NATIONAL ENERGY TECHNOLOGY LABORATORY

Accelerating Commercialization and Deployment of Advanced Gasification Technology Through Multiphase Modeling

Chris Guenther[1], Ken Williams[2], Dale Snider[2], Sam Clark[2]

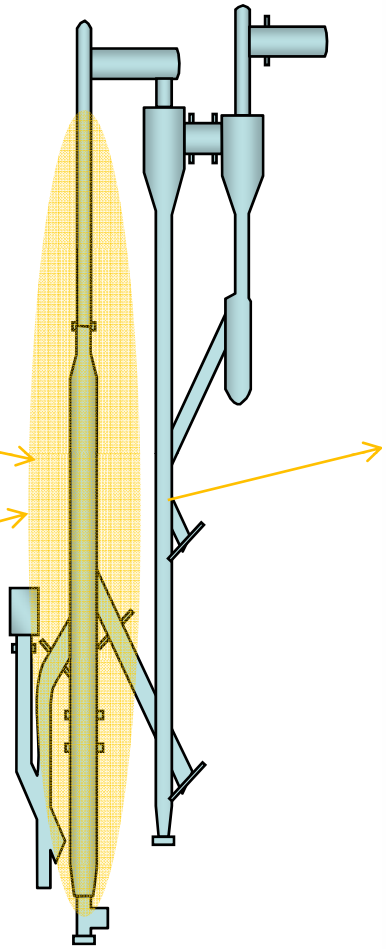
[1]National Energy Technology Laboratory (NETL), Computation Science Division

[2]Computational Particle Fluid Dynamics (CPFD) Software LLC

Gasification Technologies Conference, Oct. 31-Nov. 3, 2010 Washington, DC

Agenda

- **NETL Multiphase Activities**
- **Success Stories in Multiphase Modeling**
  - The role CFD can play in gasification
  - Transport gasifier
  - Hydrogasification
- **Current Multiphase Modeling Activities**
  - Chemical Looping
  - Sorbent based CO_2 capture
  - Additional areas of concentration
- **Questions**



MFIX validation and scale-up of a NCCC Transport Integrated Gasifier (gas temperature predictions of a commercial scale transport gasifier).

M Syamlal, Guenther C, Gel A, Pannala S, "High performance Computing: Clean Coal Gasifier Designs Using Hybrid Parallelization", Fluidization XIII, May 16-20, Gyeong-ju, Korea.

NETL Multiphase Activities

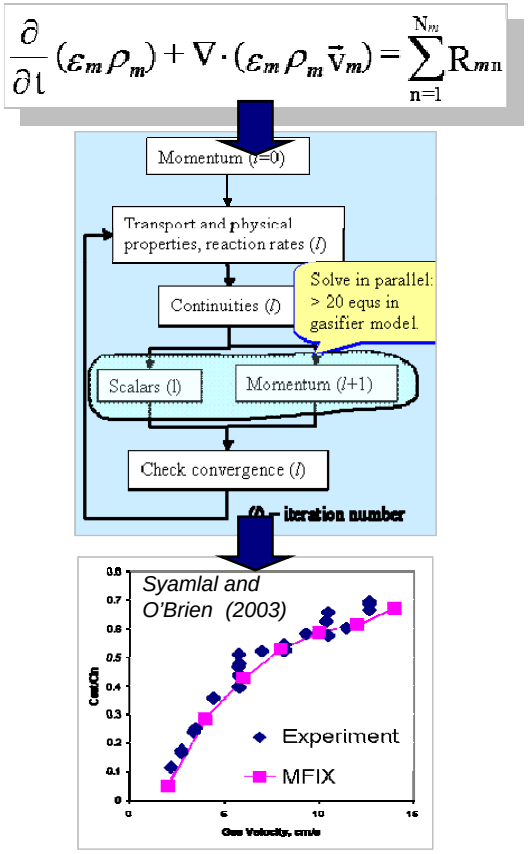
Advanced Gasification Team
Funding support through NETL's Gasification Technology Area: Program Manager Jenny Tennant

- **Biomass**
  - Frictional strengths and rheologies and gas transport characteristics for blended mixtures of coal-biomass under compactive stresses relevant to continuous feed systems will be evaluated.
  - Conduct mechanical property measurement of torrefied biomass materials and develop a correlation to grinding energy requirements.
- **Refractory**
  - Research and develop improved or new advanced gasification liner materials for entrained bed slagging gasifiers utilizing mixed carbon feedstocks (coal, petcoke, and/or biomass) and evaluate physical and thermodynamic properties of mixed carbon feedstock.
- **Co-Gasification Reactions and Kinetics**
  - Experimental measurement of pyrolysis and gasification rates for coal, biomass and coal-biomass mixtures for both transport and entrained flow gasification conditions
  - Development of coal/biomass kinetic data based for computational modeling
- **Device/Systems Modeling**
  - Dynamic process-level simulations for optimization and deployment of real-time dynamic simulators with full-scope operator training system
  - Multiphase CFD modeling (gasification, transport desulfurization), multi-scale modeling

NETL Multiphase Activities

Advanced Simulation Team
Funding support through NETL's Gasification, Advance Research, And Sequestration Technology Areas

- **Theory development**: drag relations, granular stress, chemistry models …
- **Numerics development**: solvers, high resolution schemes, hybrid discrete/continuum models, explicit schemes, parallelization, GPU acceleration,…
- **Computational Software development:** MIFX https://mfix.netl.doe.gov/ , *Carbonaceous Chemistry for Computational Modeling (C3M)*
- **Validation studies**: bubbling, circulating, and spouted beds, gas-solids jets, …
- **Reduced Order Model (ROM):** Fast models based on high fidelity models
- **NETL Multiphase Flow Workshop:** annual meeting with 100+ attendees from around the world representing government labs, academia, and industry



NETL Multiphase Activities: *Carbonaceous Chemistry for Computational Modeling (C_3M)*

Motivation

Currently gasification kinetics information taken from literature needs to be reprogrammed for different CFD and process simulation software.

