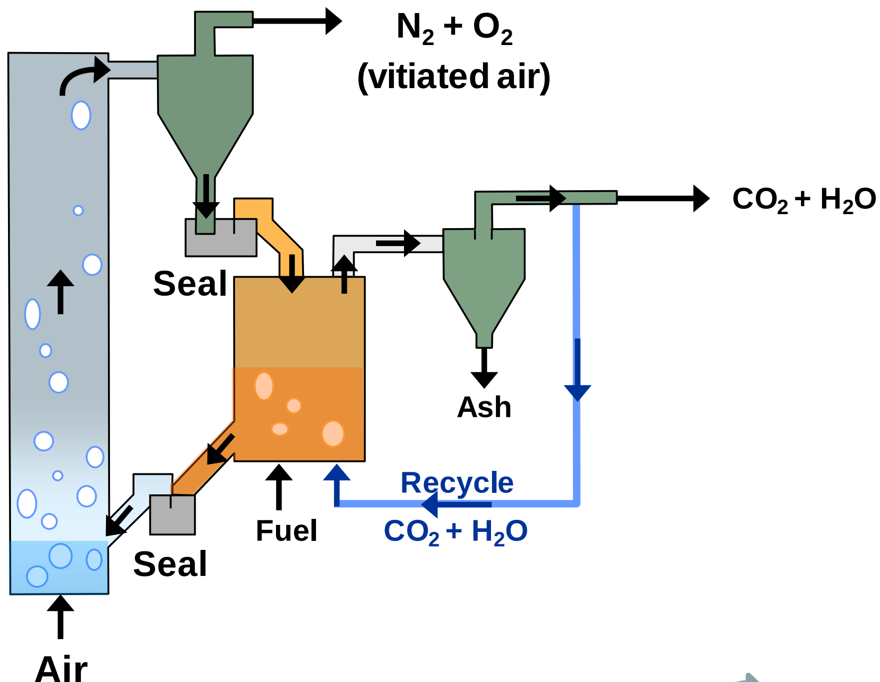
A different approach to CO2 capture.

Chemical Looping



CANMET Energy Technology Center mini pilot-scale sorbent looping test facility.*

- **Shares advantages of oxy-fuel**
  - Product is just CO_2 and H_2O
- **No separate oxygen production is needed**
- **Significant interest/development worldwide**



Carbon + metal oxide = CO_2 + metal

Metal + air (oxygen) = metal oxide

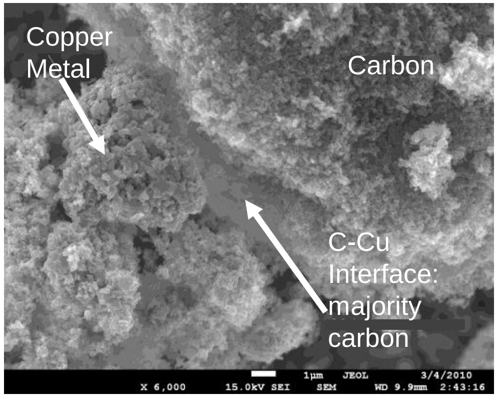
*120 kW Chemical Looping test rig (TU, Austria) **

*Pilot-scale calcium looping rig (30 kW) at INCAR_CSIC, Oviedo, Spain**

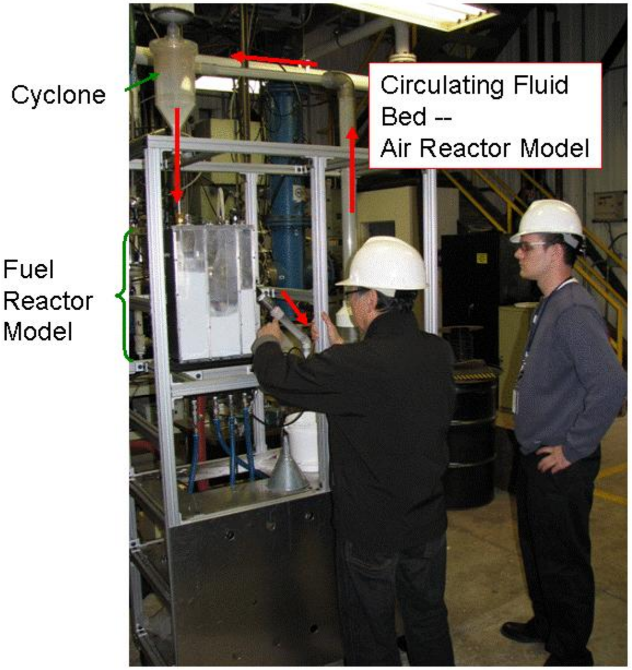
•Photos used with permission from the IEA web-site for the chemical looping network

