Introduction to Barracuda VR®

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Outline

- Introduction to CPFD Software and the Barracuda Virtual Reactor®
- Fluid-Particle flows
  - Examples
  - What is different than single phase flows?
  - Modeling approaches
- The CPFD® modeling approach
  - Overview
  - Advantages and disadvantages
- Validation
- Commercial examples and case studies
  - Biomass CFB combustor
  - FCC regenerator

CPFD Software, LLC

- Inventors of the CPFD technology and the Barracuda Virtual Reactor

- Founded by CFD pioneers, Dr. Ken Williams and Dr. Dale Snider, as a vital supplement to general CFD software packages

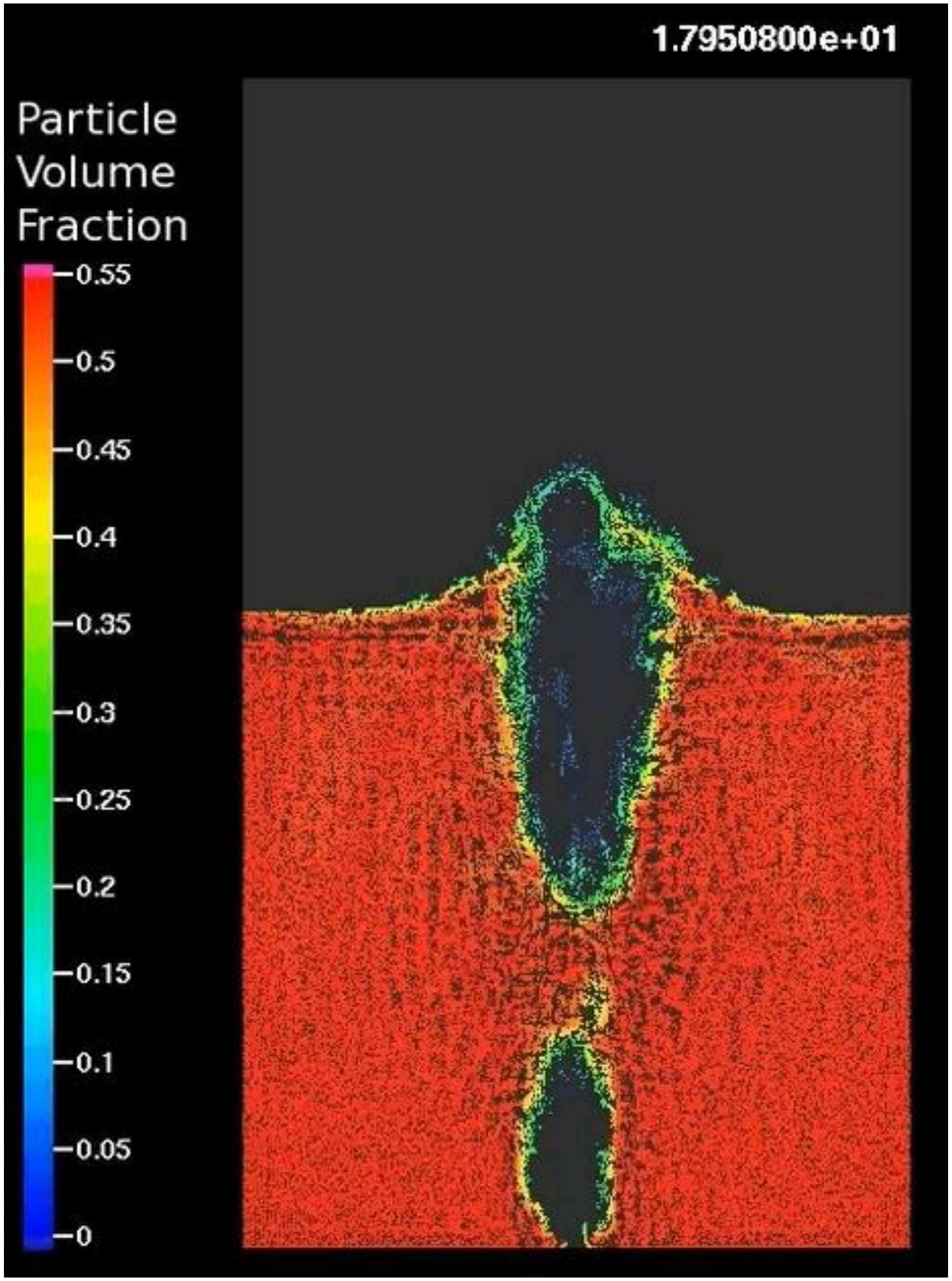
- Barracuda VR is the only commercial software package focused on chemically-reactive gas/particle flow