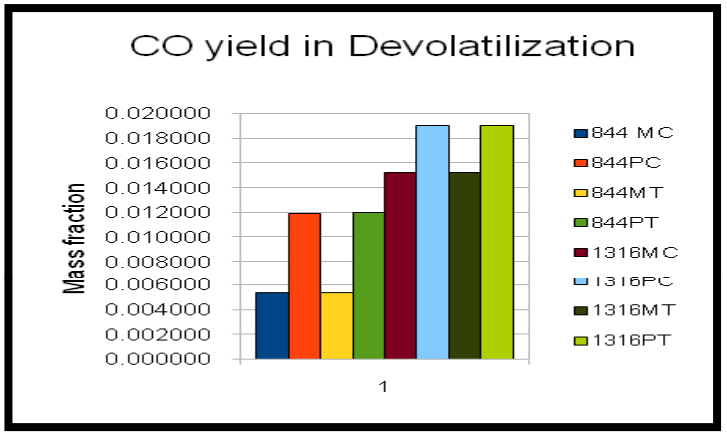
Goal

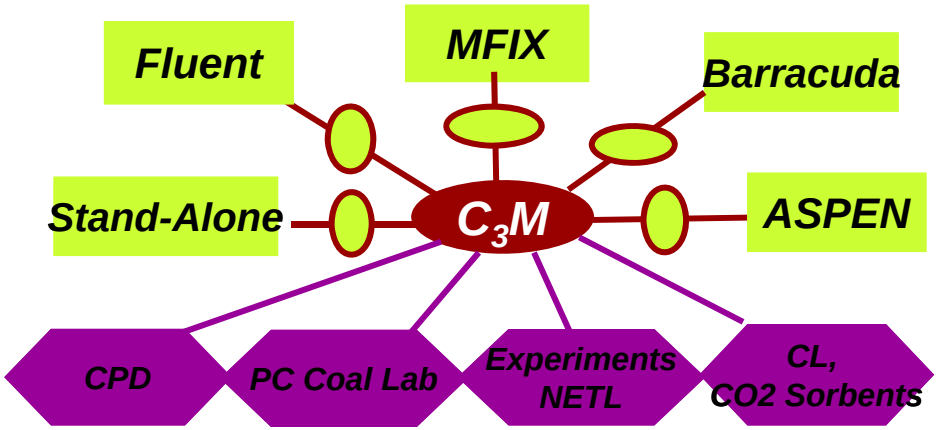
Develop a repository of data and unified interface such that CFD and process simulation software can access kinetic rates and yields for various coals and biomass

Current Status

A seamless connection between PC Coal Lab™, C_3M, and MFIX and FLUENT EE models has been developed for devolitization and tar chemistry and soot formation.

CO devolitization yields for 844 °C and 1316 °C from different kinetic sources



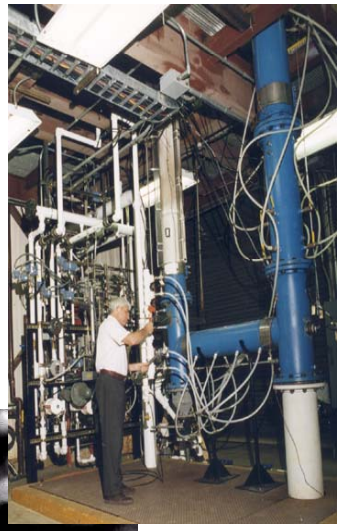


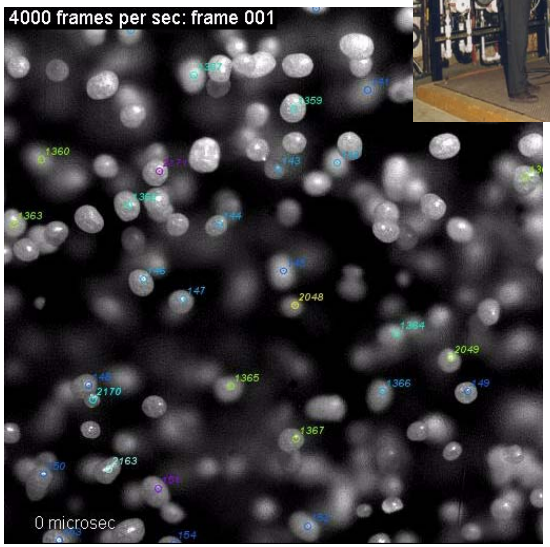
Architecture of C_3M

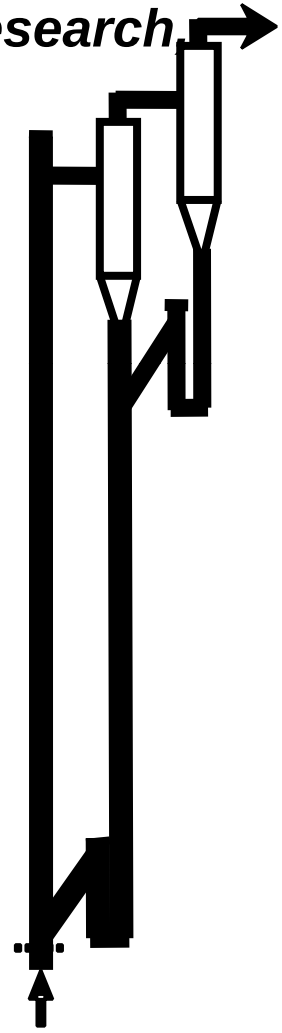
NETL Multiphase Activities

Other activities (Advance diagnostics and validation data)
Funding support through NETL's Gasification, Advance Research And Sequestration Technology Areas

- **Industrial scale and bench scale cold flow reactors**
  - Solids Circulation Rates
  - Optical probes
  - Capacitance Imaging System (Tech 4 ECVT)
  - High speed pressure transducers
  - LDV
  - Fiber Optic Probe
  - High Speed Particle Imaging Velocimetry



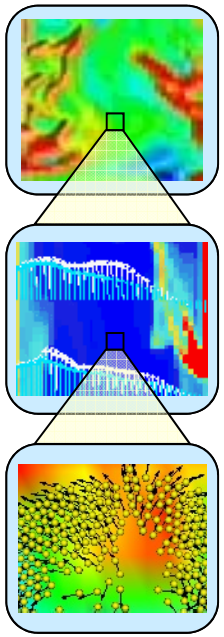




NETL Multiphase Activities

Other activities (UCR, HBCU, SBIR, FWP)
Funding support through NETL's Advance Research Area: Program Manager Robert Romanosky

- **University Coal Research (UCR's)**
  - Colorado University (Polydispersity for EE models)
  - University of Michigan (Horizontal jet studies: experiments and modeling)
  - UC-Merced (Radiation sub-models for gas-solids applications)
- **Historically Black Colleges and Universities (HBCU's)**
  - UT-San Antonio (DNS solver)
- **Small Business Innovative Research (SBIR's)**
  - CPFD-Barracuda (GPU acceleration)
- **Field Work Proposals (FWP's)**
  - Iowa States, Ames Laboratory (Multiphase CFD model development)
  - Oak Ridge National Lab (Multiphase CFD model development)



Three scales of description in NETL's multiphase code MFIX: discrete particles to continuum to filtered-continuum models