NETL on-site Research on Chemical Looping

- **Evaluating carrier behavior & options**
  - Physics of solid-fuel & MeO reaction.
  - Evaluation of metal "commodity" carriers from waste or natural sources.
- **Leverages NETL capability in multi-phase flow:**
  - Cold Flow Facility
    - Investigating **ash, coal, carrier separation** and handling.
    - Validate model predictions.
  - Hot Flow Facility
    - Address reaction performance
    - Detailed design in progress.
  - Reactor simulations.
    - Accelerate understanding & scale-up



C/CuO Interface Regions



ICMI – Industrial Carbon Management Initiative:
1.) Industrial Chemical Looping (natural gas and coal)
2a.) CO2 Storage in depleted Shale
2b.) CO2 re-use

Approach for chemical looping

- **Conduct needed research on oxygen carriers, hydrodynamics, process design to develop chemical looping for:**
  - Industrial applications (heat, steam)
  - Power
- **Not a single design, but data to enable design choices explored with numeric simulations.**
- **Complements specific developments by others.**
- **Assess process economics, performance.**
- **Information to NETL leadership on performance potential.**
- **Partnerships for continued *commercial* development.**

Chemical Looping Development

- *Develops/demonstrates breakthrough carbon management technology*
- *Utilizes NETL strength in simulation based engineering/visualization*
- *Flexible/distributed infrastructure a model for collaborative R&D portfolio*

RUA Universities, other laboratories, industrial partners

The Physical Lab

Air (minus process oxygen)

CO_2

Industrial process heat

Air

Natural gas

Sensors and diagnostics
- *Hot solids flow rate*
- *Real solids temperature*
- *Solids conversion*
- *Hot particle image velocimetry*

Material Science/ Engineering
- *Oxygen carrier particle design*
- *Material durability & reactivity*
- *Coking resistance*

Control
- *Thermal balance*
- *Bed dynamics*
- *Hardware in the loop simulation*
- *(for simulating full-scale behavior)*

Fluid & Thermal Science/ Engineering
- *Reaction kinetics & diffusion limits*
- *Reactor configuration*
- *Heat transfer & thermal management*
- *Bed hydrodynamics*

A chemical looping dual-reactor process reported on in the literature is currently being designed and built at NETL.

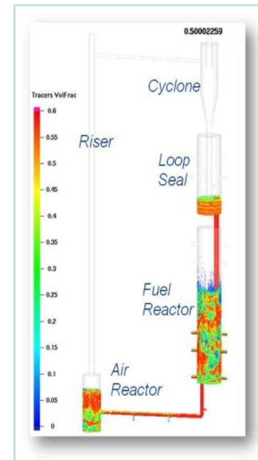
Connecting physical data with detailed simulations

The Virtual Lab

- Accelerates commercialization of systems and technologies,
- Minimizes deployment risk/cost,
- Identifies “gaps” for further targeted R&D

Simulation Based Engineering
- *Industrial application modeling*
- *Component validation models*
- *Particle models*

Collaborative Data Management
- *Lab portal development*
- *Reduced order models*



Virtual Industrial Design and Operation

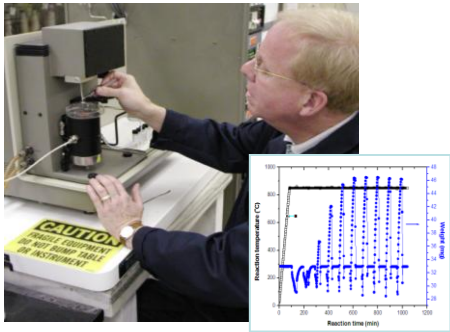
Simulation and Experimental Facilities

Existing Clusters

Attrition Tests

Fluid Bed Reactors

Existing TGA Lab



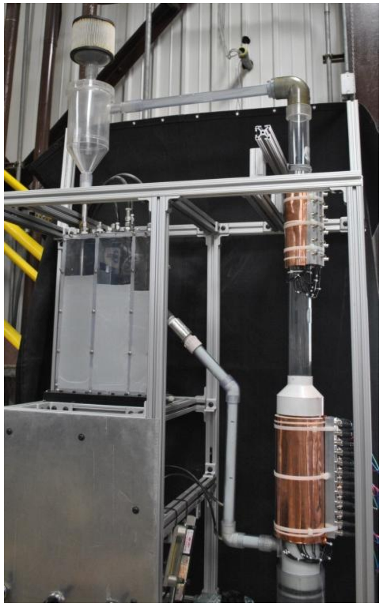
NETL O2 carrier - cyclic studies in progress