- CPFD Software offers
  - Software licensing
  - Engineering services
  - Training
  - Collaborative programs

CPFD Software, LLC
Albuquerque, New Mexico, USA

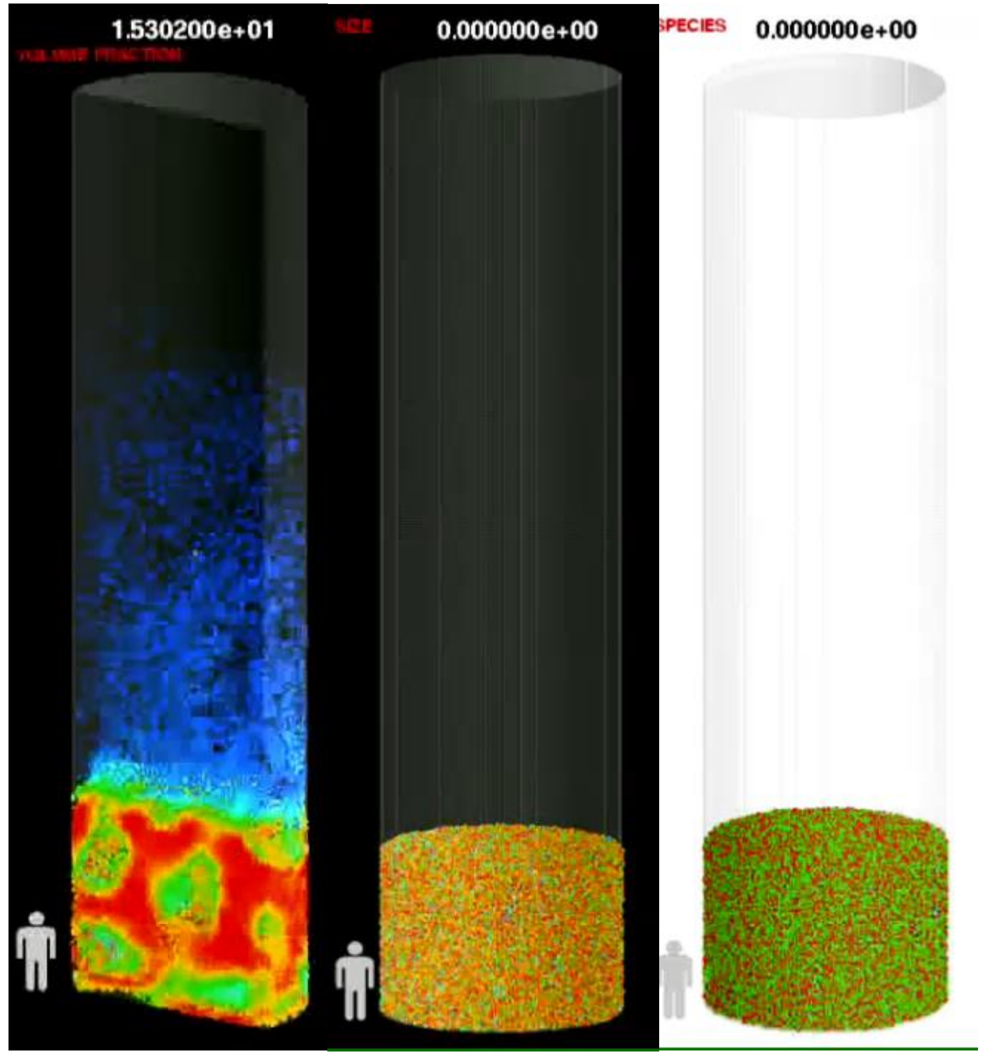
Particle Flow Examples

- Fluidized Beds (experiments)
  - Air (fluid) field important
  - Particle field important
    - Dilute to dense
  - Particle properties important
    - Size
    - Density



