Industrial Applications of CFD for Clean Coal Plant Design

Optimization, Reliability Improvement and Emissions Reductions

NETL Workshop on Multiphase Flow Science

August 6-7, 2013

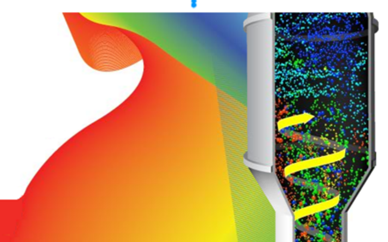
BARRACUDA VR®

Kenneth A. Williams, PhD, PE

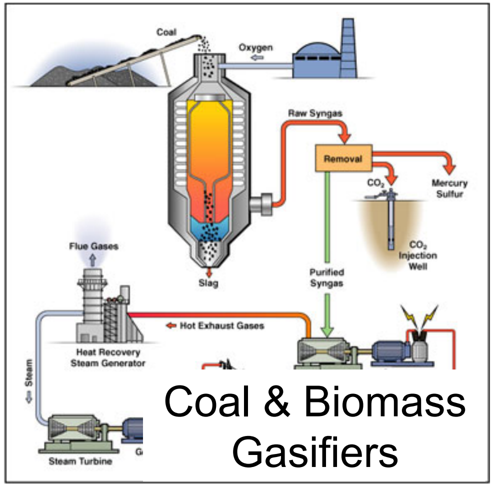
CPFD Software, LLC

Albuquerque, NM USA

cpfd COMPUTATIONAL PARTICLE FLUID DYNAMICS

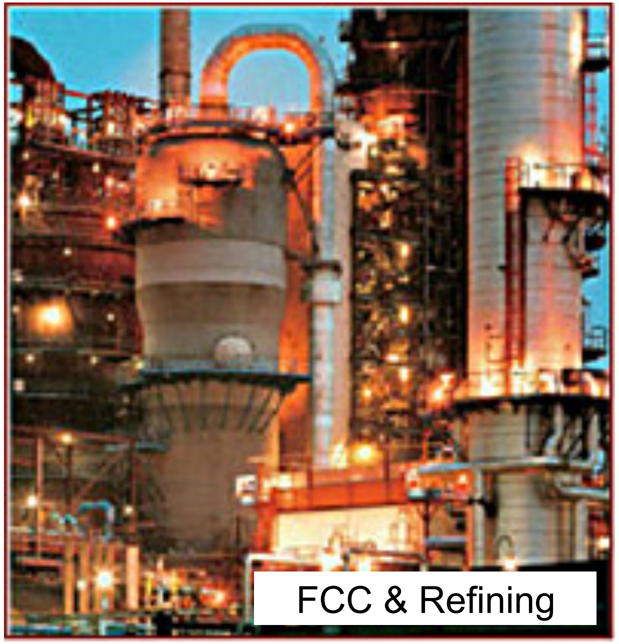


Why are particle flows in Fluidized Bed Reactors (FBRs) of such commercial importance?



Coal & Biomass Gasifiers

PV Materials Production



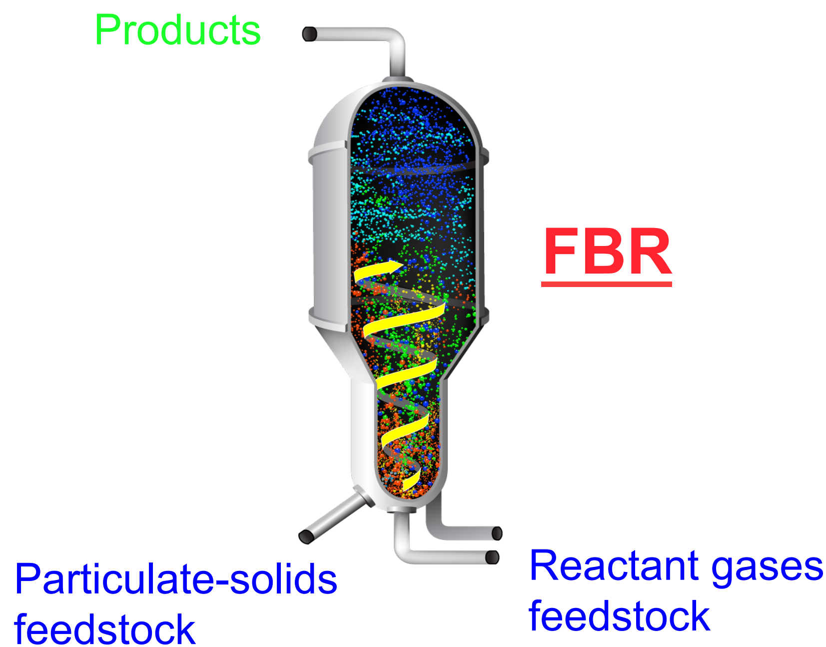
FCC & Refining

CFB Coal Power Plants

Chemical Manufacturing

Commercial CAE for FBRs - Barracuda Virtual Reactor®

- **What is Barracuda VR ?**
  - ✓ A physics-based 3D virtualization and simulation software package capable of *predicting* all fluid, particulate, thermal and chemically reacting behavior inside a fluidized bed reactor (FBR)
- **What does a FBR produce?**
  - ✓ Gasoline; diesel; jet fuel
  - ✓ Plastics; polypropylene; nylon 6-6; polyethylene
  - ✓ Coal & biomass combustion – heat or syngas
  - ✓ Metals refinement: gold; titanium; polysilicon (PVs)
  - ✓ Carbon capture / gas cleanup scrubbing
- **How is Barracuda VR used?**
  - ✓ Reactor operations troubleshooting
  - ✓ Reactor reliability and 'yield' improvements
  - ✓ Reactor scale-up
  - ✓ Reactor new design or feedstock change-out
  - ✓ Reactor emissions reductions
- **What is Barracuda VR value to Industry**
  - ✓ Addresses multi-million dollar issues
  - ✓ Oil refinery shutdown: $1MM per day
  - ✓ Refinery emissions control: $20-100 MM per unit
  - ✓ Elimination of a pilot plant: $150-250MM

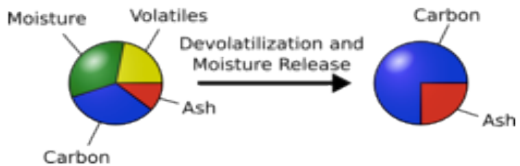


Barracuda VR® – A physics-based "Virtual Reactor"

Multi-material particulate solids with discrete-particle chemistry

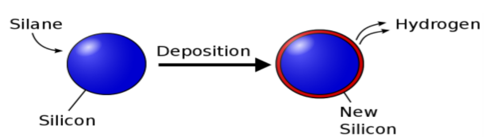
Coal & Biomass Gasification

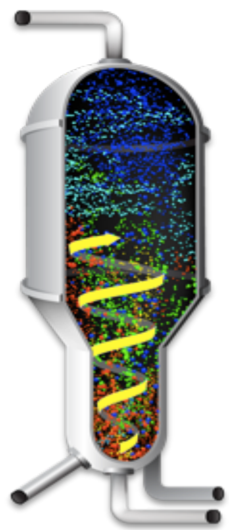
- Multi-media particles allow any coal composition to be accurately modeled
- Include temperature-dependent devolatilization CH_4, CO, H_2O



Polysilicon FBRs

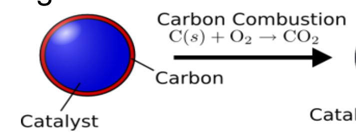
- Particle-level CVD chemistry for silicon deposition from silane or trichlorosilane in a fluidized bed reactor
- Model heating and cooling requirements for the fluidized bed
- Model direct or hydrochlorination FBRs





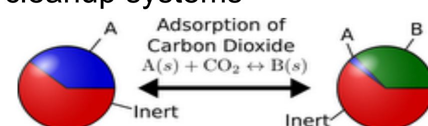
FCC Catalyst

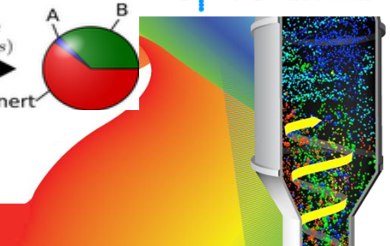
- Discrete particle-level chemistry calculates coke burn-off from spent catalyst during regeneration, and can help reduce NOx / SOx levels with a full-scale regenerator model



Carbon Capture & Gas Cleanup

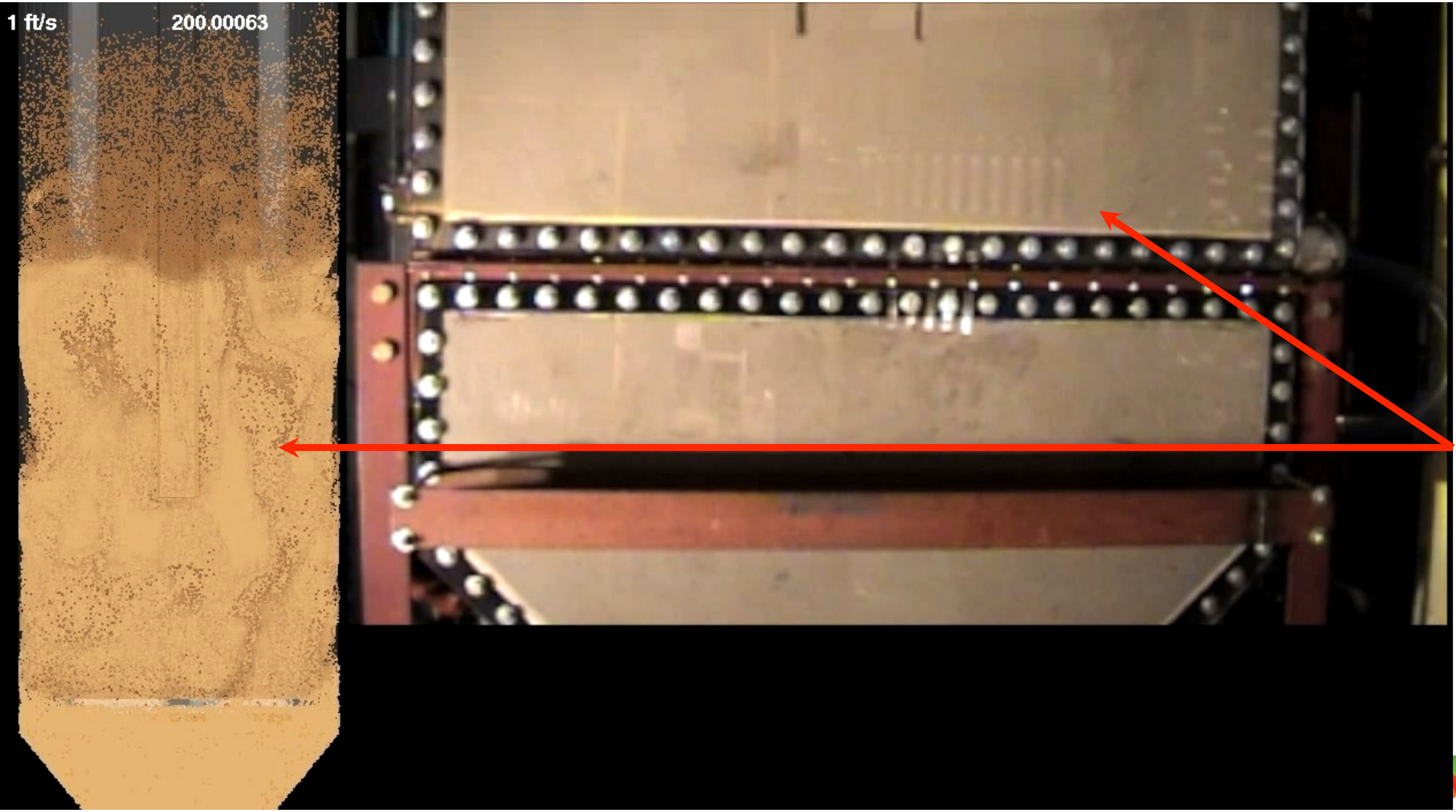
- Model adsorption of gases onto sorbent solids with multi-material particles and particle level chemical kinetics
- Model full-loop CO_2 capture systems
- Optimize sorbent regeneration in sulfur cleanup systems