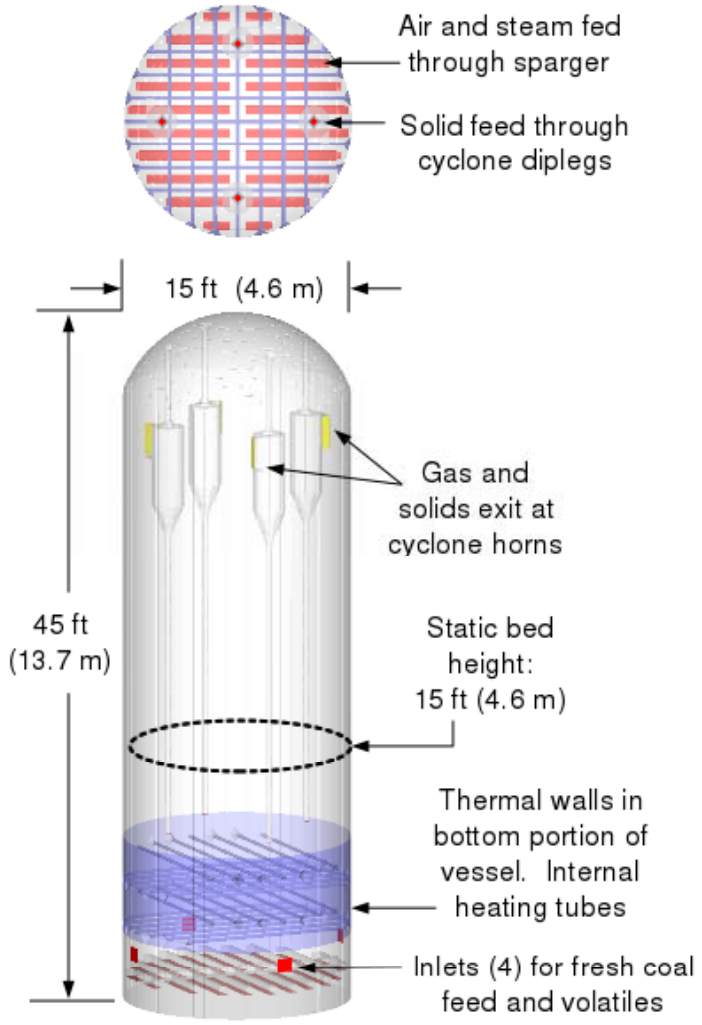
Multiphase Modeling: The role of CFD

CPFD-Barracuda Demonstration Simulation

- *Performed as a demonstration of currently available modeling capabilities.*

- *Features:*
  - *Transient, 3D, commercial-scale geometry*
  - *Complex internals: gas sparger, heating tubes, cyclones*
  - *Thermal + chemistry*
  - *Full PSD for solids*

- *Publication is pending.*

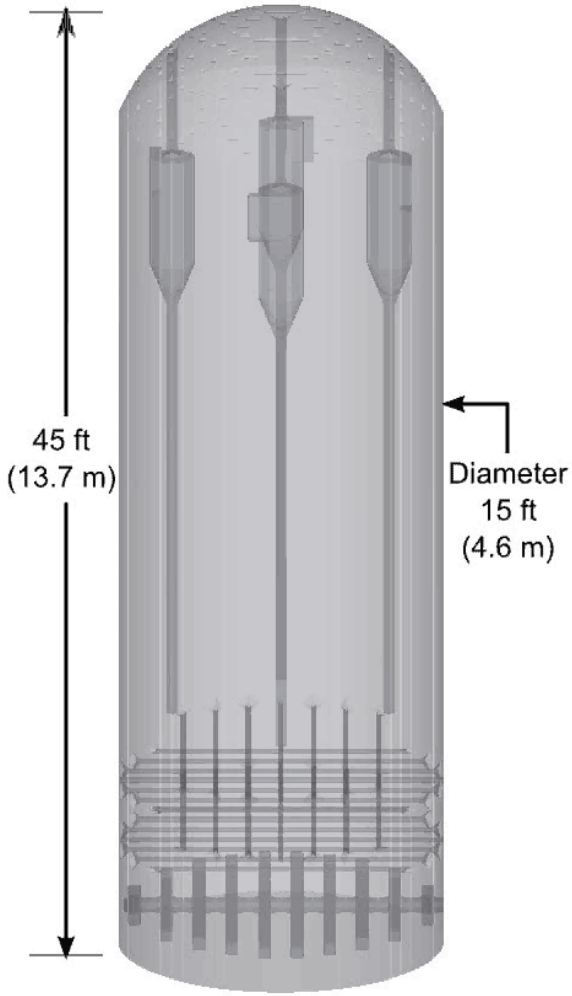


Multiphase Modeling: The role of CFD

CPFD-Barracuda Demonstration Simulation

- *If this were an operating unit, what would you know about how it is running?*
  - *Temperature readings*
  - *Pressure readings*
  - *Gas compositions from cyclones*

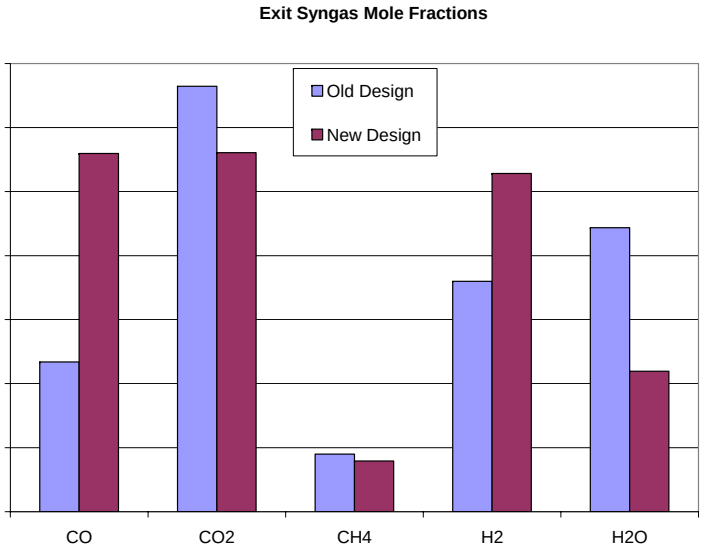
- *What can the simulation help us learn?*
  - *Gas-solids flow patterns*
    - *Formation of stagnant particles above central sparger arm*
    - *Gas tends to flow around rather than through these particles*
  - *Hot-spots from chemistry*
    - *Hottest near sparger due to carbon combustion*
  - *How to improve performance*
    - *Different sparger design could help*

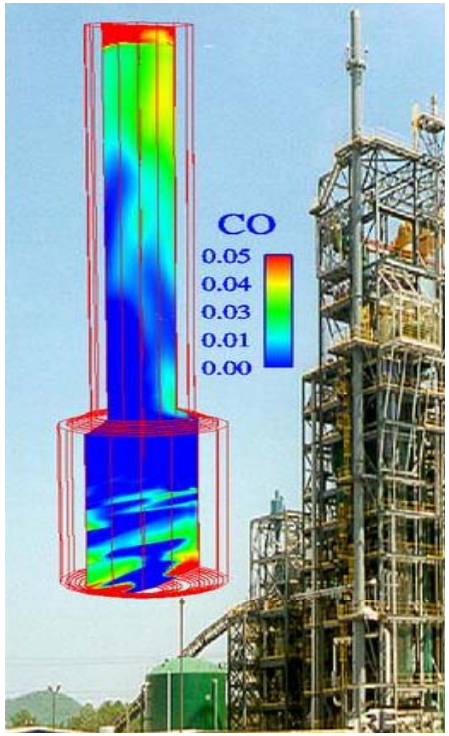


Multiphase Modeling:Transport Gasifier

National Carbon Capture Center at the Power Systems Development Facility (PSDF), Wilsonville, Alabama, Transport Integrated Gasifier (TRIG)

- **Validation**
  - Bituminous, sub-bituminous and lignite coals under both air and oxygen blown conditions
    - Pressure , axial temperature, exit syngas
- **Model predictions later confirmed experimentally**
  - Oxygen break through
  - **Exit effects**
  - **Reactor design**