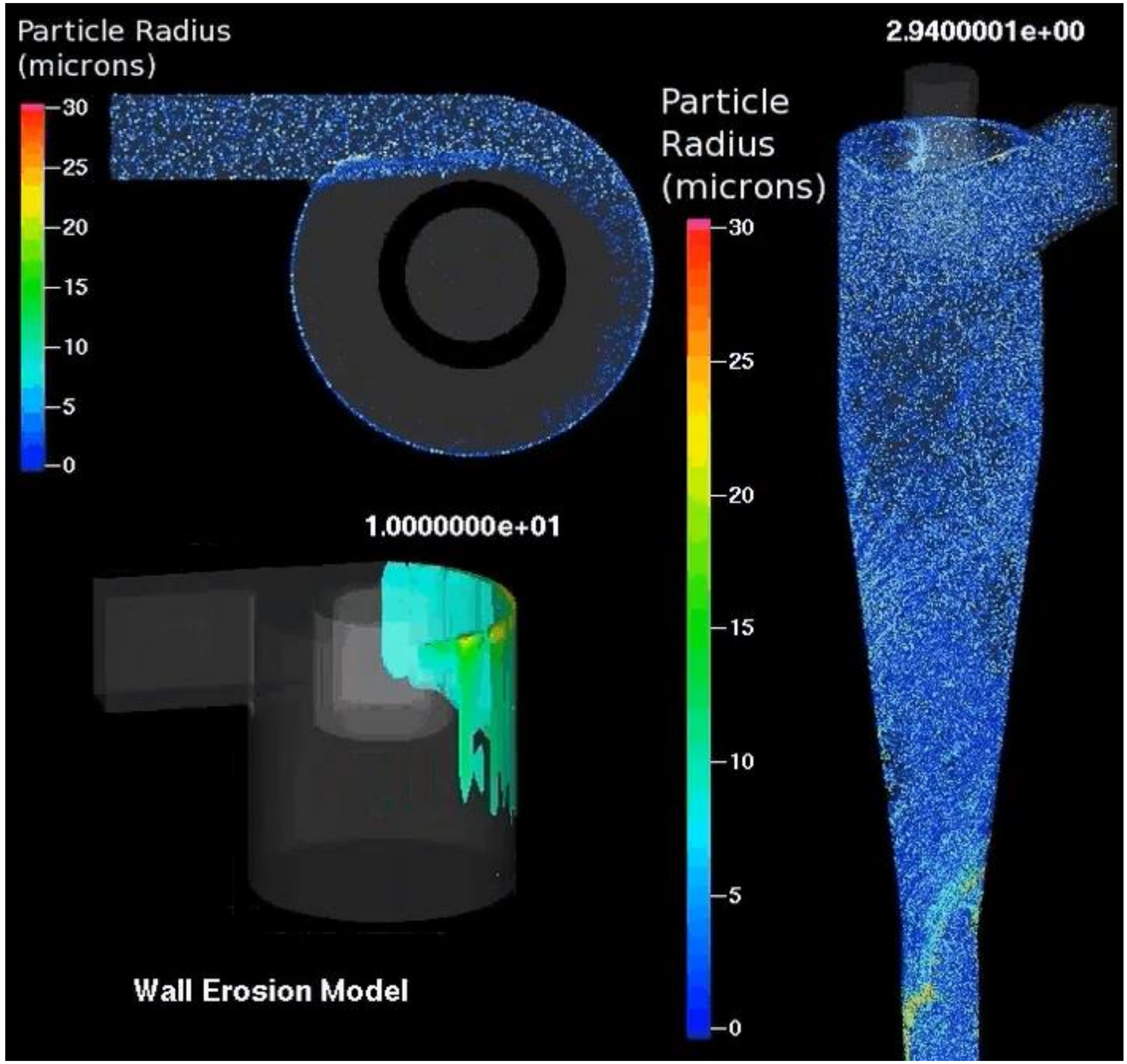
Particle Flow Examples

- Ore Reactors (Industrial)
  - Gas (fluid) field important
  - Particle field important
    - Dilute to dense
  - Particle properties important
    - Size distribution
    - Different materials with different densities