Candidate SBEUC Systems

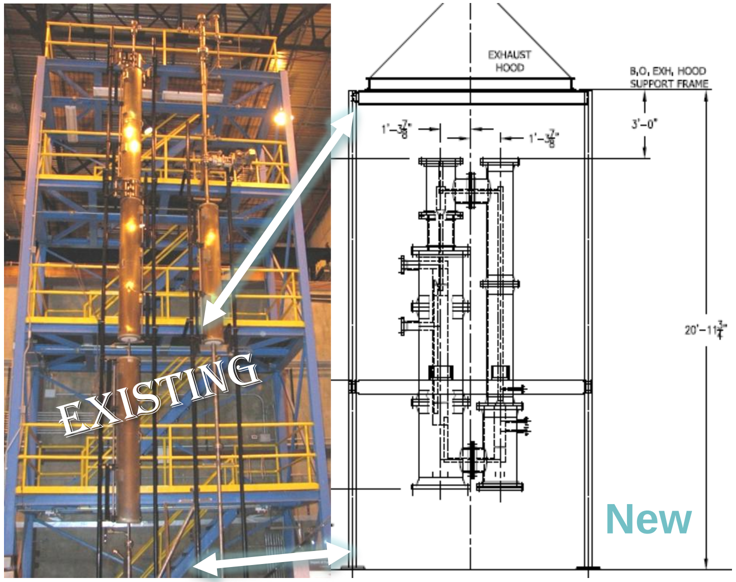
Portable Modular System

Performance Optimized System

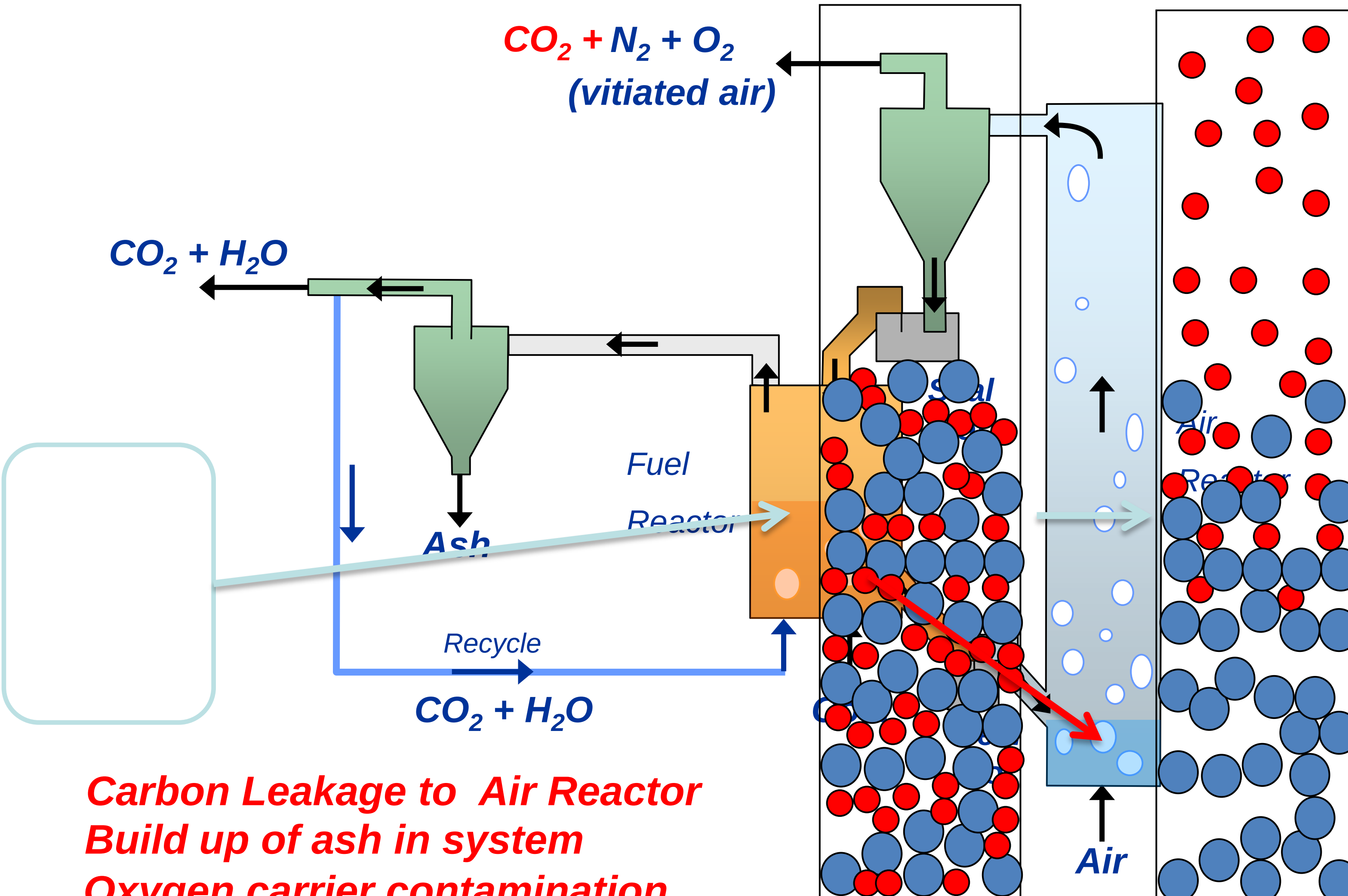
Cold Flow with ECVTs