CFD must be well Validated and with large-scale Experimental Data

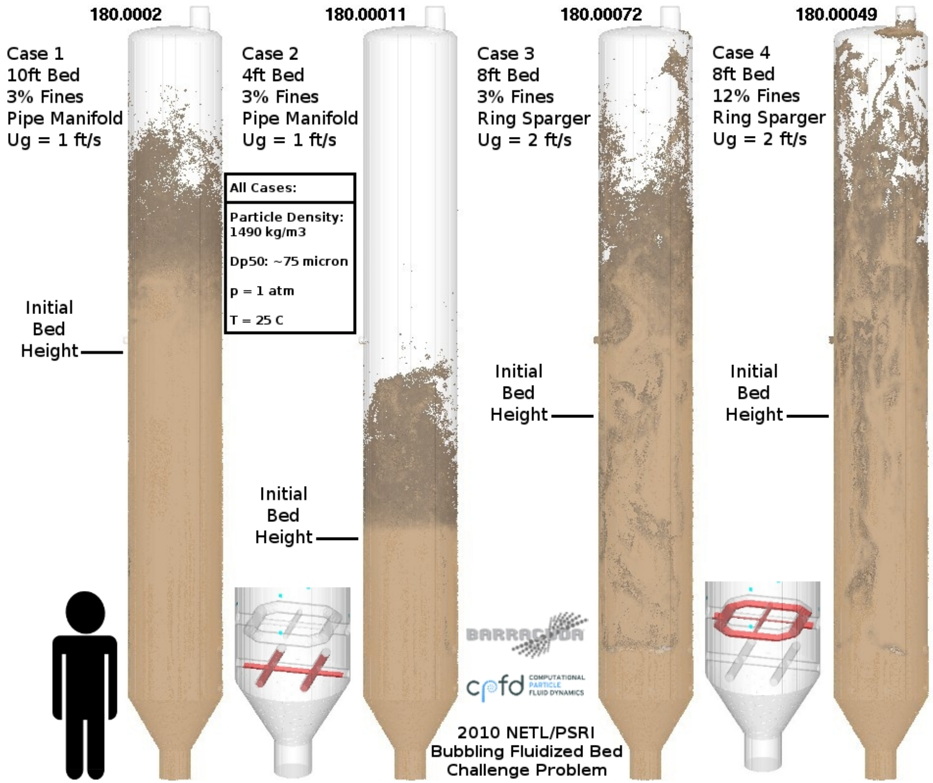
- Particulate Solid Research Inc. (PSRI)
  - www.psrichicago.com
- Extensive experimental facilities
- Deep-bed units, with a variety of powder types, often ‘Group A’
- Results widely published
  - T. Knowlton, R. Kerri, R. Cocco
- CPFD Software is Member Company
  - Model development, Validation



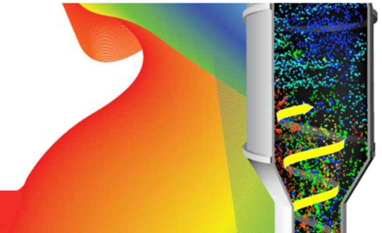
Gas streamers form at walls and can penetrated entire bed height

Barracuda® prediction of gas streamer in PSRI Fluidized Bed Experiment (2008)

CPFD participated in U.S. DOE 2010 'Challenge Problem' Bubbling Fluidized Bed

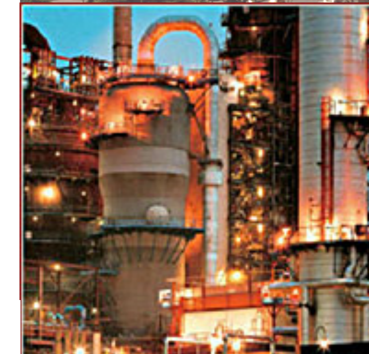


- Experimental data were provided by PSRI for the purpose of validation CFD software worldwide
- Vessel was 3-foot in diameter with a deep bed
- Range of gas velocities: 1 ft/s and 2 ft/s
- Range of static bed heights
- FCC particles with the 'fines content' (diameter < 44 microns) varying from 3% to 12%
- Data revealed a significant effect on fluidization mode from variations in particle size distributions (PSD), that is 'fines content'
- Barracuda results submitted to US DOE for pressure variation in the bed, surface, and freeboard



Industrial Fluidization Case Studies

- Case 1: Biomass-fired CFB Boiler: Erosion Minimization, Strongoli, Italy
- Case 2: 250MW CFB Furnace: Flow Maldistribution in Deep Bed, Duisburg, Germany
- Case 3: Sorbent-based Warm Syngas Clean-up System: Design Optimization of Regeneration Process with Sorbent Chemistry, Florida, USA
- Case 4: Biomass and MSW Gasifiers: Validation, Design and Optimization Study, USA



Case Study #1: CFB Combustor Primary Loop Erosion

- The overall objective of this work was to assist the plant operator, Biomasse Italia SpA, to choose effective design modifications to reduce erosion damage at multiple locations in the CFB units operating at the Strongoli plant.
- This work was undertaken in three stages:
  1. **Baseline analysis** – understand current erosion and the 3D, transient, multiphase flow inside the current design
  2. **Design Alternatives Assessment** – model several alternatives for each component to understand effects of potential changes on erosion
  3. **Redesign Assessment** – evaluate the candidate final redesign, which may include several components of different design alternatives
- The primary evaluation criteria are:
  - Minimizing erosion due to particle impingement on surfaces
  - Maximizing cyclone efficiency, which relates directly to erosion on suspension tubes
  - Ensuring proposed changes do not lead to detrimental flow behavior within the system
  - Ensuring proposed changes do not create problems with heat transfer in the FBHE

Example Courtesy of:

BiomasseItalia

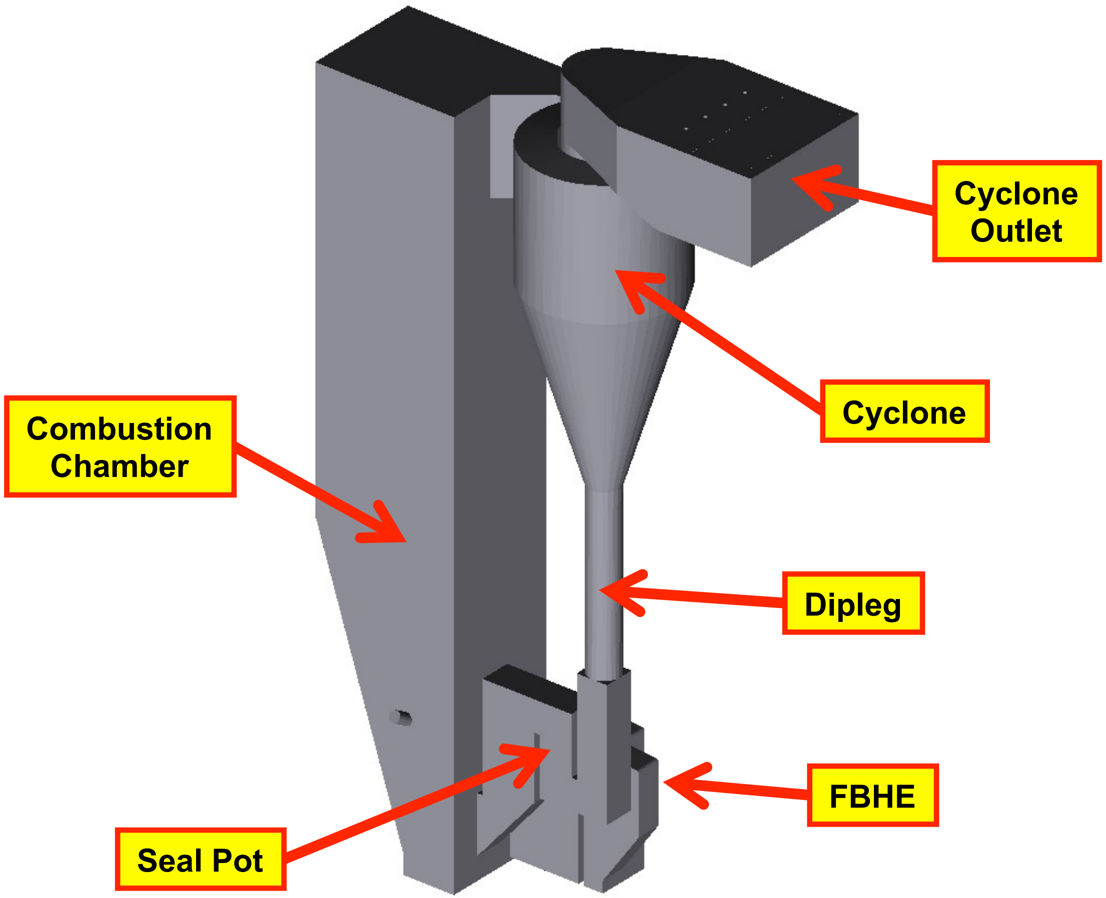
Erosion Damage in Strongoli CFB Plant

Cyclone Inlet

Fluidized Bed Heat Exchanger (FBHE)