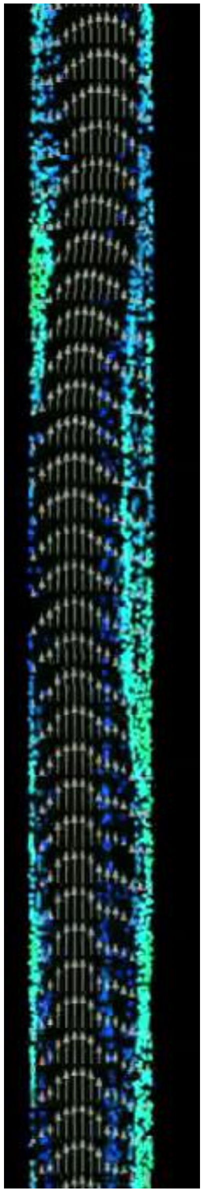


Particle Flow Examples

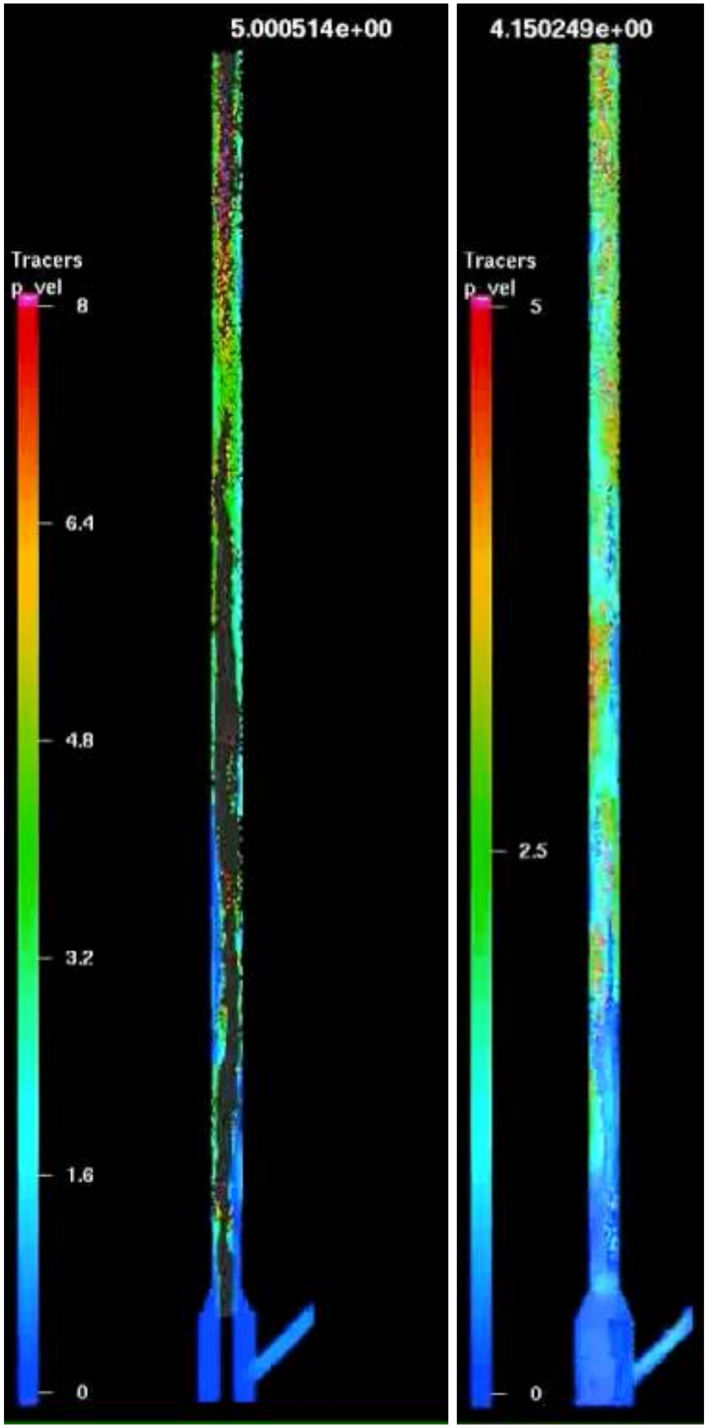
- Cyclones
  - Gas field important
  - Particle field important
    - Typically dilute
  - Particle properties important
    - Size and size distribution
    - Density
  - Areas of interest:
    - Overall efficiency
    - Efficiency vs. size
    - Erosion
    - Pressure drop