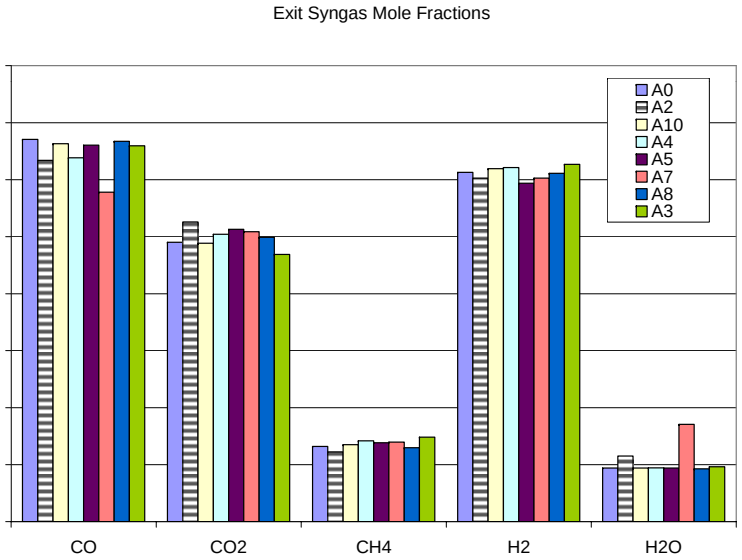
Exit effects: High CO levels at the exit region inside the NCCC-TRIG, Wilsonville, Alabama

Reactor Design: Model predictions showed clustering and downflow along The wall which resulted in longer residence times and improved mixing

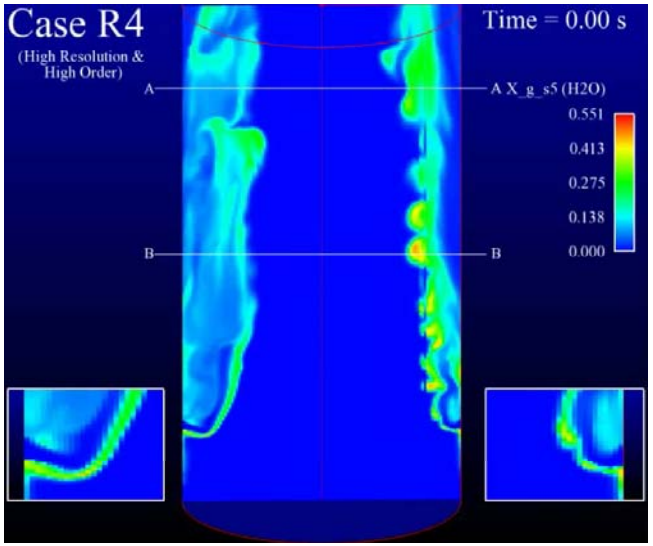
Multiphase Modeling: Transport Gasifier Scale-Up

Scale-up of the NCCC'sTransport Integrated Gasifier (TRIG) Model

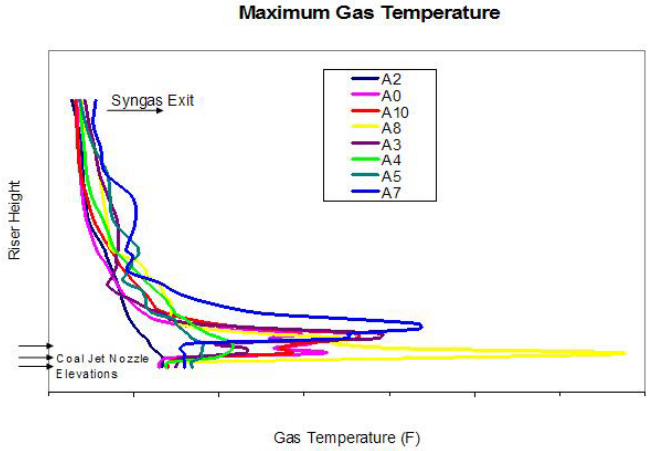
- L/D parametric study
- Coal feed rate
- Solids circulation rate
- Effect of recycled syngas
- Effect of coal jet penetration



[M. Syamlal, Guenther C, Cugini A, Ge W, Wang W, Yang N, and Li J, "Impact of computational science on technology development", Accepted International Journal for Computational Science, 2010.

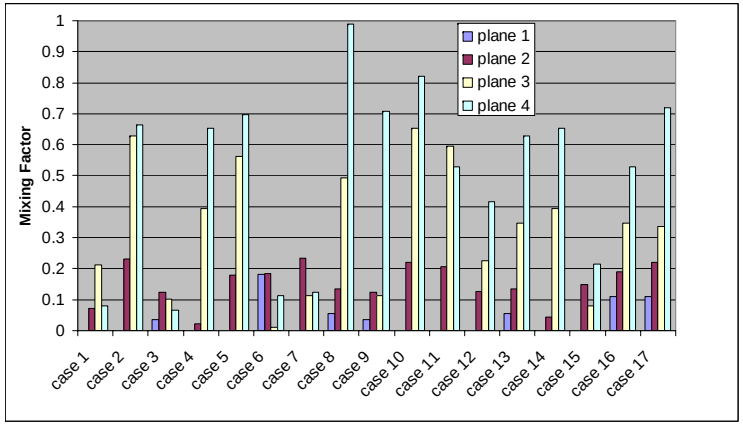


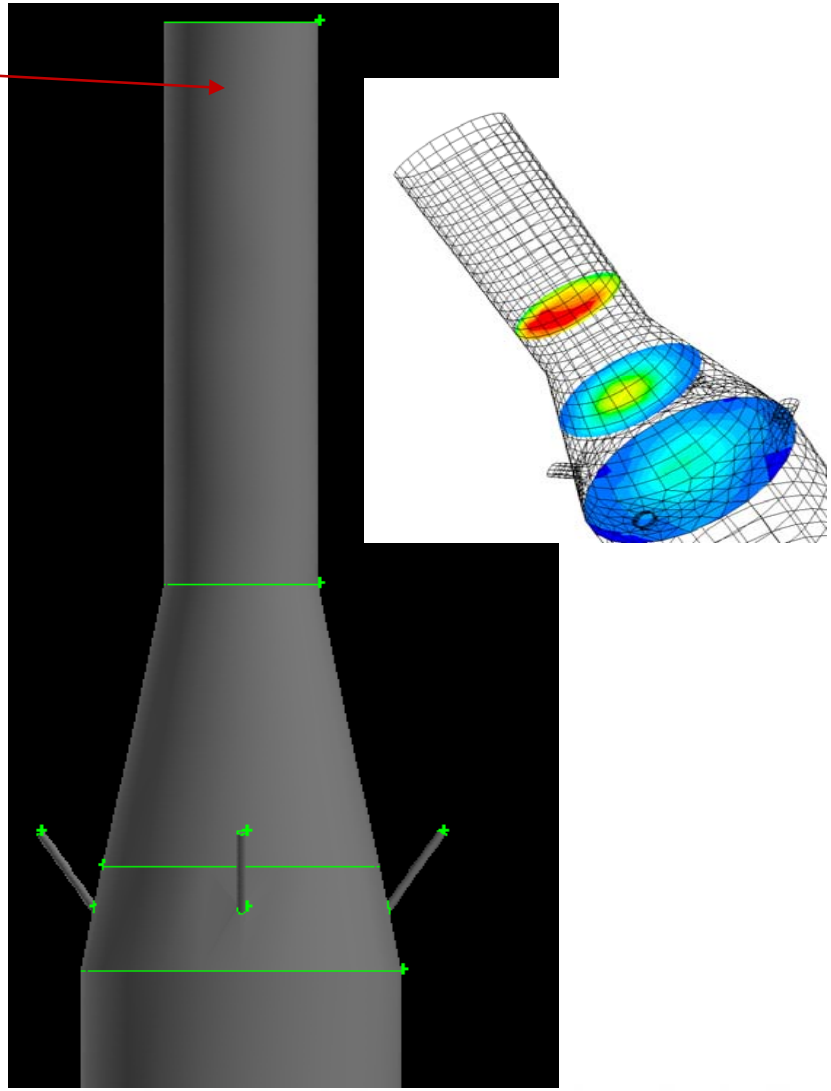
Coal jet penetration study (INCITE Award): Mass fraction of steam
A. Gel, Pannala S, Sankaran R, Guenther C, Syamlal M, and O'Brien T, "Accelerating Clean Coal Gasifier Designs with Hybrid MPI/OpenMP High Performance Computing", Proceedings of the 21st International Conference on Parallel Computational Fluid Dynamics, May 18-22, 2009, Moffett Field, CA. pp: 224-228.