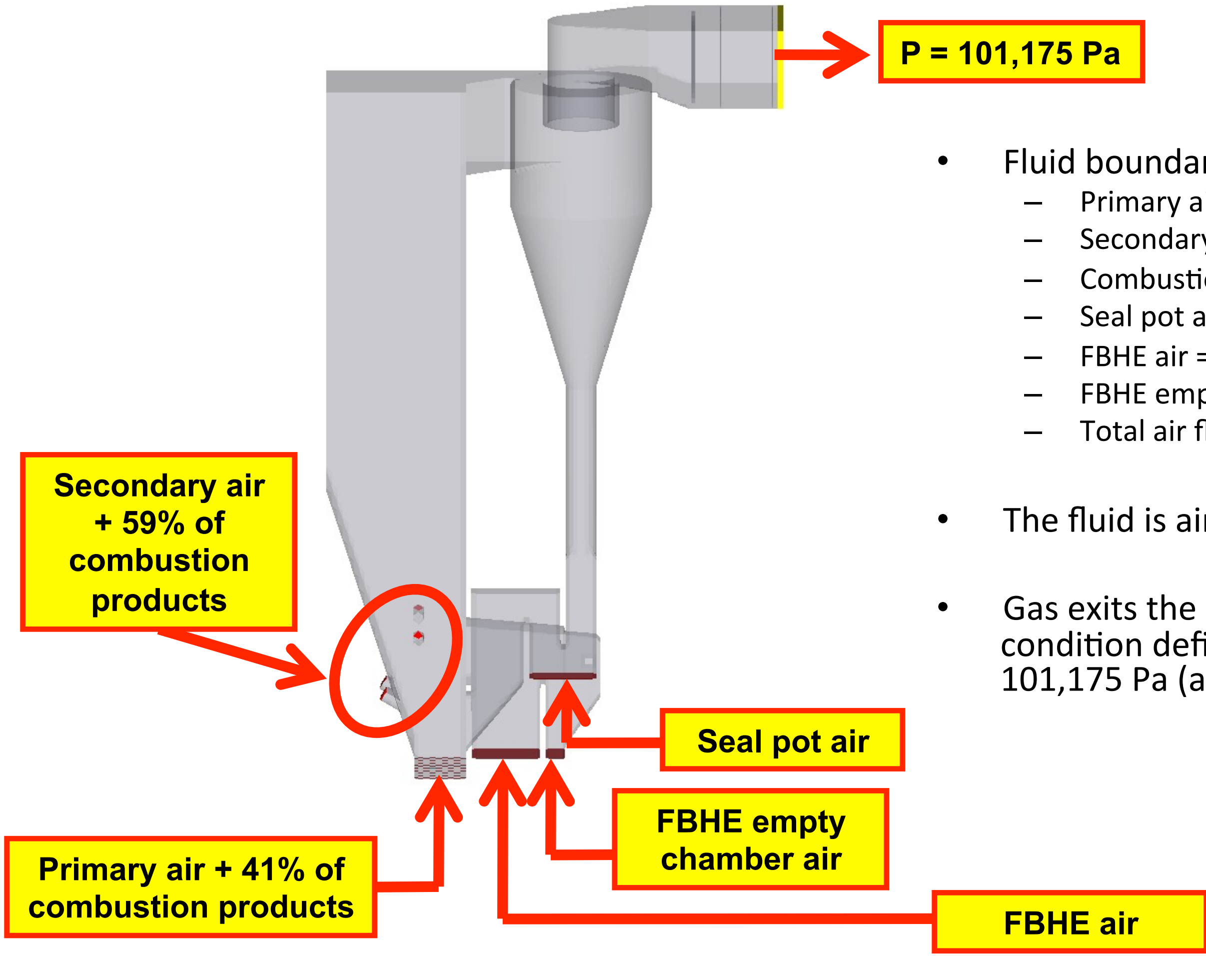
Suspension Tubes

3-D Computational Model – Entire CFB Loop



- The details of the geometry were provided by Biomasse Italia through various drawings and images
- A 3D solid model of the primary CFB loop was created including:
  - Combustion chamber
  - Cyclone
  - Dipleg
  - Seal pot
  - Fluidized Bed Heat Exchanger (FBHE)
  - Cyclone outlet (including suspension tubes)

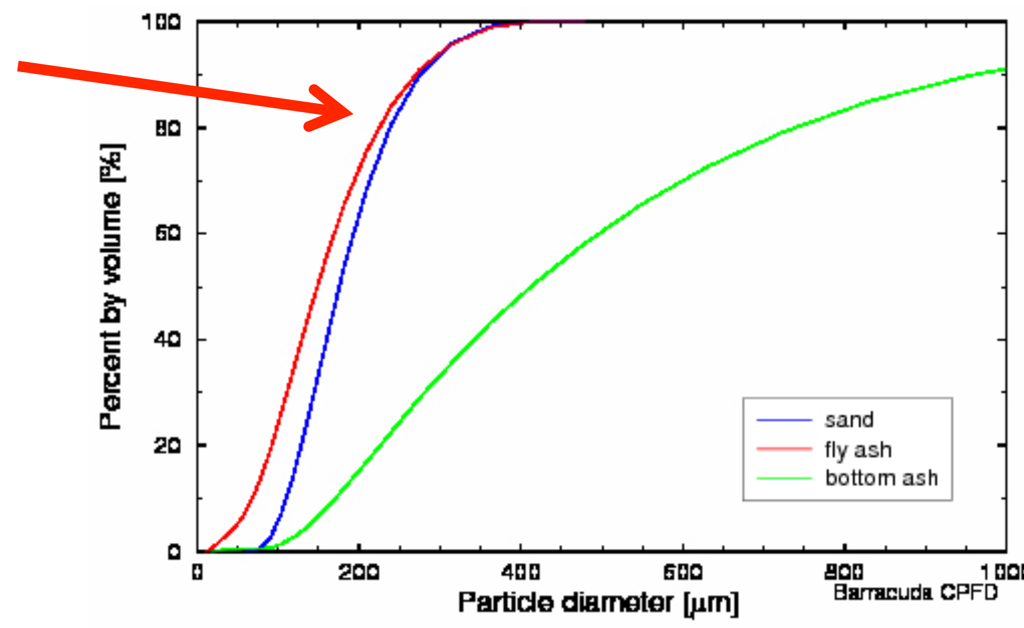
Boundary Conditions



- Fluid boundary conditions were applied as shown
  - Primary air = 31,000 Nm^3/h
  - Secondary air = 44,000 Nm^3/h
  - Combustion products = 17,121 Nm^3/h
  - Seal pot air = 1,800 Nm^3/h
  - FBHE air = 3,800 Nm^3/h
  - FBHE empty chamber air = 1,500 Nm^3/h
  - Total air flow through system = 99,221 Nm^3/h
- The fluid is air at 850°C = 1123.15K
- Gas exits the domain at the pressure boundary condition defined on the cyclone outlet: -1.5mbar = 101,175 Pa (absolute)

Particle Properties

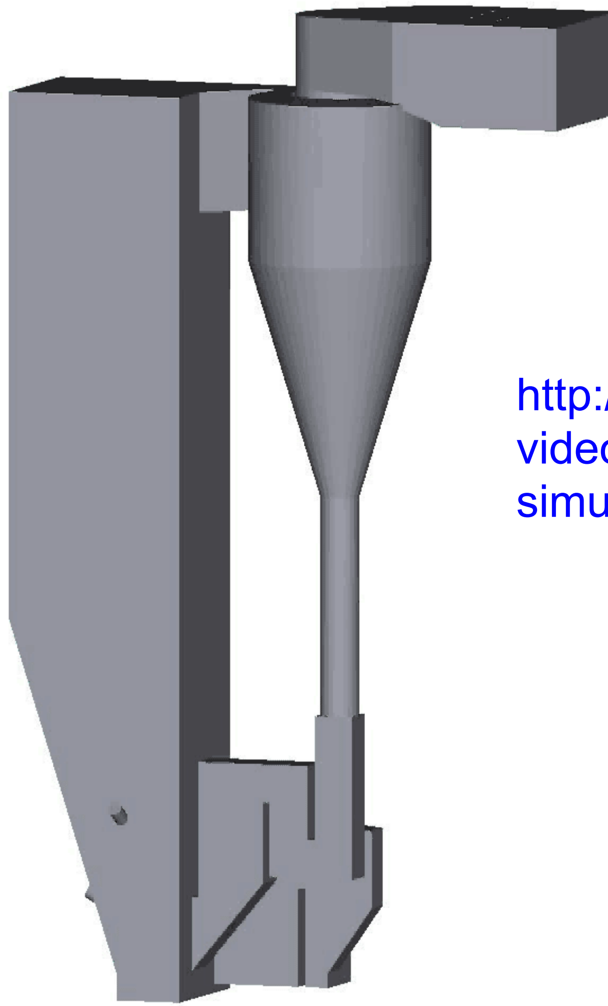
- Three particle species were defined with the PSDs shown
  - Note, the bottom ash represents some particles as large as 2188 micron (scale clipped in image)
- The CPFD method computes the particle phase with discrete, Lagrangian entities. Thus, each particle has its own, unique size, determined at random from the PSD curves
- The particle densities are:
  - Sand: 2650 kg/m3
  - Ash: 1500 kg/m3
- Over 1.4 million computational particles are used to represent the solids phases



Example Courtesy of BiomasseItalia

CFB Simulation

- STL geometry
- Computational Grid
- Boundary Conditions
- Particle Flow

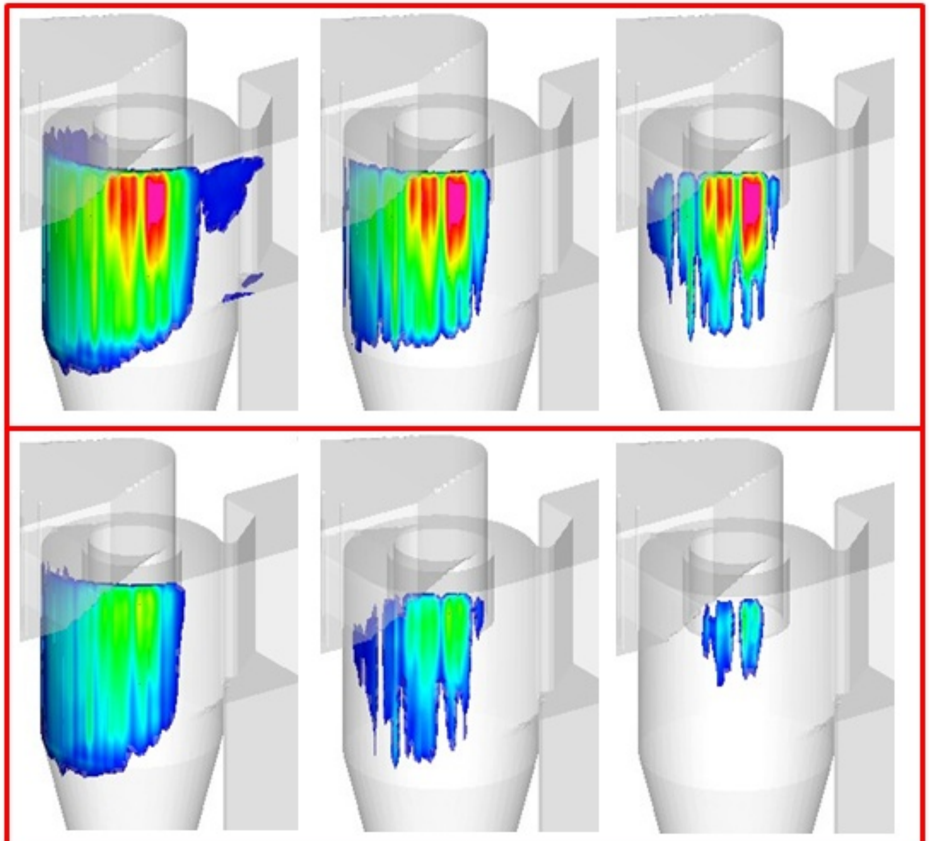


http://cpfd-software.com/resources/videos/cfb-combustor-3d-cfd-simulation-in-cpfd-barracuda-vr