Particle Flow Examples

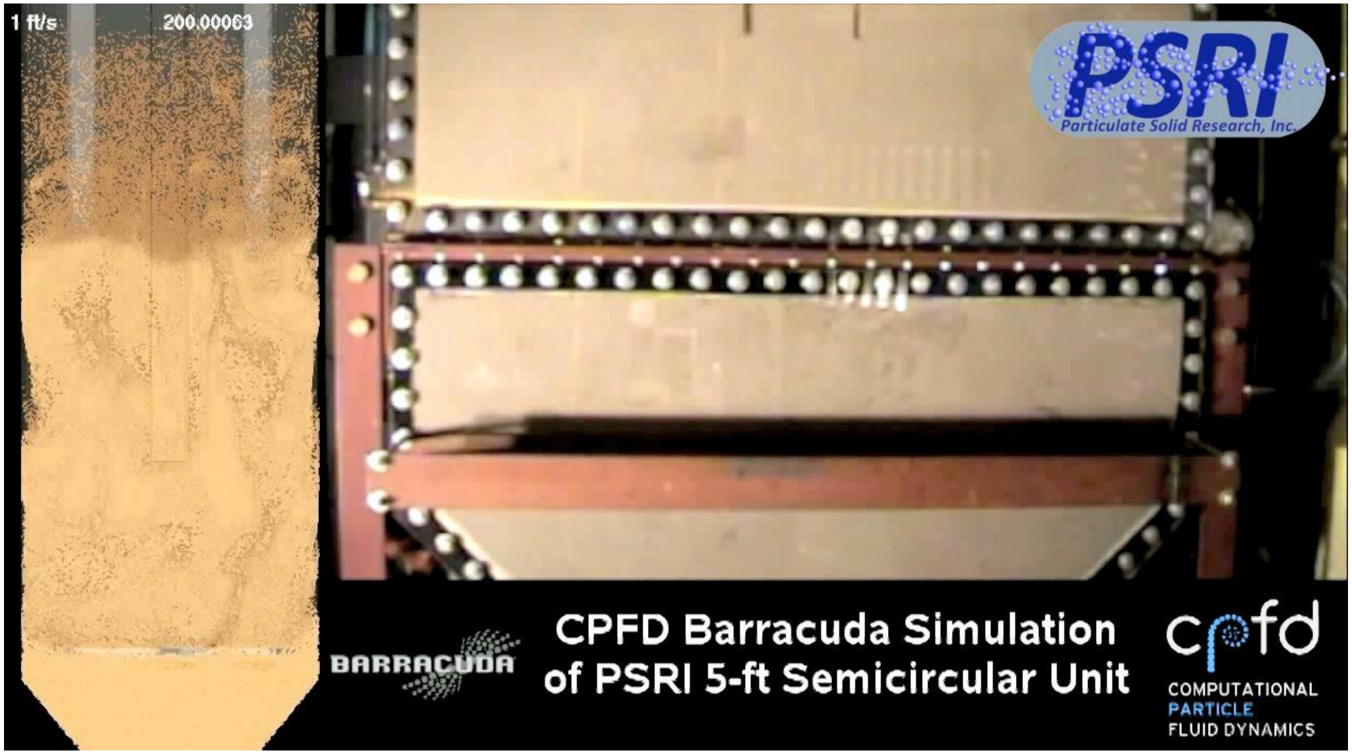


- Risers
  - Gas field important
  - Particle field important
    - Dilute to dense
  - Particle properties important
    - Size and size distribution
    - Density



Particle Flow Examples

- Deep Beds
    - Gas field important
    - Particle field important
        - Dilute to dense
    - Particle properties important
        - Size and size distribution
        - Density
    - Areas of interest
        - Mixing
        - Gas bypass
        - Entrainment
        - Yield