Integrated Chemical Looping Reactor

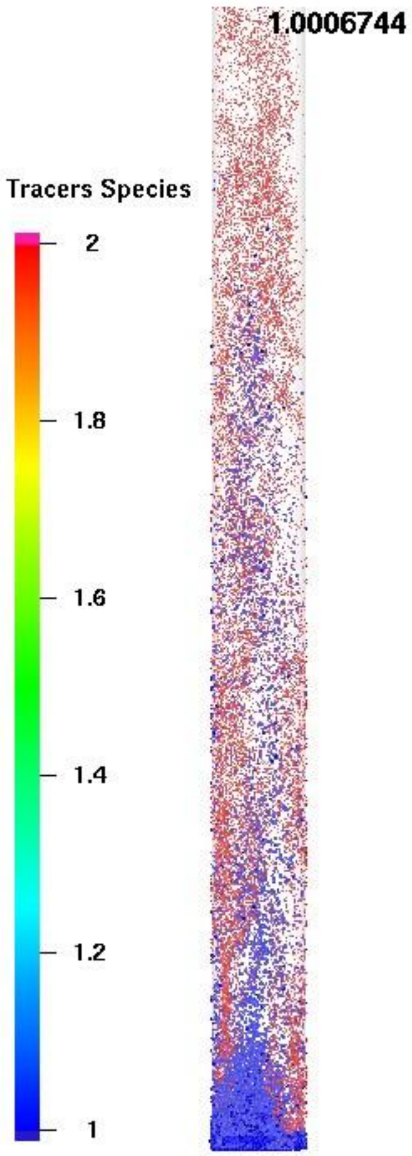


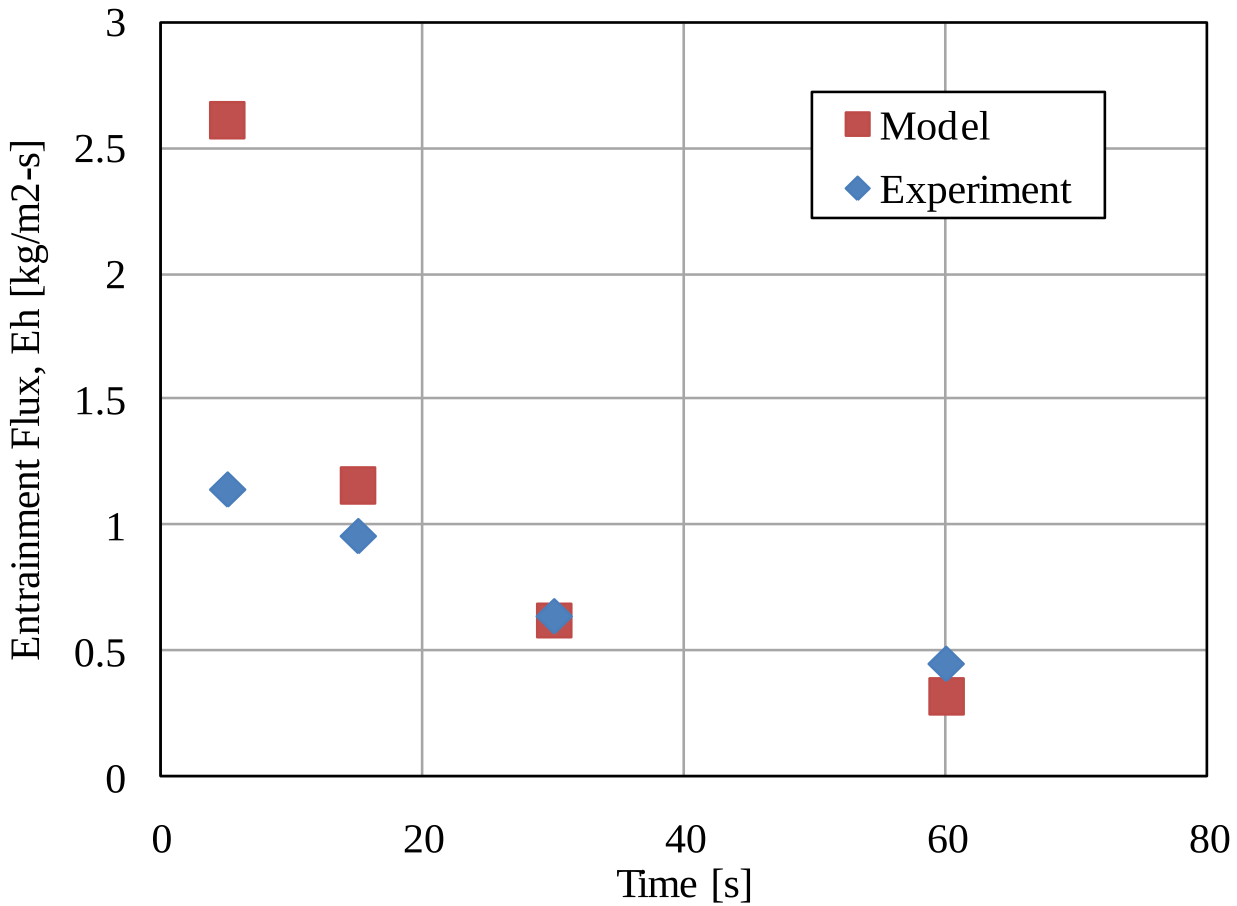
Issues with a CLC?
Solutions: Aerodynamic Separation