Validation of Erosion Model Based on Plant Data

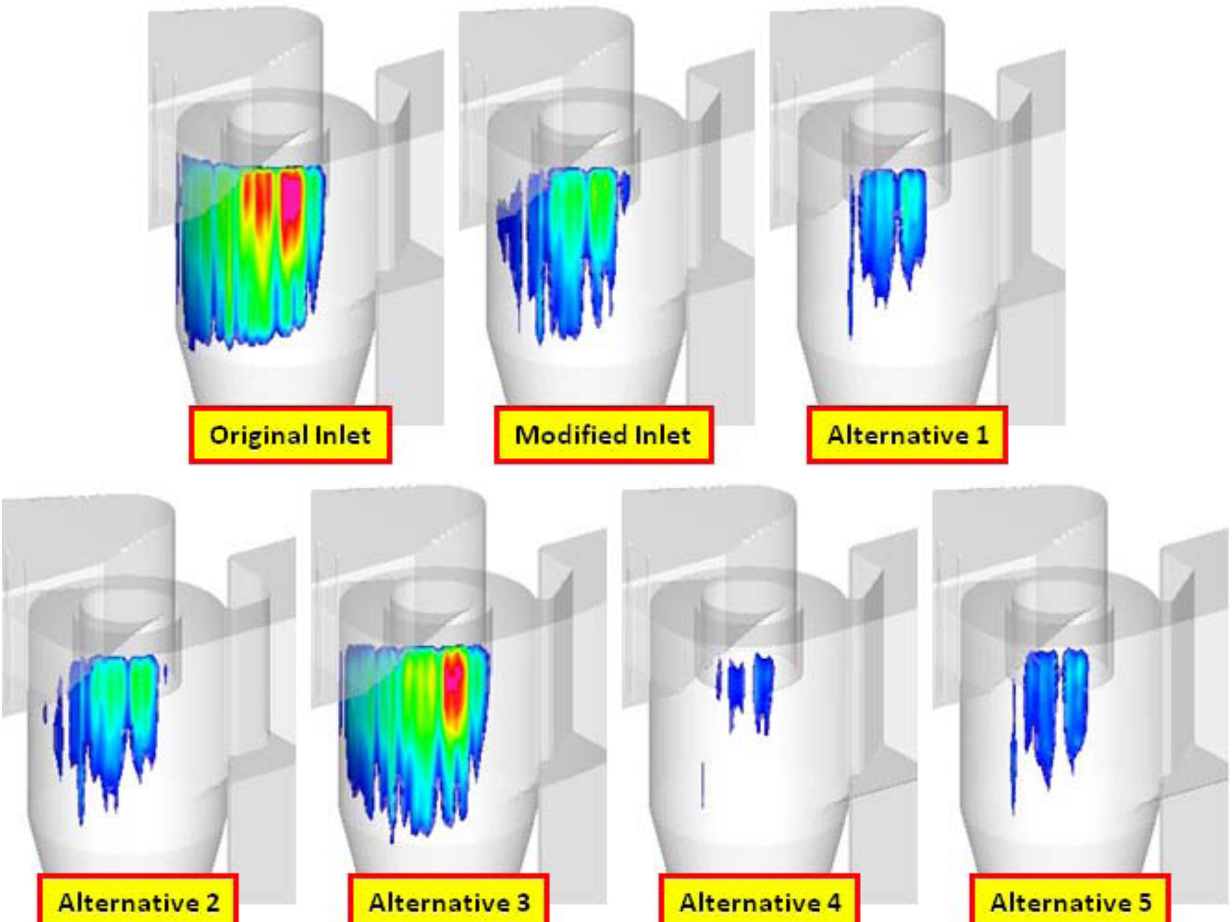
Original Inlet

Modified Inlet



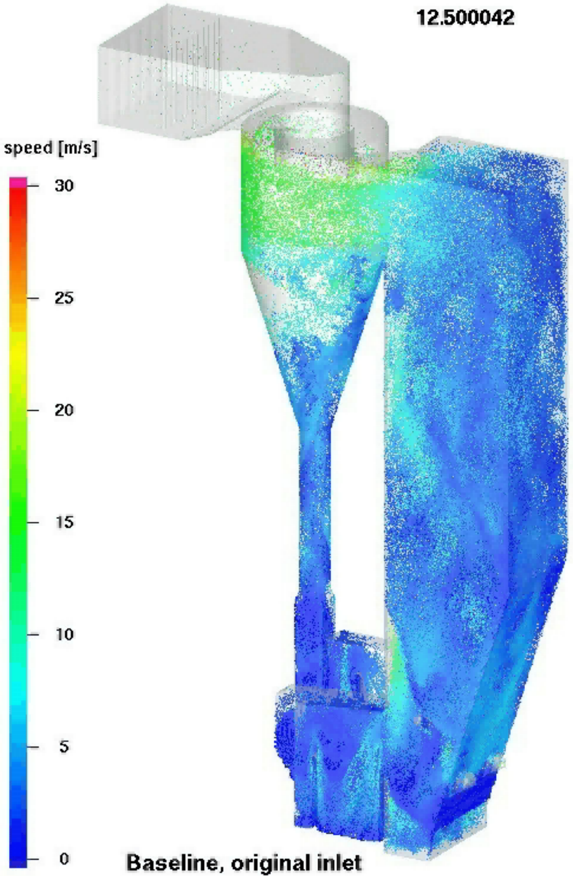
- Validation of the erosion prediction was accomplished by comparing simulations to the known erosion results from a prior plant modification.
- The original inlet design had resulted in even more erosion damage than the unit as operating today.
- A modified inlet was previously designed and installed. The erosion dropped sufficiently to allow the plant to run 3X longer than with the original design.
- It was based on this success that the current project was undertaken to make further improvements and to make them based on the system performance as a whole.
- Results from the two simulations (original and modified inlet) agreed closely with observed damage from inspection in the field.

Cyclone Erosion: Comparison for Different Designs



- Alternatives 2 and 3 were rejected as having similar or worse erosion characteristics than the current as-operated design.
- Erosion indices for Alternatives 1, 4, and 5 all show dramatic reduction in predicted erosion levels and are actually very similar to one another in their reduction from the base case.
- Alternative 1 was selected because Alternatives 4 and 5 exhibited unacceptable increases in the pressure drop across the cyclone.
- Erosion performance at the cyclone was balanced against erosion predicted in suspension tubes and fluidized bed heat exchanger (not shown).
- Overall, ~50% reduction in erosion was predicted, which should result is much more than a 50% increase in service life due to the non-linearity of erosion damage.
- Full results are not yet known as the plant is still operating. Plant has already operated longer than its previous maximum operating period.

CFB Erosion Study Conclusions



The CPFD multiphase CFD method enabled plant engineers to select the best trade-offs for maximizing service life and performance.

- Full-scale commercial unit
- Compared well to operational data
- Modifications completed in early 2011
- Full service life extension is not yet known because plant is still operating

Reference: Blaser, P. and Corina, G. "Validation and Application of Computational Modeling to Reduce Erosion in a Circulating Fluidized Bed Boiler", *International Journal of Chemical Reactor Engineering*, 10, A51 (2012).

Case Study #2: CFB Combustor – Flow Maldistribution

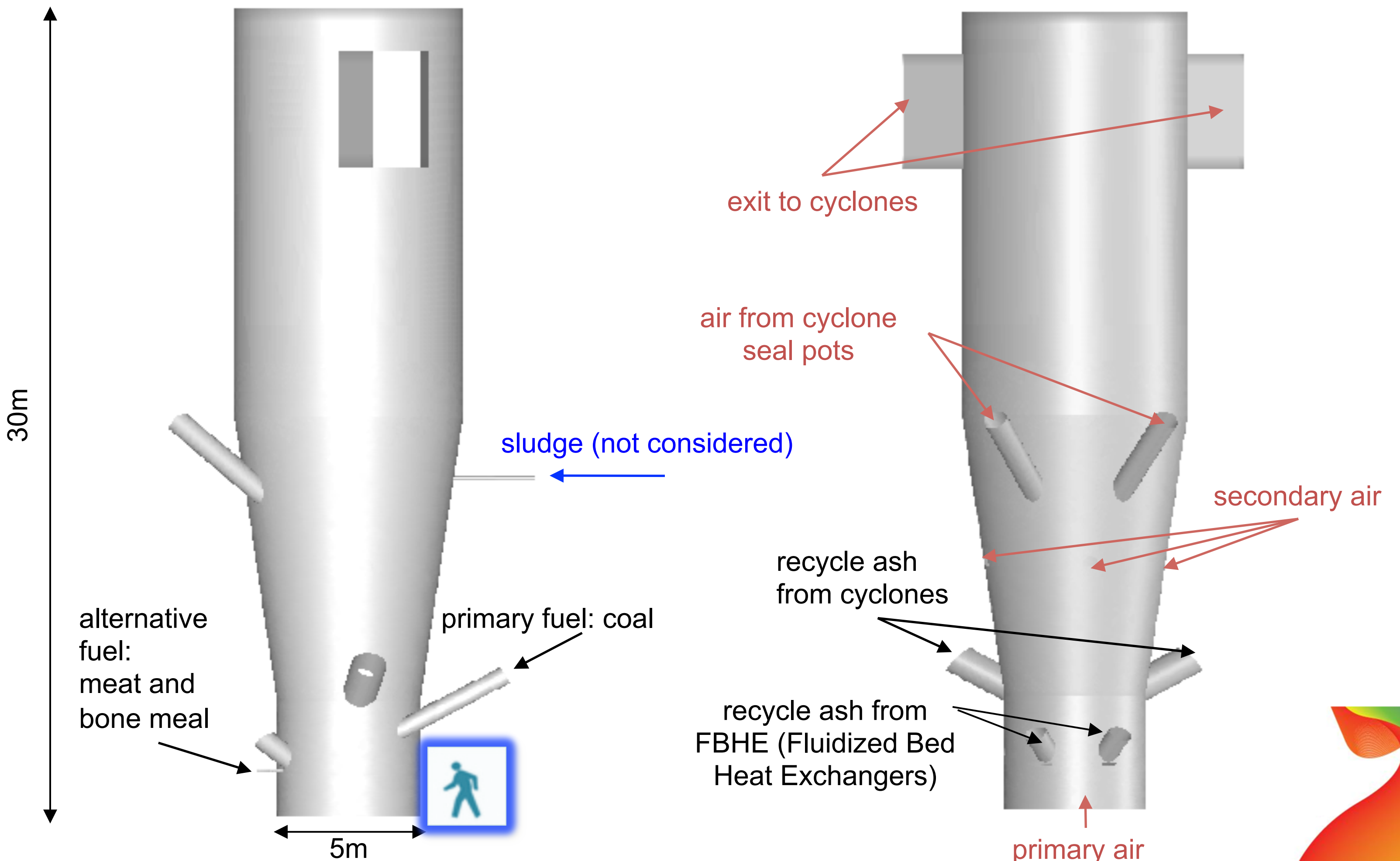
- Simulation of a 250 MW Circulating Fluidized Bed (CFB) combustion chamber at Duisburg power plant (Germany)
- Exploration of the influence of the substitution of coal by alternative fuels
- Computer-based design of an additional secondary air addition in order to avoid temperature peaks and achieve optimized mixture
- Barracuda VR® was selected for its speed and accuracy for understanding CFB systems, combining chemical reaction kinetics with accurate particle-fluid flow prediction