Multiphase Modeling: Hydrogasification

- **Hydrogasifier model used to answer preliminary design questions**
  - Single wall design
  - Double wall design
- **Proprietary set of kinetics implemented into NETL's Carbonaceous Chemistry for Computational Modeling (C3M)**
- **CFD model developed for the design of Arizona Public Service's Hydrogasifier**
  - Model based on C_3M, MFIX and FLUENT
  - Simulations conducted based on different parameters: shooting angle, swirl, coal and H_2 feed rates, and nozzle ID
  - Statistical analysis of CFD results using solids flux and temperature as response variables
- **Final bench scale design parameters selected based on CFD analysis**
  - Large H_2 nozzle ID, 45º Downward H_2 injection
  - 30º degree swirl for improved mixing
  - Low H_2/Coal ratio





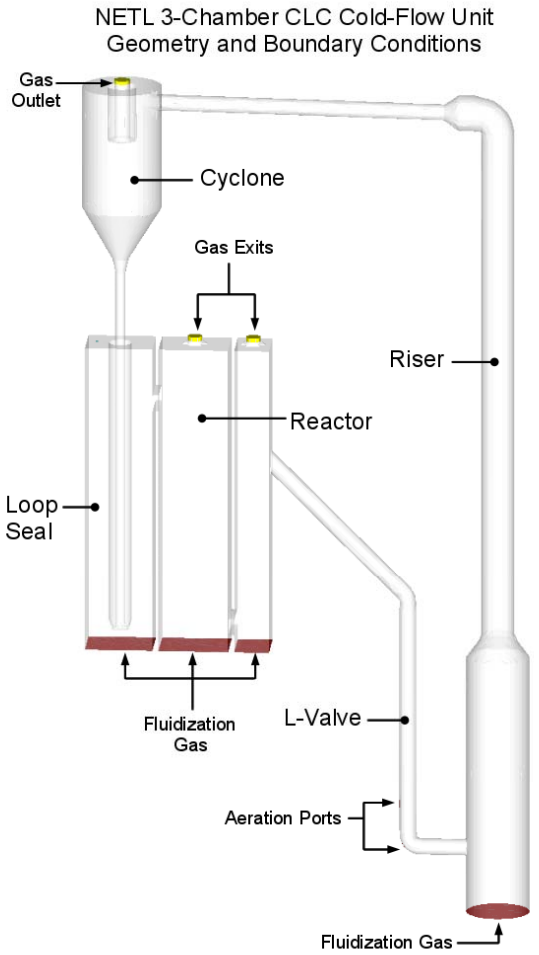
NETL's Chemical Looping Experiment

Experimental Unit at NETL

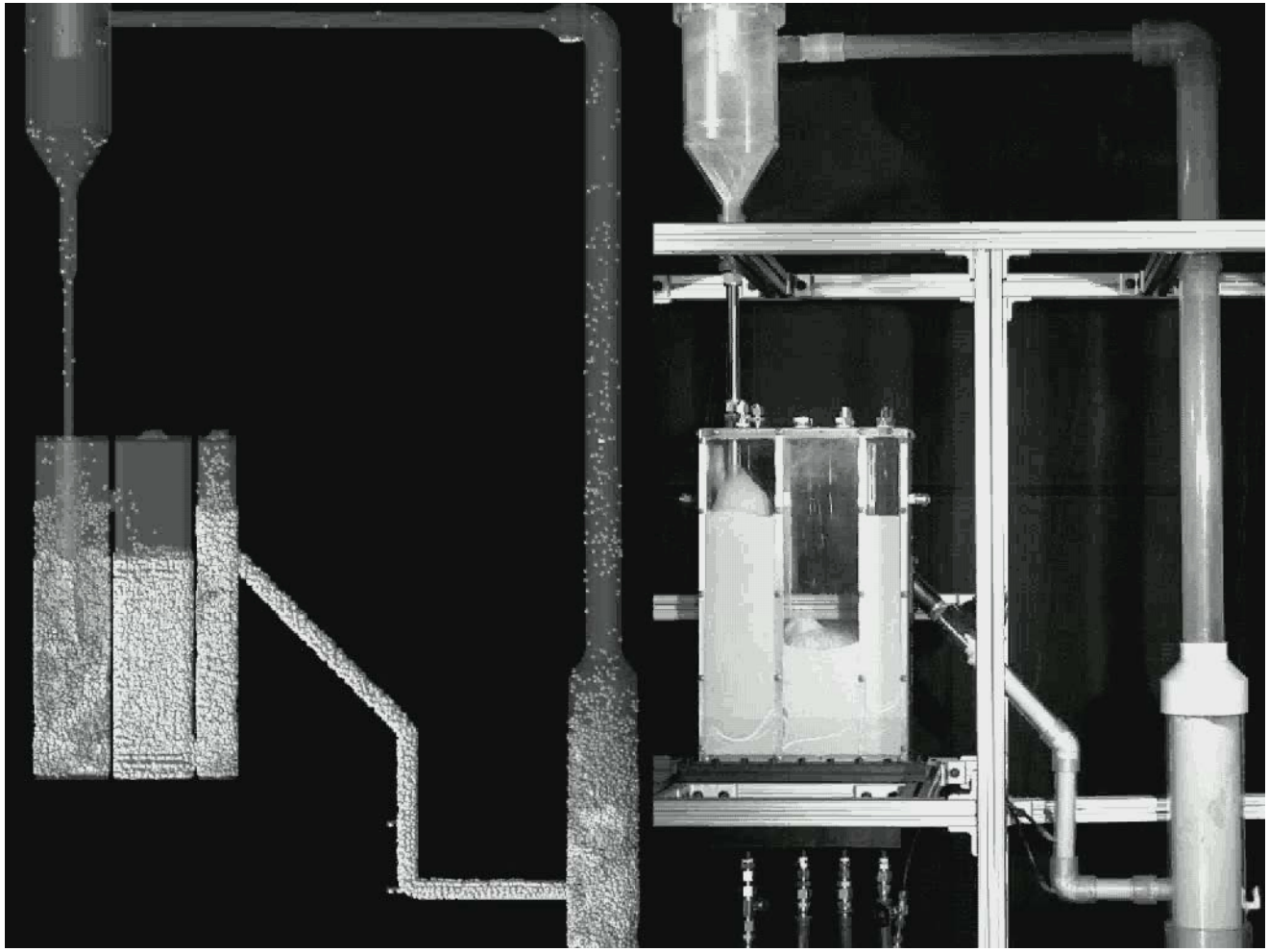
- *3-Chamber, transparent, cold-flow unit to test fluidization behavior.*
- *Useful for validation of simulation results, since flow behavior can be compared visually.*