Carbon Leakage to Air Reactor
Build up of ash in system
Oxygen carrier contamination

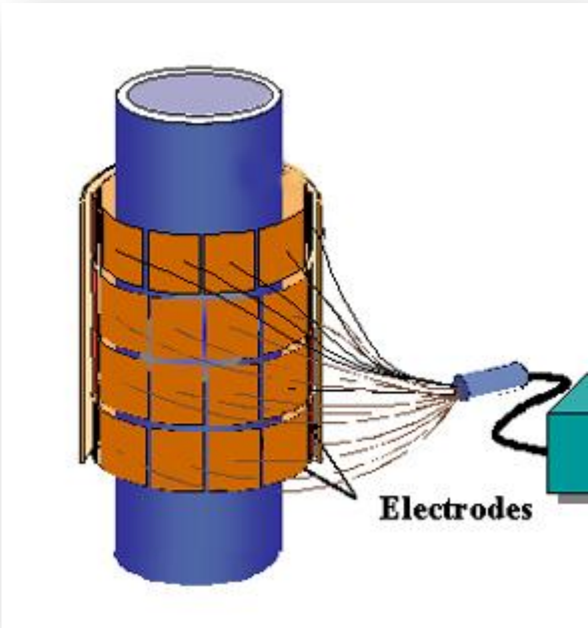
How does CFD Compare?