Municipal Power Plant
Duisburg, Germany

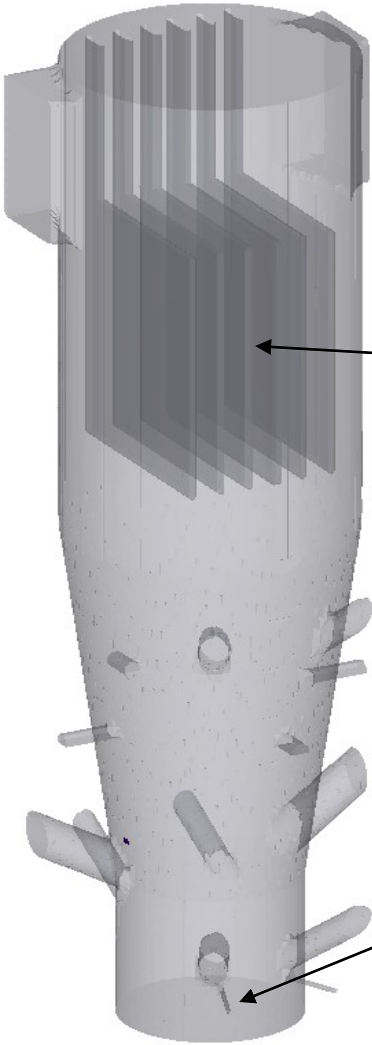
COMPUTATIONAL PARTICLE FLUID DYNAMICS

Example courtesy of:
aixprocess

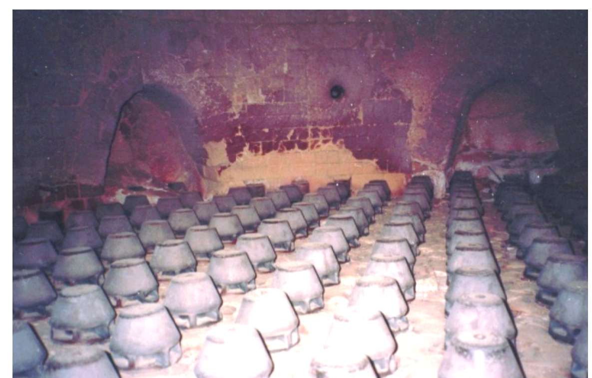
CFB Inlet/Outlet Configuration



CFB Geometric Details

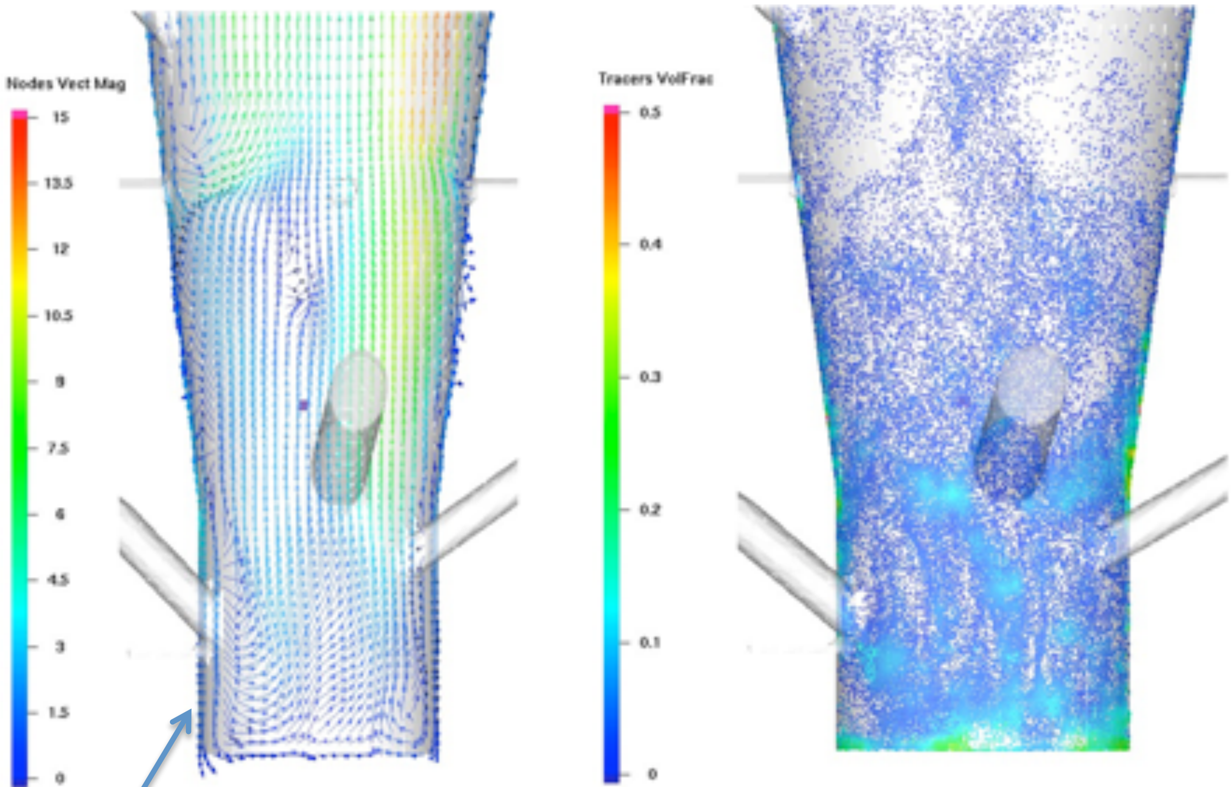


Heat Exchanger Modules

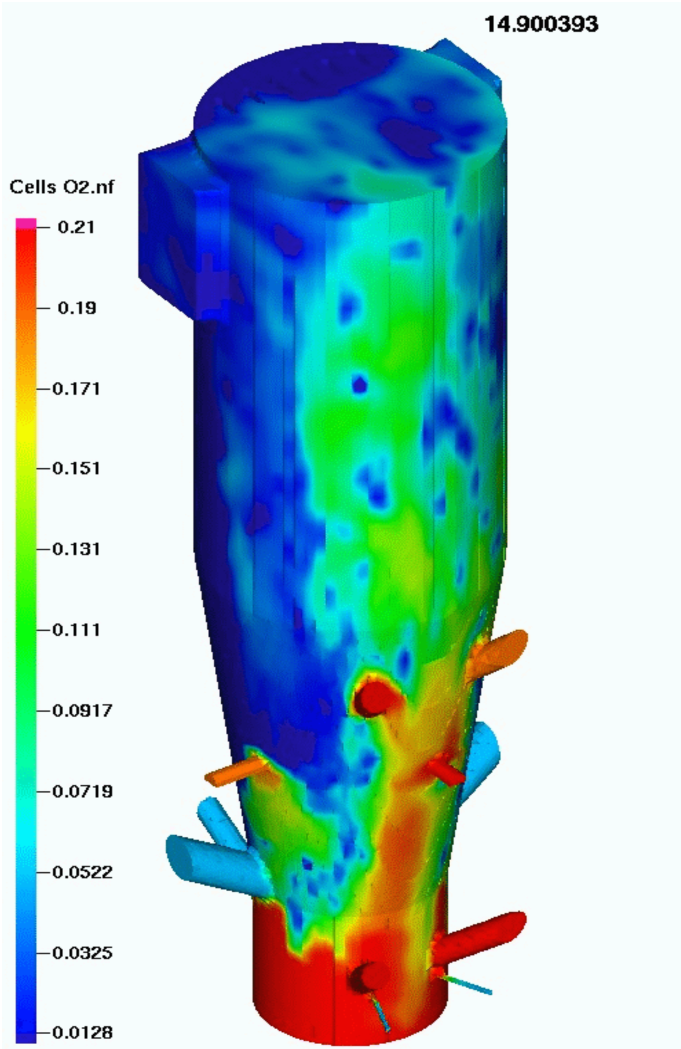


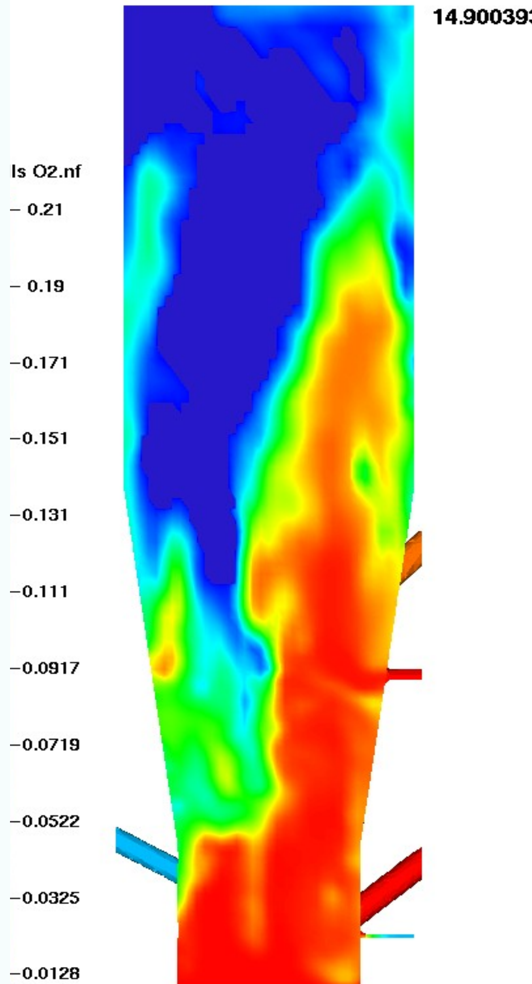
Gas Nozzles

Particle Velocities



Near-wall *downward* velocity of ~2 m/s



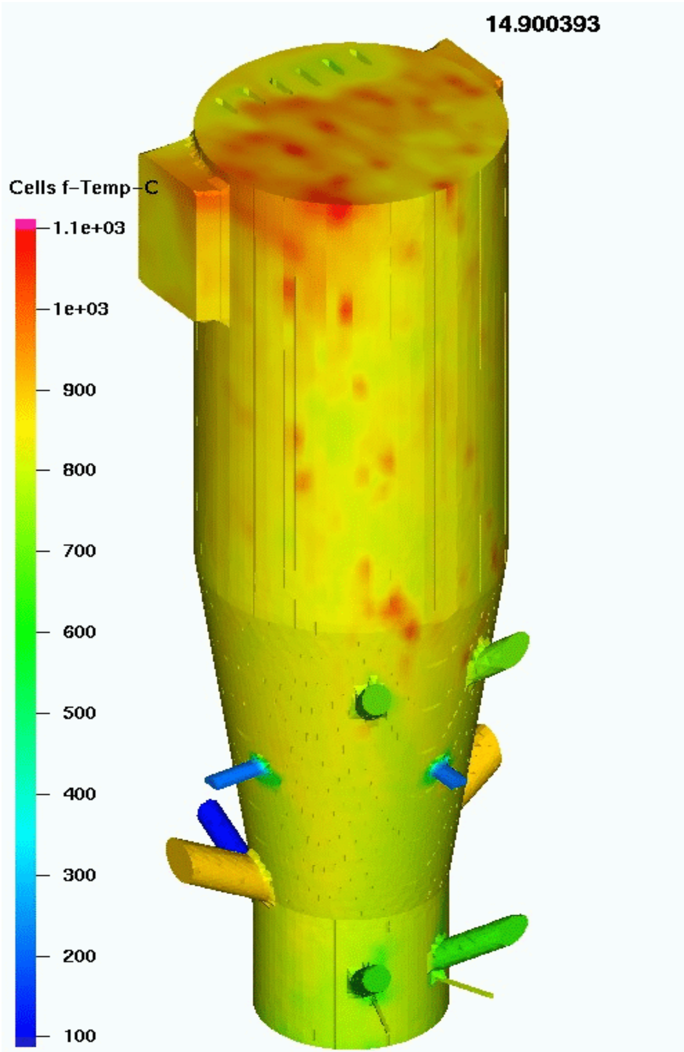


Oxygen Distribution:

Near Wall and at Center Plane

- One side exhibits an oxygen deficit with corrosion-critical values near the heat exchanger modules.