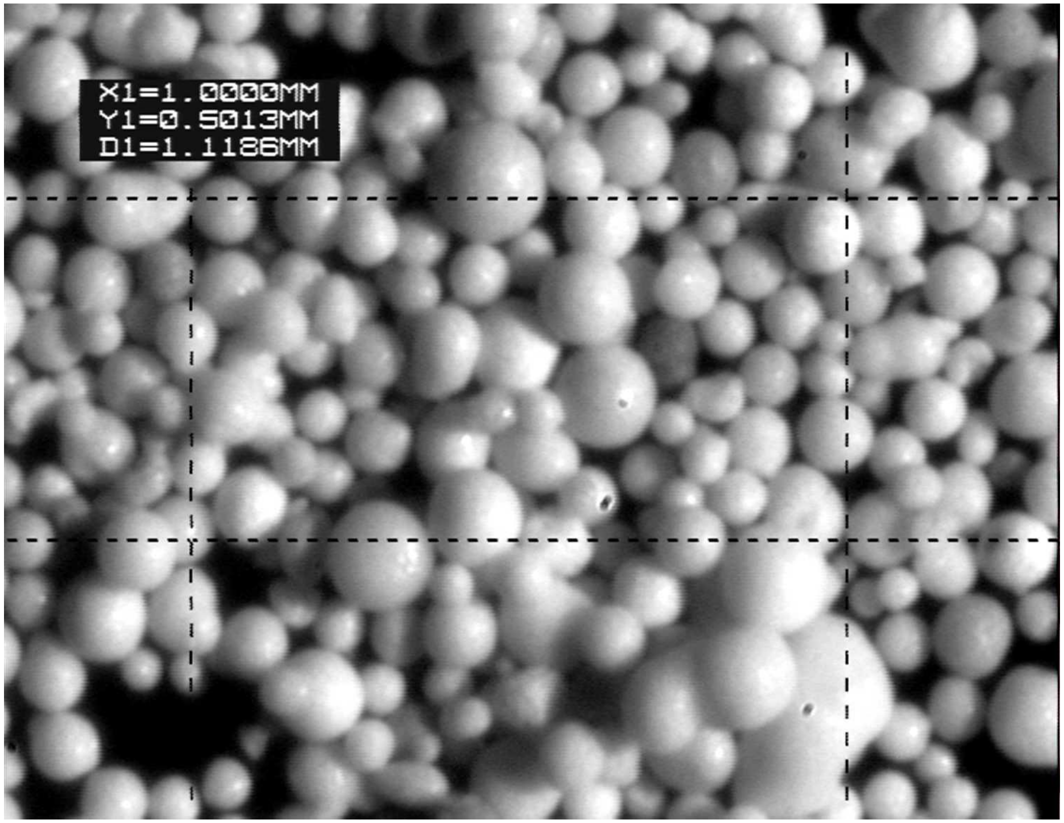
Question:

What's different about modeling fluid - particle flows compared with most CFD simulations?

Answer:

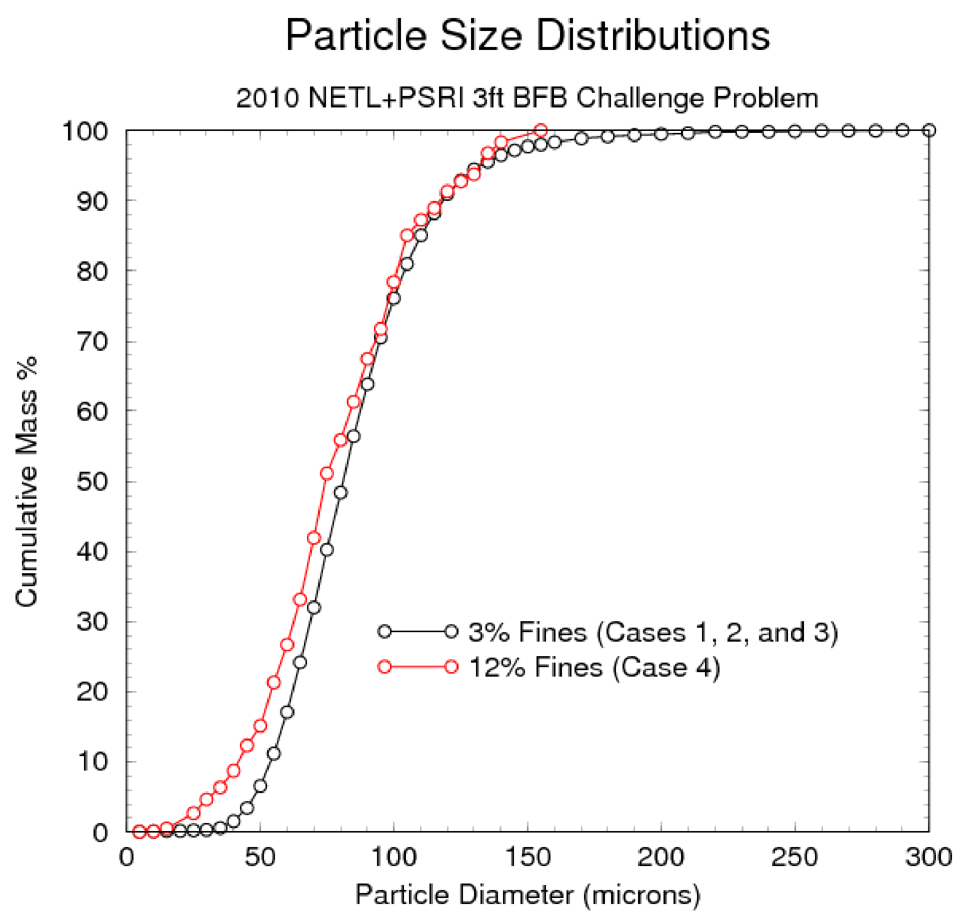
Particles are NOT fluids.