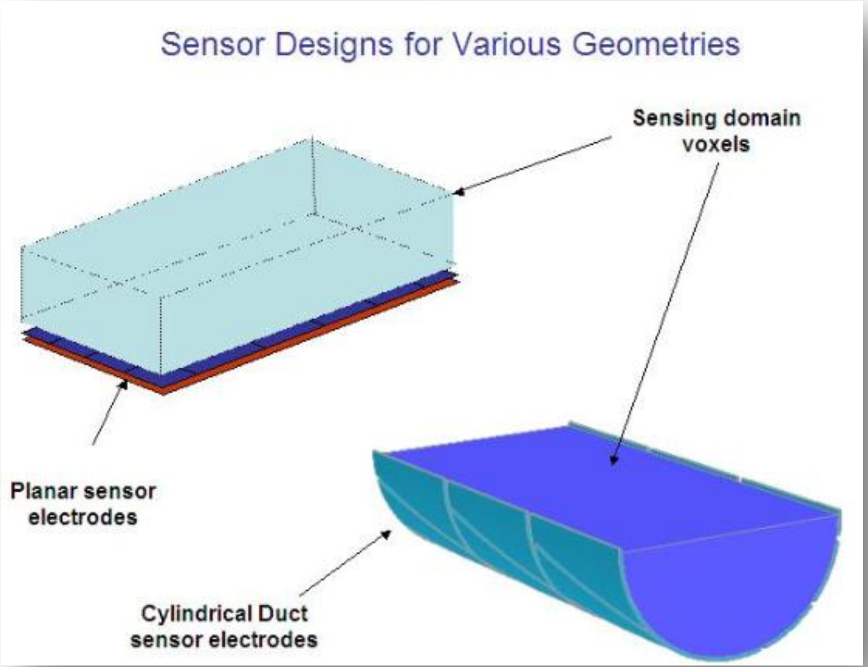




- CPFD's Barracuda
- 43k cells
- CuO/Acrylic 1.5*Ut

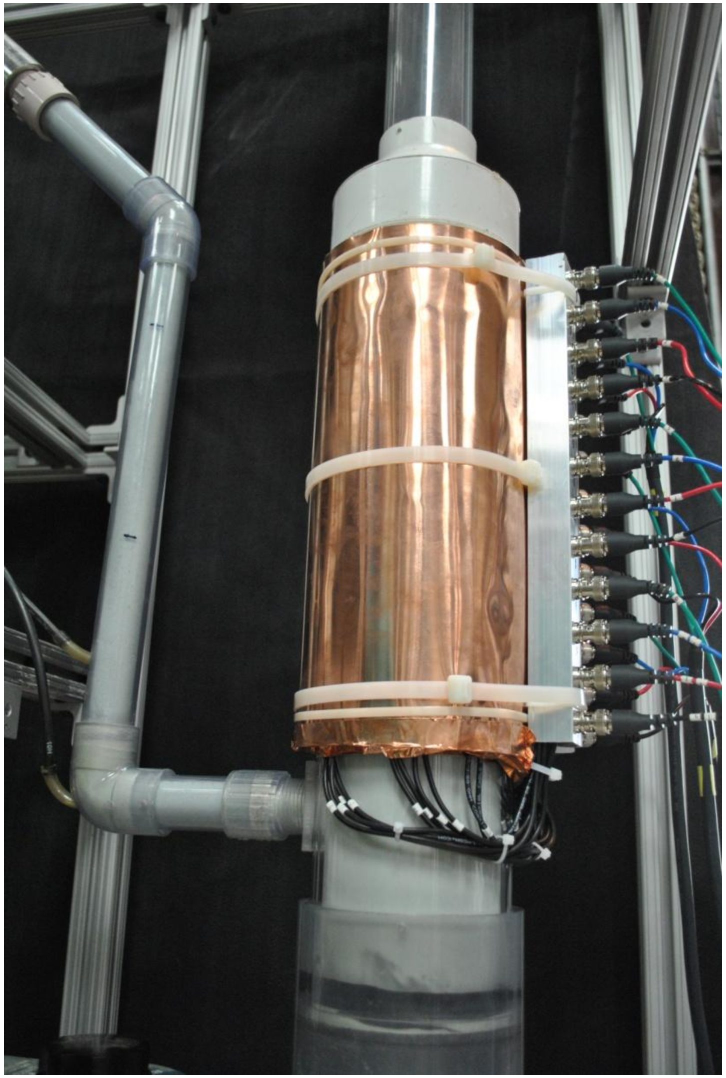
ECVT Sensor Overview



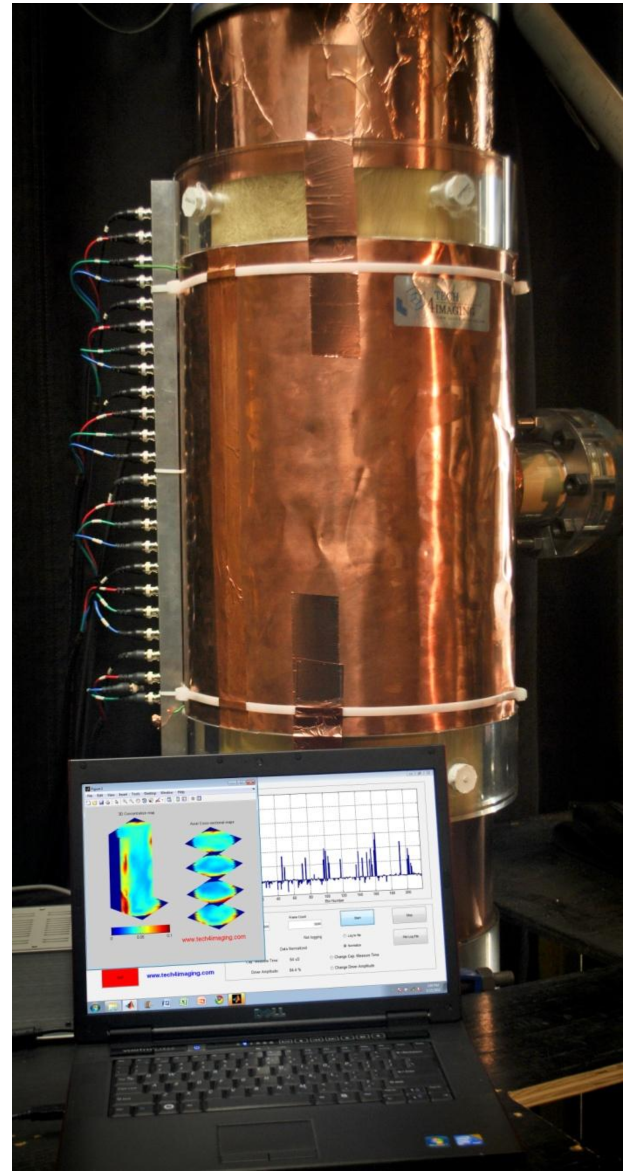


Data Collection → Reconstruction → Post Processing

1 Frame ~1s

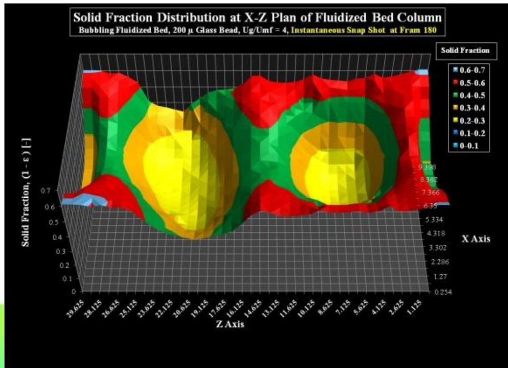


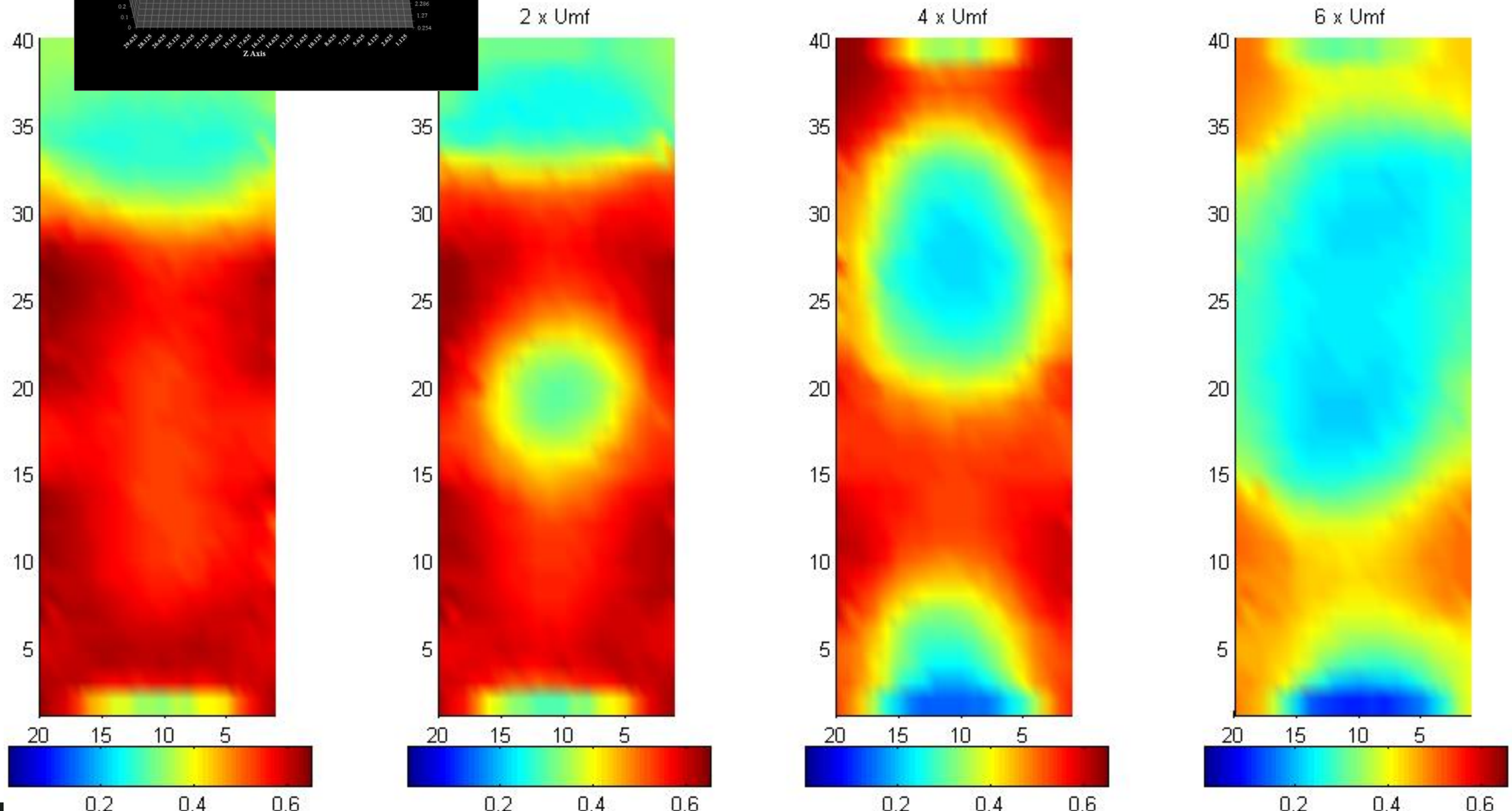
4in ECVT sensor on CLC Demo Unit