Barracuda Simulation

- *Full loop, complete system, transient, 3D, isothermal, no chemistry.*
- *Full particle size distribution (PSD)*
- *Simulation success stories:*
  - *Simulations capture qualitatively all the different flow regimes (frictional, turbulent, transport, dilute, …)*
  - *Identified plugged pressure outlet on middle chamber*
  - *Identified solids backing up in cyclone dipleg*
- *Current in-progress work : compare simulation results with pressure, HSPIV, and ECVT measurements.*



CL: Side-by-Side Video Comparison



D. Snider, Guenther C, Dalton J, Williams K., "CPFD Eulerian-Lagrangian Numerical Scheme Applied to the NETL Bench-top Chemical Looping Experiment", 1st International Conference on Chemical Looping, Lyon, France March 17-19, 2010.

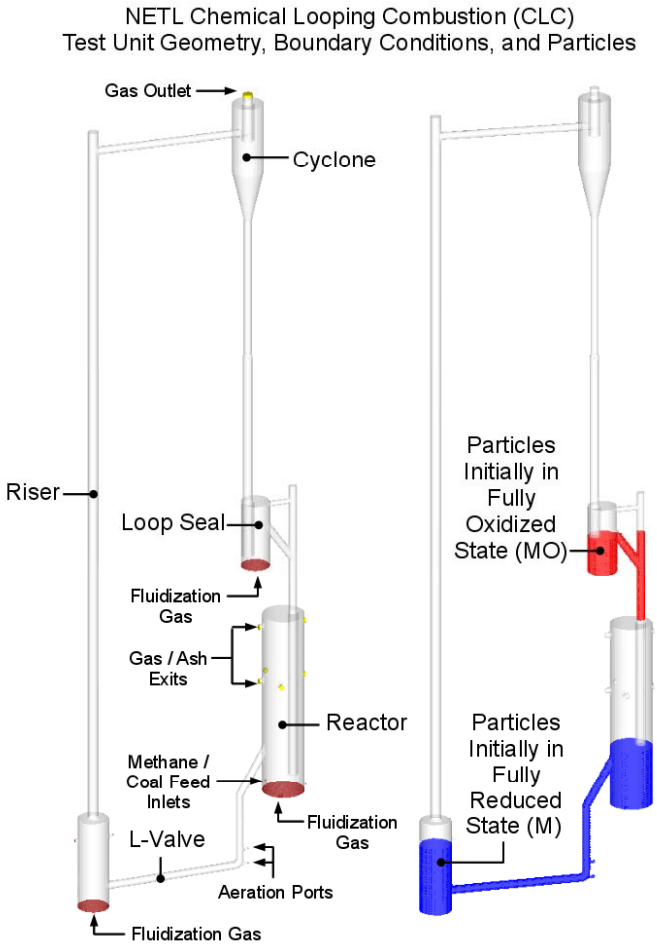
Planned Hot-Flow CL Experiment

Planned Experimental Unit at NETL

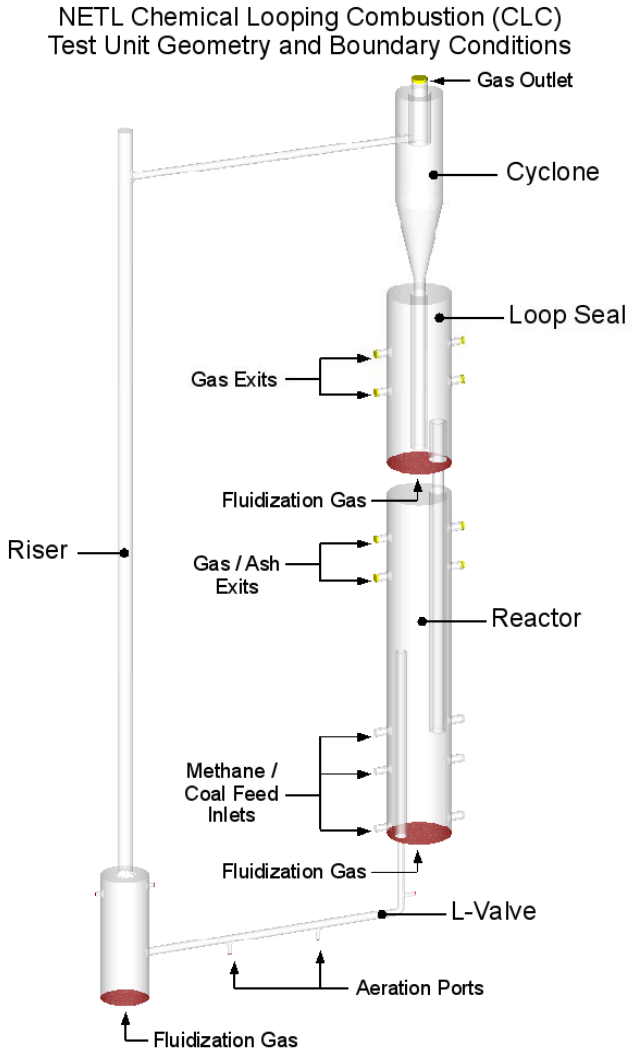
- *Bench-scale, hot-flow unit to test CL chemistry and kinetics.*
- *Will be instrumented for comparison of experimental data with simulation results.*
- *Design phase completed*