Particles Are NOT Fluids



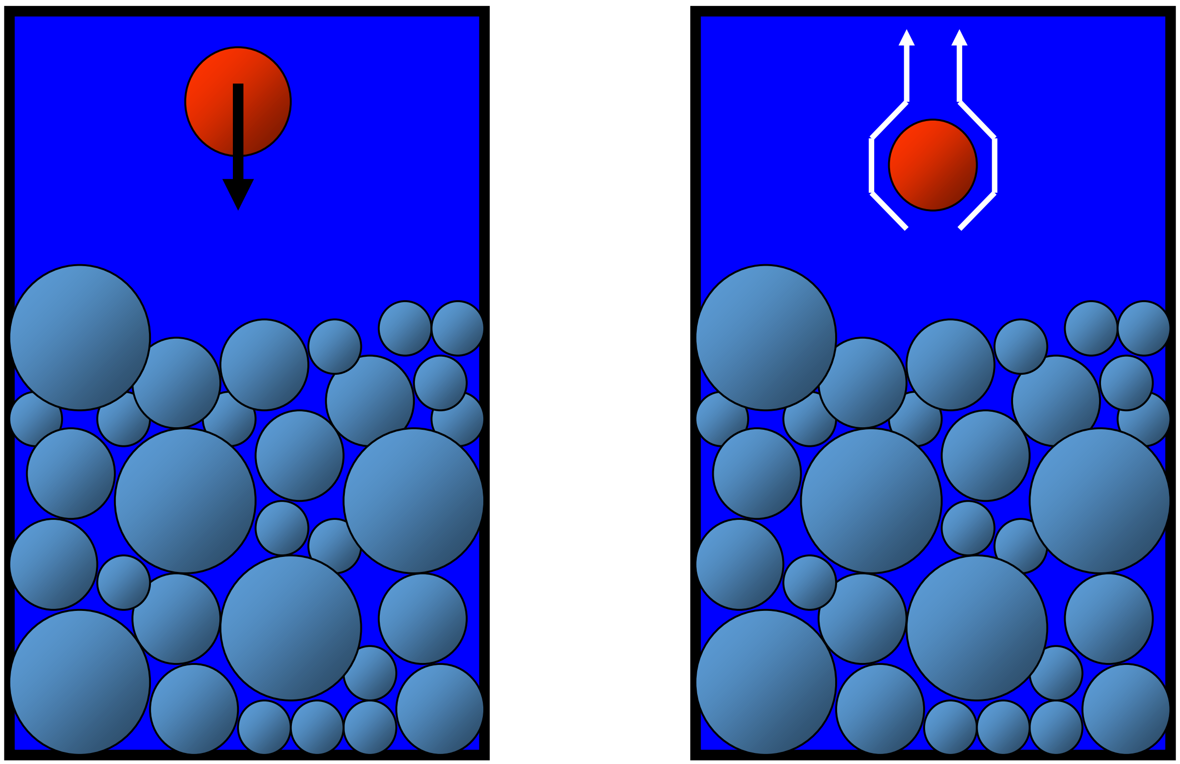
- Particles are discrete entities (cannot be subdivided like a fluid)