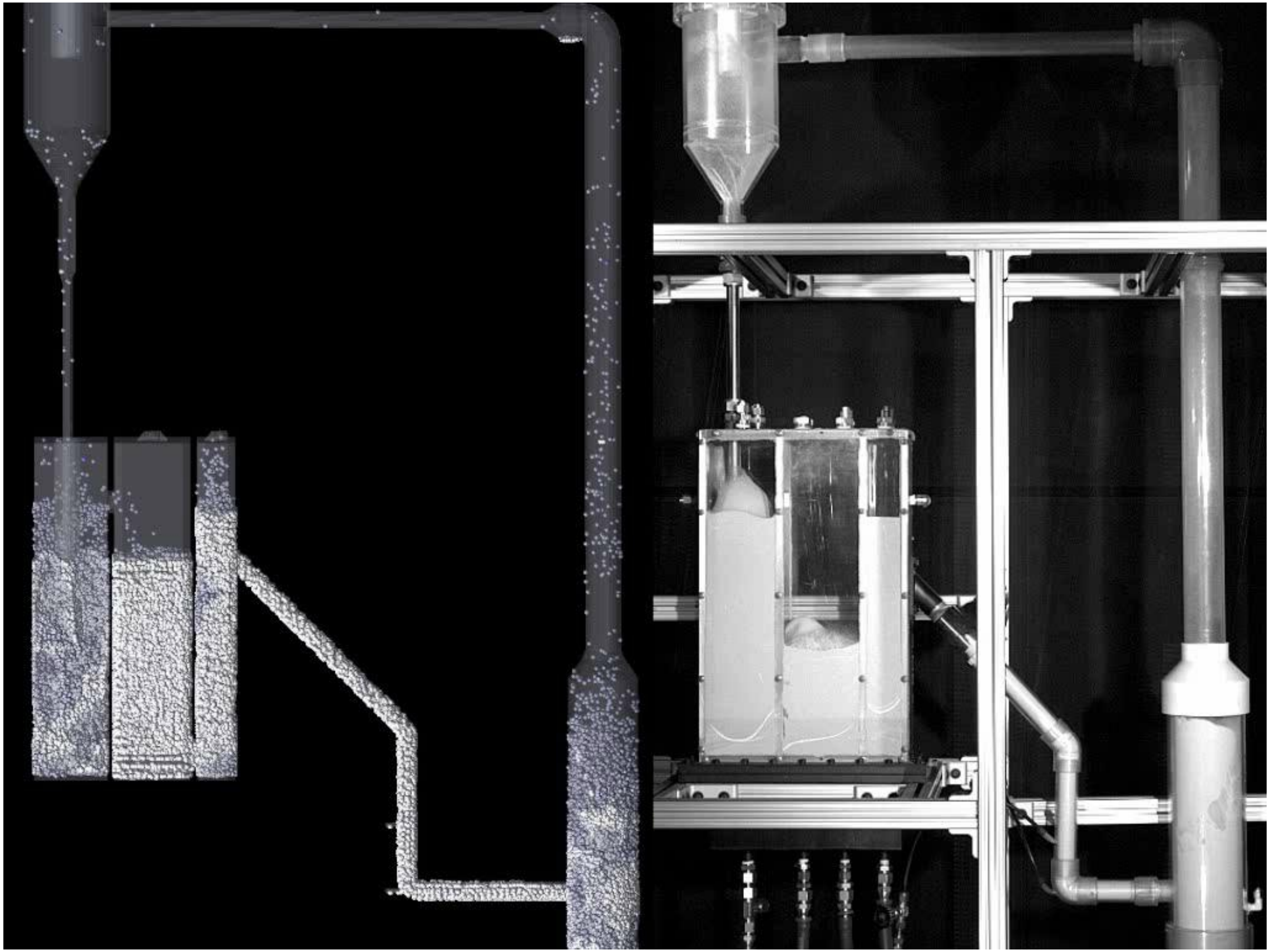
12in ECVT sensor on CFB

<u>Quantitative</u> measurement of bubble dynamics – unique validation data & important insight for chem looping reactors.





Comparison of CFD and Cold Flow Rig



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- **Attrition !**

- **Can multi-phase flow models be used to predict *<u>or prevent</u>* attrition in chemical looping systems?**

Summary

- **Multi-phase flow is a key to existing and future energy technologies:**
  - Entrained-flow, slagging gasifers
  - Fluid bed gasifiers for low-rank coal
  - Future CO2 sorbent capture systems
  - Future chemical looping systems

- **Progress and needs:**
  - Fundamental validation with reacting flow
  - Unsteady, transient behavior
  - Prediction of attrition