- Low penetration depth of secondary air flow due to high solids momentum.

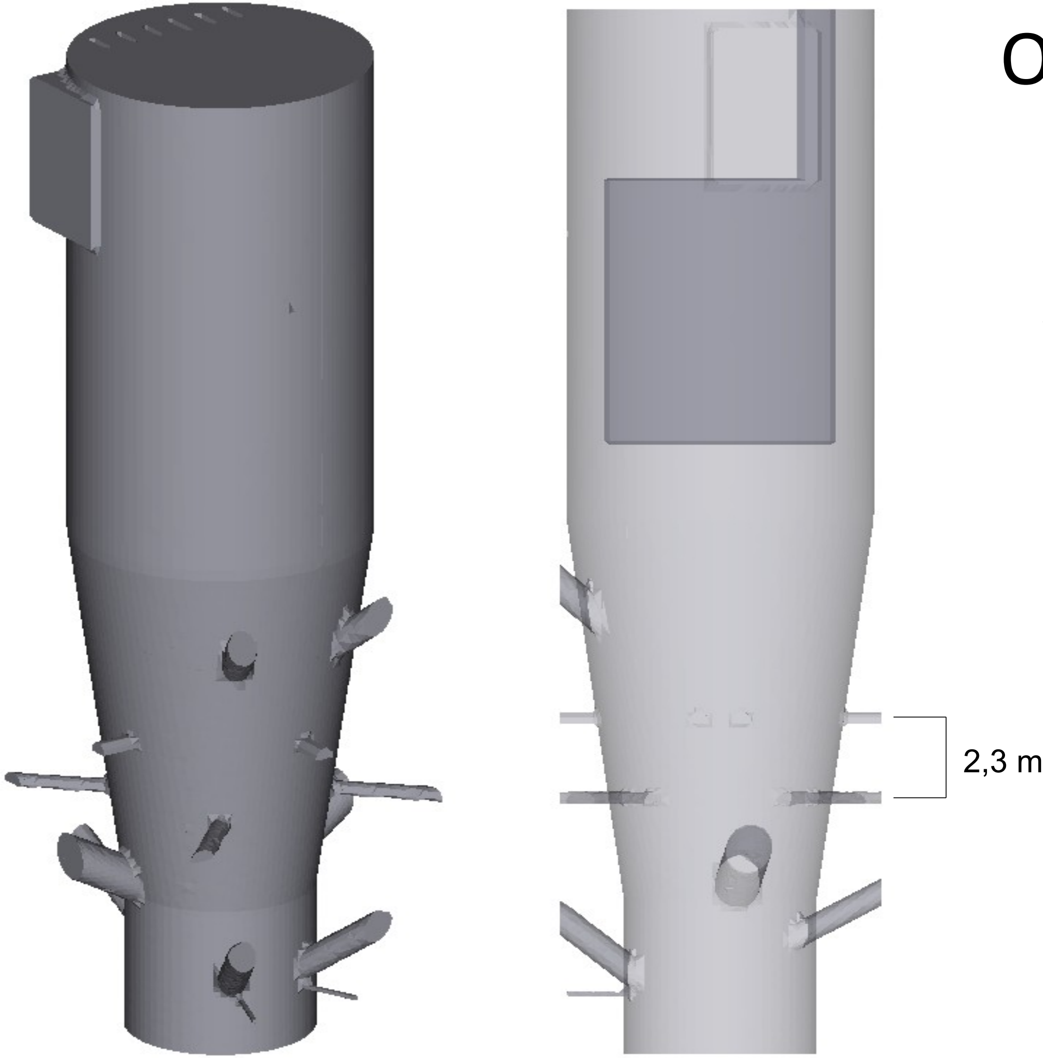
COMPUTATIONAL PARTICLE FLUID DYNAMICS



Gas Phase Distribution

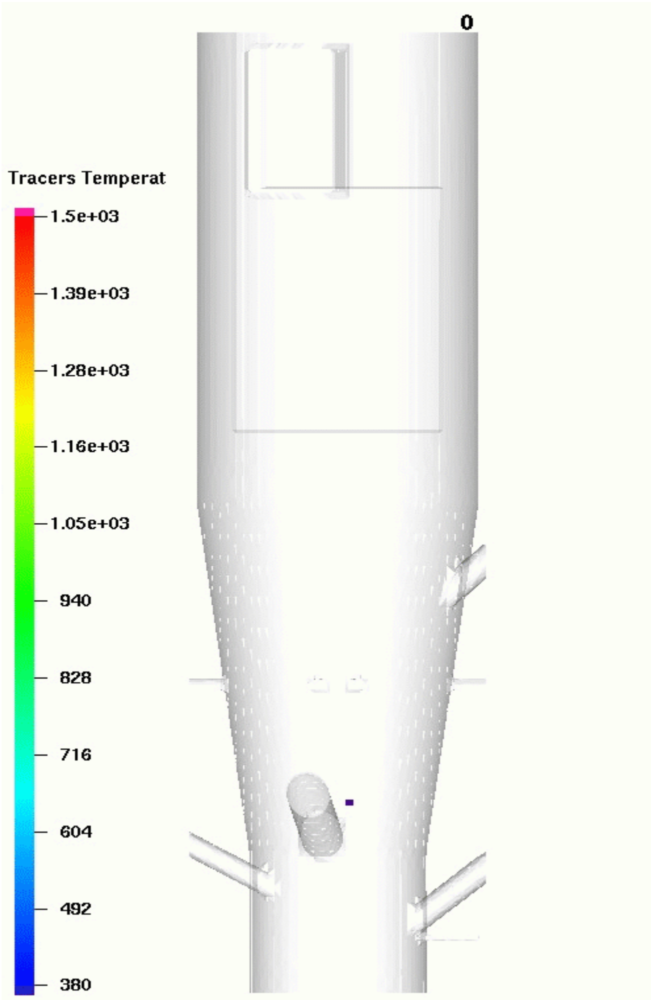
- Temperature peaks on the fuel injection side and near the top

Simulation reveals mal-distribution in the deep-bed of injected fuel is the root-cause of operational problem

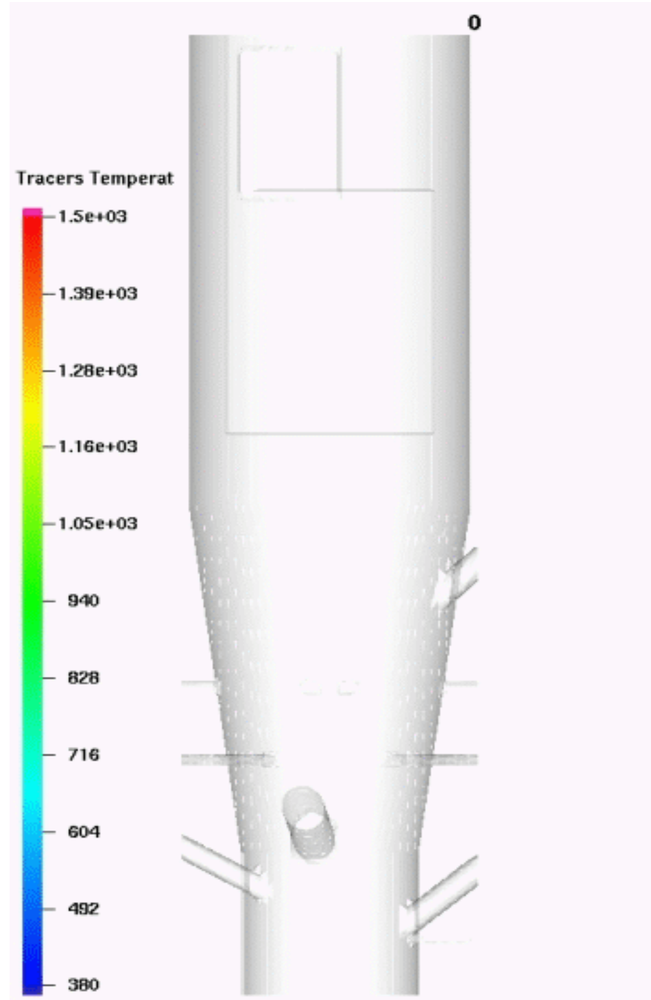


Optimization: Additional Secondary Air Nozzles

- ✓ Recommendation for optimizing combustion was to add and locate additional secondary air nozzles, with specific flow rate distribution to overcome oxygen mal-distribution.