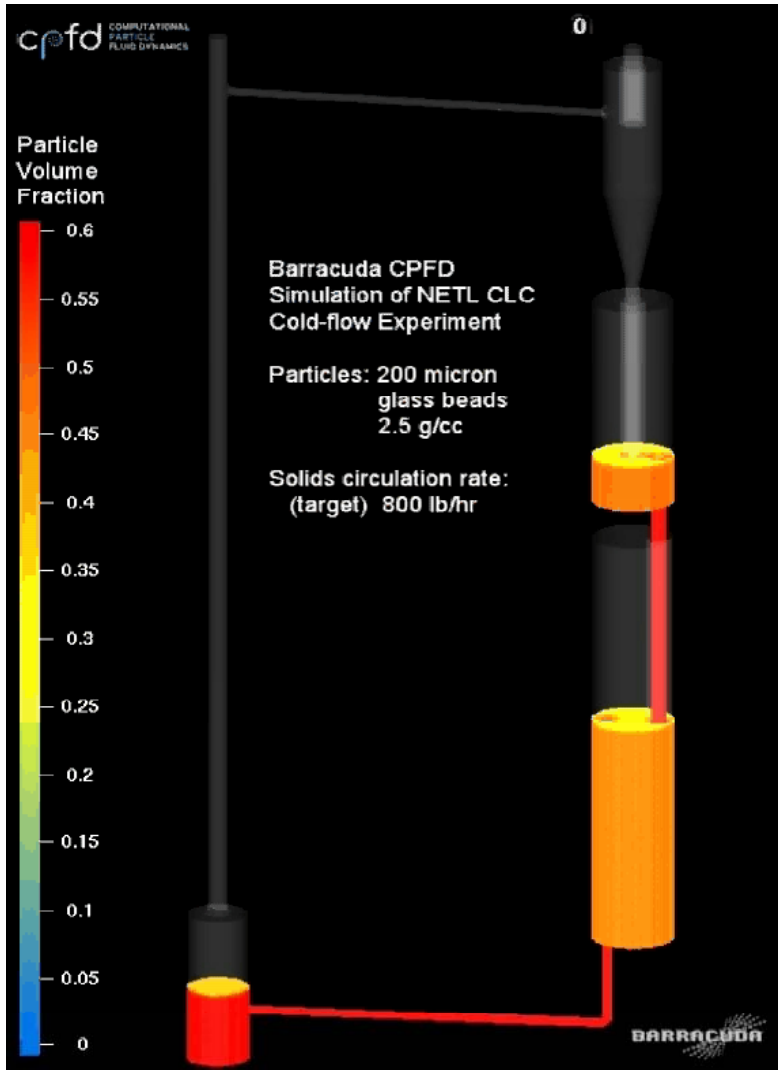
CPFD-Barracuda Simulation

- *Initial simulations:*
  - *Full loop, complete system, transient, 3D, isothermal, no chemistry.*
  - *Full particle size distribution (PSD)*
  - *Studied fluidization behavior without chemistry and results used in the design cycle.*
- *Current in-progress work: add chemical reactions, use multi-material particles as oxygen carriers.*



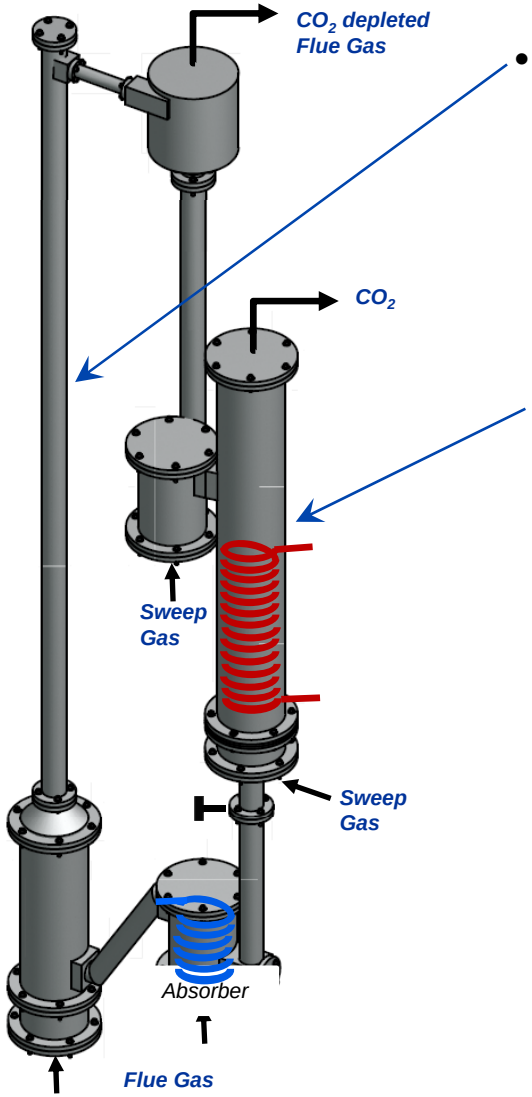
Initial Simulations of Hot Flow CL Experiment





NETL's Carbon Capture Unit (C2U)

Bench scale circulating fluidized bed with energy management



- **Adsorber**
  - Bubbling bed, long residence times ww/o heat ex.
  - Sufficient pressure head for solids transport
  - Cyclone – Gas/particle separation
- **Regenerator**
  - Fluidized Bed
  - Sorbent minimally fluidized with sweep gas (nitrogen, CO2, or air)
  - Heated interior tubes.
- **Adsorber/Regenerator Solids Return Loopseals**
  - Segregates flue gas from enhanced CO_2 stream

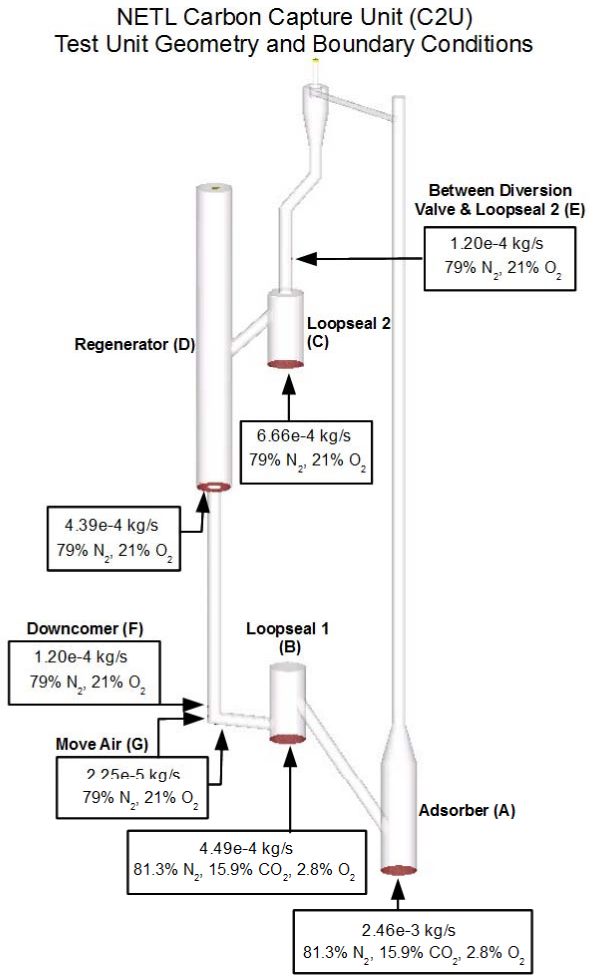
NETL's Carbon Capture Unit (C2U)

Experimental Unit at NETL

- *Bench-scale, hot-flow unit to test sorbents for carbon capture.*
- *Will be instrumented for comparison of experimental data with simulation results.*
- *C2U under fabrication*

CPFD-Barracuda Simulations

- *Current simulations are in-progress:*
  - *Full loop, complete system, 3D, isothermal, no chemistry.*
  - *Full particle size distribution (PSD)*
  - *Goal: study fluidization behavior without chemistry.*
- *Future work:*
  - *Add chemical reactions.*
  - *Use multi-material particles as sorbents.*



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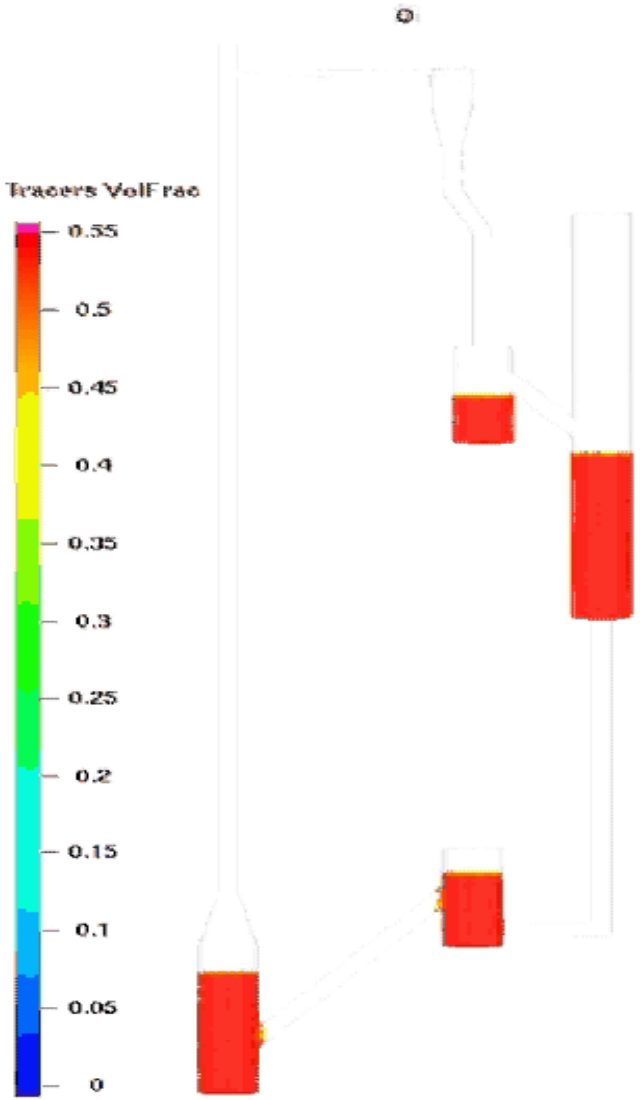


NETL Dynamic Simulator Research & Training Center

- Located at NETL & WVU/NRCCE
- R&D, education, and training for design, operation, and control of advanced energy systems
- Real-time dynamic simulators w/ operator training systems (OTS)
- Immersive training systems (ITS)
- IGCC plant with CO_2 capture
  - OTS: Dec 2010; ITS: Mar 2011
- NETL collaborators
  - WVU, FCS, Enginomix, EPRI
  - AEP, BP, Doosan, GRE, Southern, …
  - Invensys Operations Mgmt
    - Dynsim™, InTouch™, EYESim™

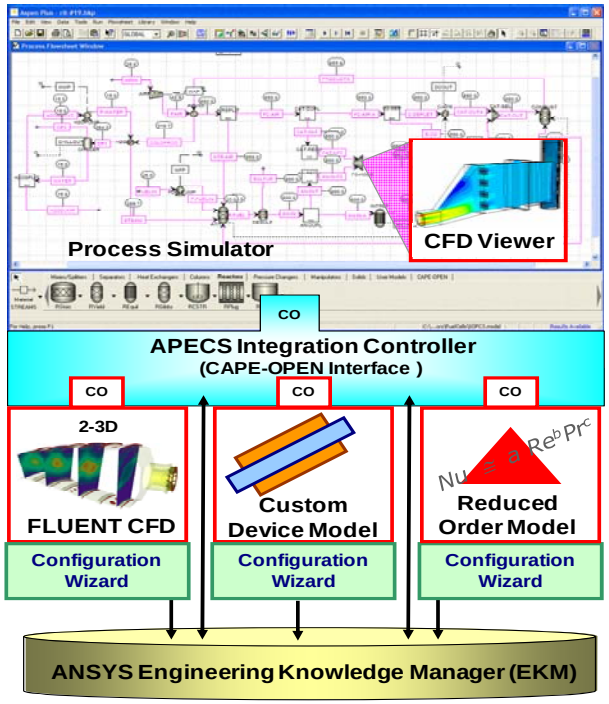
Zitney, S.E. and D. Wilbers, "NETL Advances Clean Coal Power Technology Utilizing Virtual Reality Training System," Presented at 2010 Power Plant Simulation Conference, February 21-26, San Diego, CA (2010).

Zitney, S.E. et al., "NETL to Establish Dynamic Simulation Research and Training Center to Promote IGCC Technology with CO_2 Capture," Proc. of the COAL-GEN 2009 Conference, August 19-21, Charlotte, NC (2009).

Advanced Process Engineering Co-Simulator (APECS)

High-Fidelity Design and Optimization of Energy Plants

- Process/CFD co-simulation
- CAPE-OPEN software standard
- ANSYS® Engineering Knowledge Manager™ (EKM™)
- Reduced order models (ROMs)
- Hybrid solution strategies
- Equipment design optimization
- Remote/parallel CFD execution
- CFD viewer for 2-3D analysis
- Optimization of plant performance wrt complex thermal and fluid flow



Recent Publication

Zitney, S.E., "Advanced Co-Simulation for Computer-Aided Process Design and Optimization of Fossil Energy Systems with Carbon Capture," FOCAPD 2009, Eds. M. M. El-Halwagi and A. A. Linninger, June 7-12, Breckenridge, CO, pp. 185-202 (2009).

R&D100 and FLC Awards

- ***2004 R&D100 Award (APECS)***
- ***2006, 2007 FLC Tech Transfer Awards (APECS)***
- ***2008 R&D100 Award (APECS with EKM)***
- ***2009 R&D100 Award (VE-PSI)***
- ***2009, 2010 FLC Tech Transfer Awards (VE-PSI)***

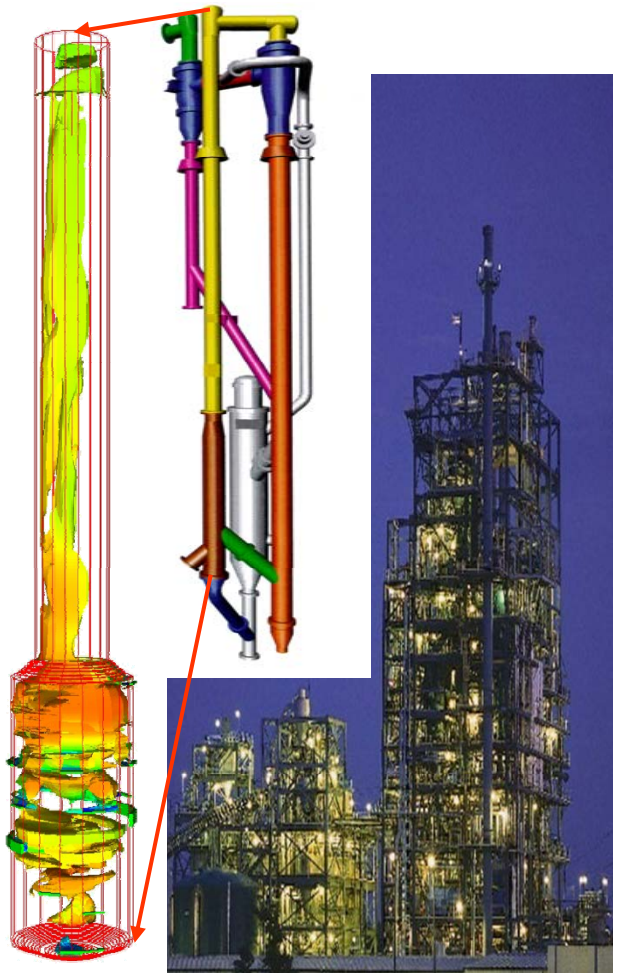
Summary

How can multiphase CFD models help advance gasification technology?

•Takes you beyond the limits of practical experiments.

• Can provide information on unexpected phenomena.

•Trouble-shoot, design, scale-up and optimize a device/process



Thank You!