As-Built



Optimized

Coal Particle Kinematics and Temperature (K)

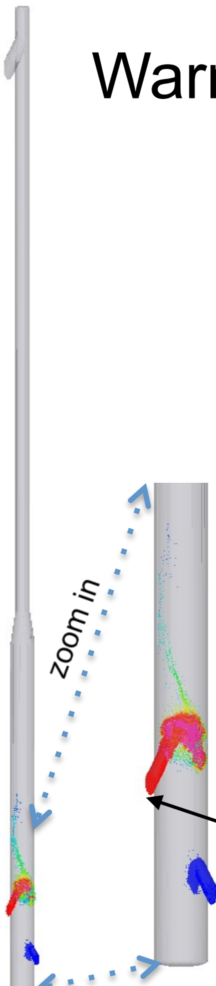
CFB Combustor Optimization Conclusions

- The multiphase Barracuda VR simulations provided deep insight into 3-D gas-particle and thermal behavior, including heterogenous coal chemistry
- As-built design reveals mal-distribution of solid fuels and volatiles in the bed
- Volatile and char burn-out is limited by local lack of oxygen
- Lateral temperature gradient and corrosion-relevant oxygen deficiency at the lower end of heat exchanger modules matches the plant operational experience
- Optimization with additional secondary air nozzles leads to moderate improvements in oxygen distribution.
- No changes yet made to plant, so full results are not yet known.

Reference: Weng, M., Nies, M., and Plackmeyer, J. *"Computer-aided Optimization of Gas-Particle Flow and Combustion at the Duisburg Circulating Fluidized Bed Furnace"*, *VGB PowerTech*, pp64-69 (2011).

Case Study #3: CFD Simulation of a Warm Syngas Cleanup System Sorbent Regenerator

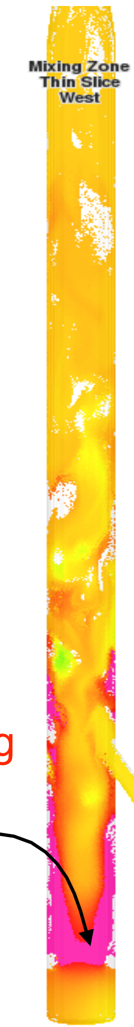
- Simulations performed for sorbent regenerator riser & mixing zone
- Goals: Optimize design and operational parameters
  - Location / orientation of solids inlets
  - Recycle ratio of regenerated sorbent
- Sorbent particles enter from 2 separate streams and have different sulfur loadings and temperatures
- Regeneration reaction is highly exothermic and kinetics increases with temperature
- Peak temperature needs to be controlled to prevent sorbent sintering



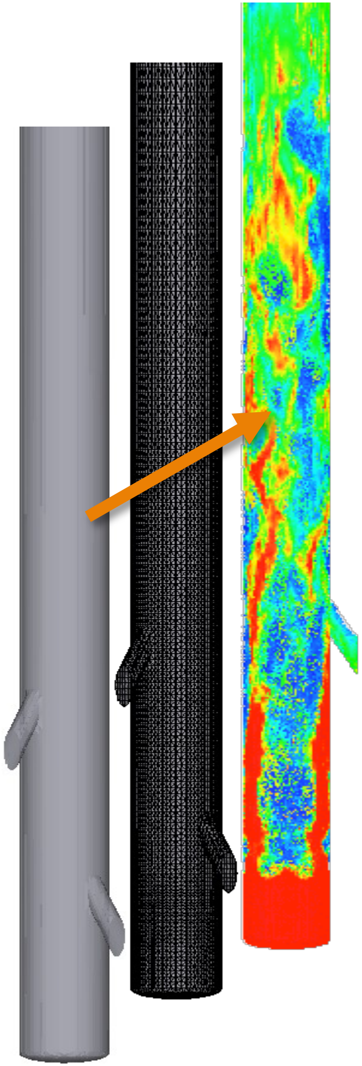
Hot regenerated sorbent (recycle stream)

Cooler spent sorbent

Air inflow from bottom to burn off sulfur



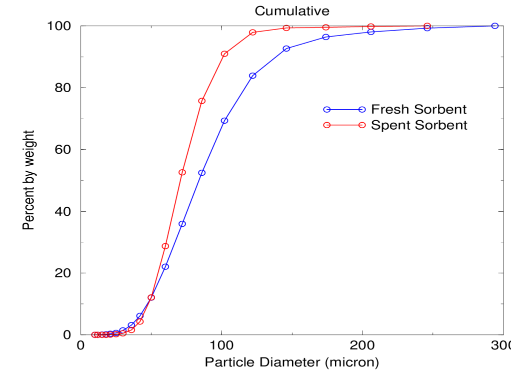
Sorbent temperature variations in regenerator



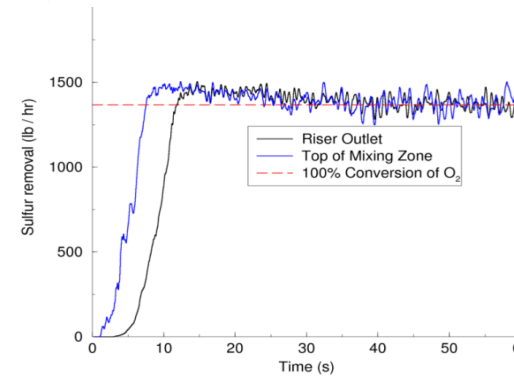
Requirements for Multiphase CFD Methodology

- Complete 3-D model of regenerator mixing zone and riser
- Must be stable at dense-to-dilute solids loadings
- Discrete sorbent particulates, each with its own diameter, sulfur load, and temperature
- Reaction chemistry must be calculated on each discrete particle due to variations in sulfur content and temperature
- Multi-component particles to handle solid-to-solid reaction as sorbent undergoes regeneration
- Simultaneous 3-D gas flow and sorbent mass and heat balance with reaction kinetics

Particle Size Distribution

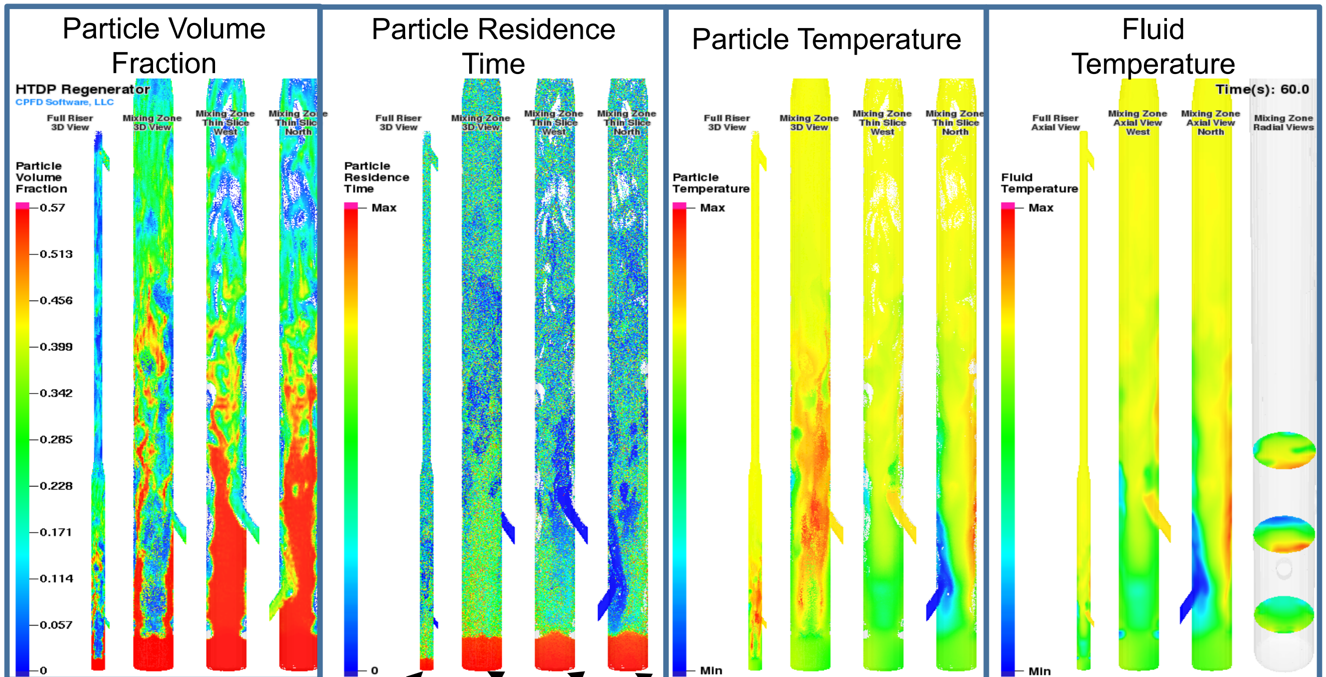


Sulfur in gas at riser outlet



CFD Simulation of Warm Syngas Cleanup System Regenerator Riser

Animation contains simultaneous views of solids and gas behavior.

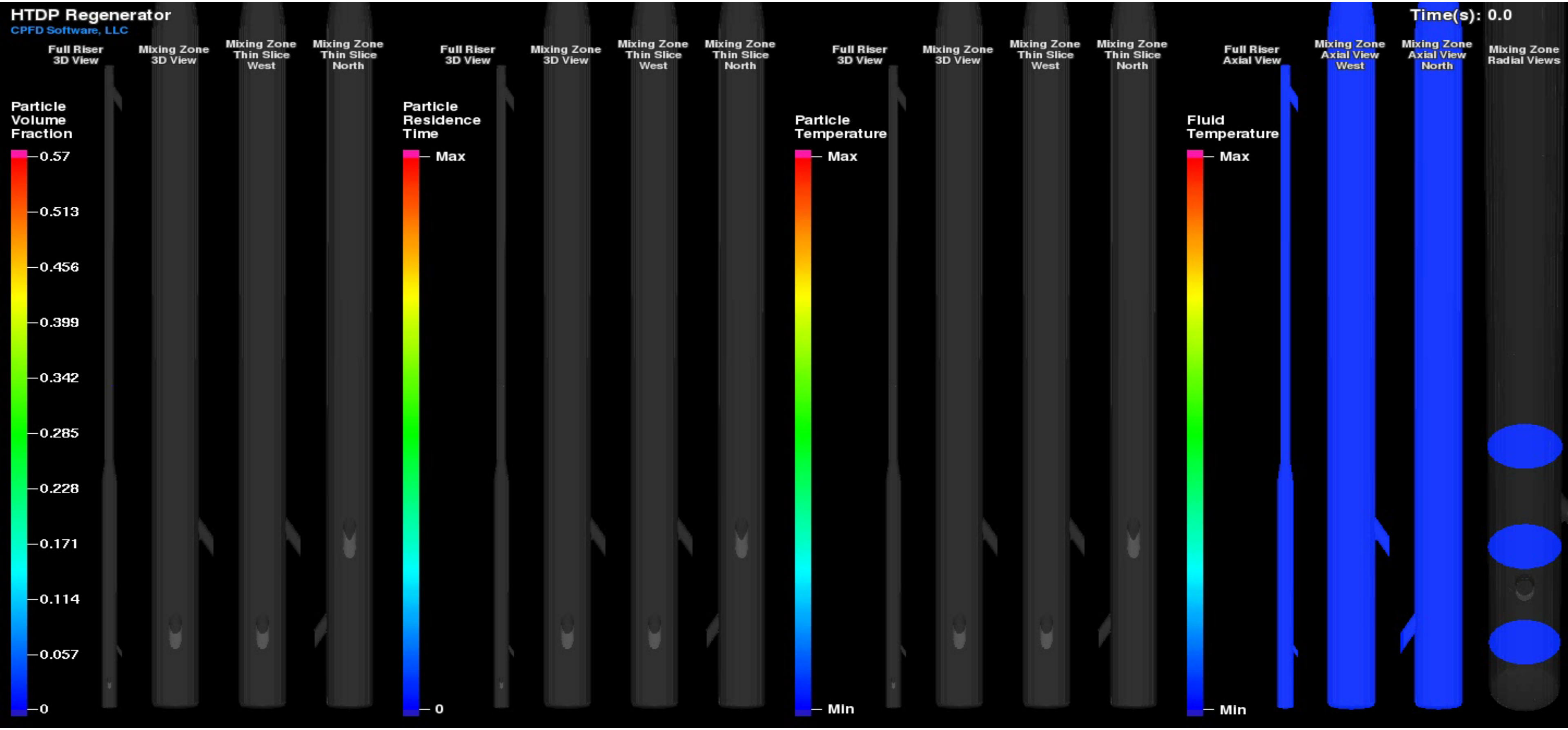


Each data set has multiple views >

Full 3D Geometry

Full Mixing Zone

Thin Slices through West and North Planes http://cpfd-software.com/resources/videos/cfd-for-sorbent-based-gas-cleanup-system



Solids Loading | Solids Residence Time | Solids Temperature | Gas Temperature

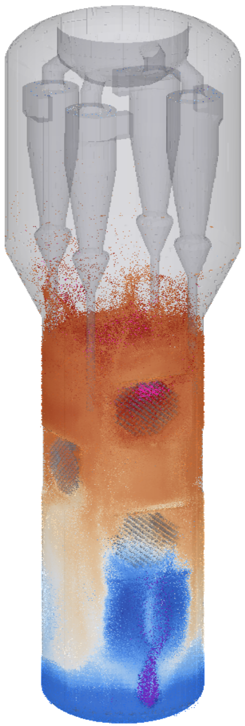
*Select scales removed intentionally; client-proprietary information.

Warm Syngas Cleanup System - Conclusions

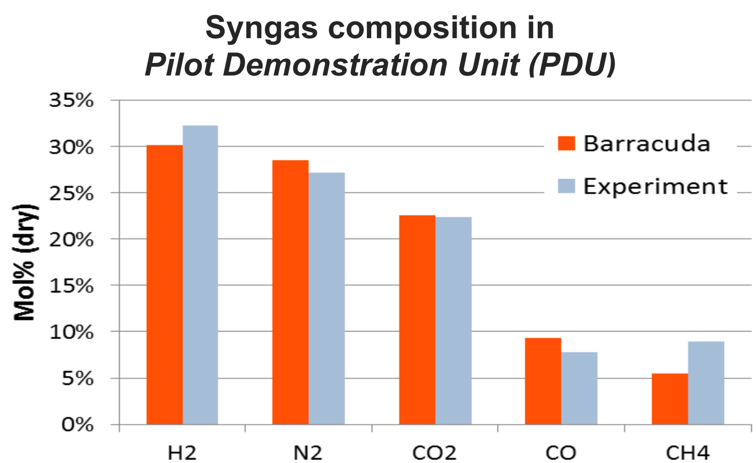
- A multiphase, 3-D CFD model was built of the warm syngas cleanup system [sorbent regenerator mixing zone and riser] with exothermic chemistry and energy balance. Chemical reactions were calculated on each particle, accounting for large variations in particle temperature and reactant composition.
- Cases were studied with spent sorbent and sorbet recycle injection points at two different locations, lower and higher.
  - ➢ Original thinking was to inject recycle (lower sulfer, higher temperature) at the lower injection point. However, this resulted in additional hot spots and affected stability of sorbent regeneration.
  - ➢ CFD results show better performance with spent sorbent (higher sulfer, lower temperature) at the lower injection point. This reduces hot spots and results in more stable sorbent regeneration.
- A study of the distribution of sulfur remaining on particles found that reduction in hot spots produces more uniformly regenerated sorbent. The CFD-optimized design lowered peak temperatures for the sorbent and resulted in more uniform sulfer burnoff, plus reduced the risk of sorbent sintering.
- Hot spots due to high reaction rates and heat release near air inlets can be mitigated by solid feed locations and angles and by adjusting recycle rates of solids into mixing zone.
- The process underwent very substantial review/redesign incorporating these results, which provided insights into the regeneration process that could have been obtained no other way.

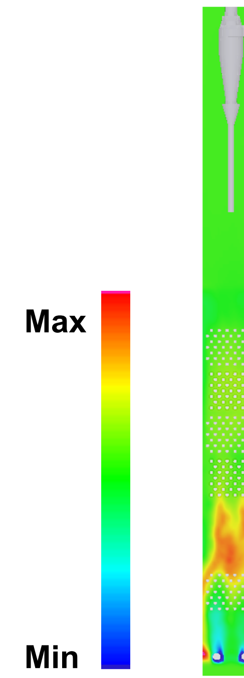
Case Study # 4: Gasifier Design

- Diverse operating gasifiers using black liquor and biomass feedstock are being simulated in conjunction with ThermoChem Recovery International (TRI) on multiple systems designs: http://www.tri-inc.net
- Barracuda models with thermal and chemical reactions have been validated and are being used to assist in design and optimization of new installations



Particle temperatures in black liquor gasification Barracuda VR simulation





PDU Time-averaged Temperatures

cpfd COMPUTATIONAL PARTICLE FLUID DYNAMICS

Barracuda VR® GPU

The Basics to Our Approach

- Philosophy has been to fit the code to parallelization and not fit parallelization to code. This has also provided advantages in physics algorithm development.
- Barracuda data restructured to1-D vectors. Barracuda internally is an unstructured-data code.
  - Allows streaming of data through all algorithms
  - Thus even out Serial Barracuda has a 2 to 20 times speed-up depending on problem
- In general, make “smart use” of all computational elements (CPU and GPU). For example, memory-read can be 10 to 100 slower than an in-place calculation. Using alignment of data keeps usable cache, etc.
- Minimize data transfer between CPU and GPU
- Test, test, test, test,……repeat

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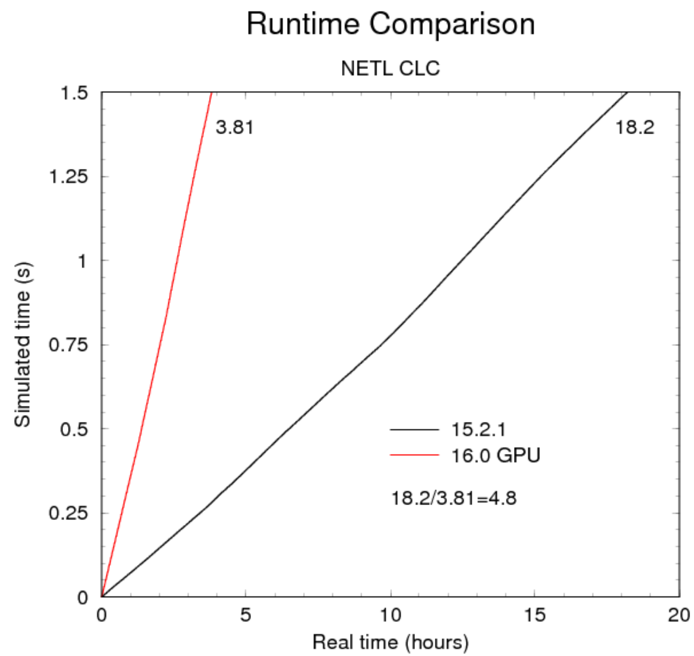
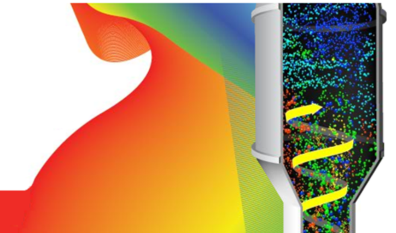
Technical Challenges and Performance

- Research required on the interpolation that maps particles to and from the grid
  - avoid “race condition” while getting high performance
- Where possible build host-device algorithms
- Keep multiple memory copies on GPU and CPU to eliminate bus traffic between CPU and GPU
- Individual algorithms are 10 to 60 times faster in GPU-parallel than the serial algorithm
- Consider: If 50% computation time is in Eulerian solution and 50% in particle Lagrangian solution, then making Lagrangian solution infinitely fast, only gives a 2-X speedup
- Partial completion of parallelization of the Lagrangian phase. One test case is NETL 3D full system CLC loop:
  - Total speed increase ~ 4.8x. If it takes 30 days to run with serial release Barracuda, now it takes <7 days



cpfd COMPUTATIONAL PARTICLE FLUID DYNAMICS



Summary

- Multiphase reacting flow science is playing a critical role with advancing the CFD technology used to design and optimize gas-solids fluidized reactors, which are used across a wide range of commercial units for manufacturing many important products:
  - Gasifiers; CFB Combustors; Chemicals; Oil Refining; CO_2 Capture; FGD…

- Commercial CFD software is now available that can virtualize in 3-D industrial-scale reactors with sufficient accuracy to help ensure:
  - ✓ Reliability improvements, component lifetime extension with reduced erosion
  - ✓ Hardware upgrades work together and as expected
  - ✓ Product ‘yields’ are maximized
  - ✓ Changes to feedstocks, catalysts and operating ranges have no surprises
  - ✓ Reactor scale-ups or turn-downs perform as promised
  - ✓ Minimize emissions and reduce need for costly ‘scrubbing’ hardware