Particles Are NOT Fluids



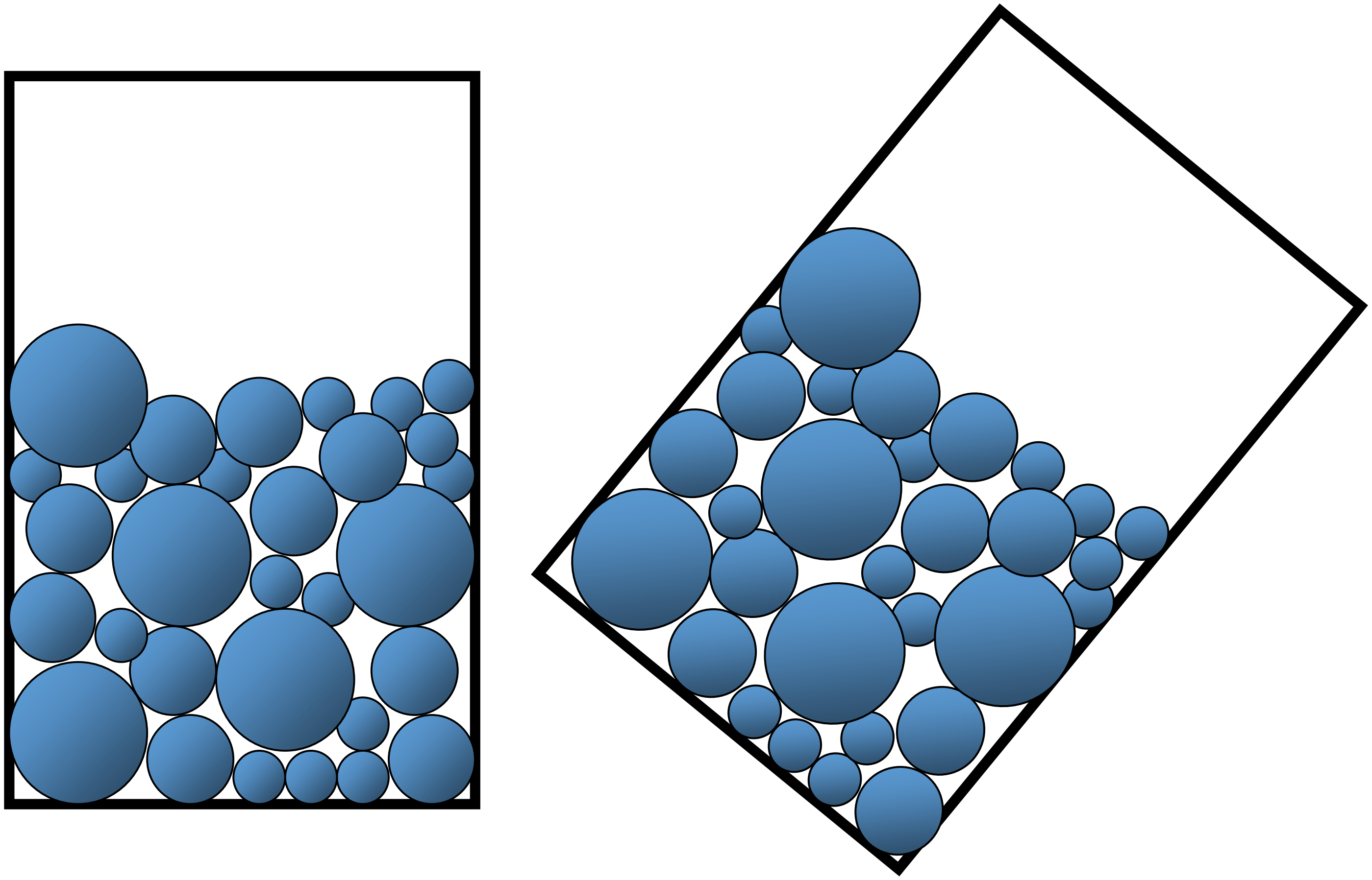
- Particles have a size distribution

Particles Are NOT Fluids



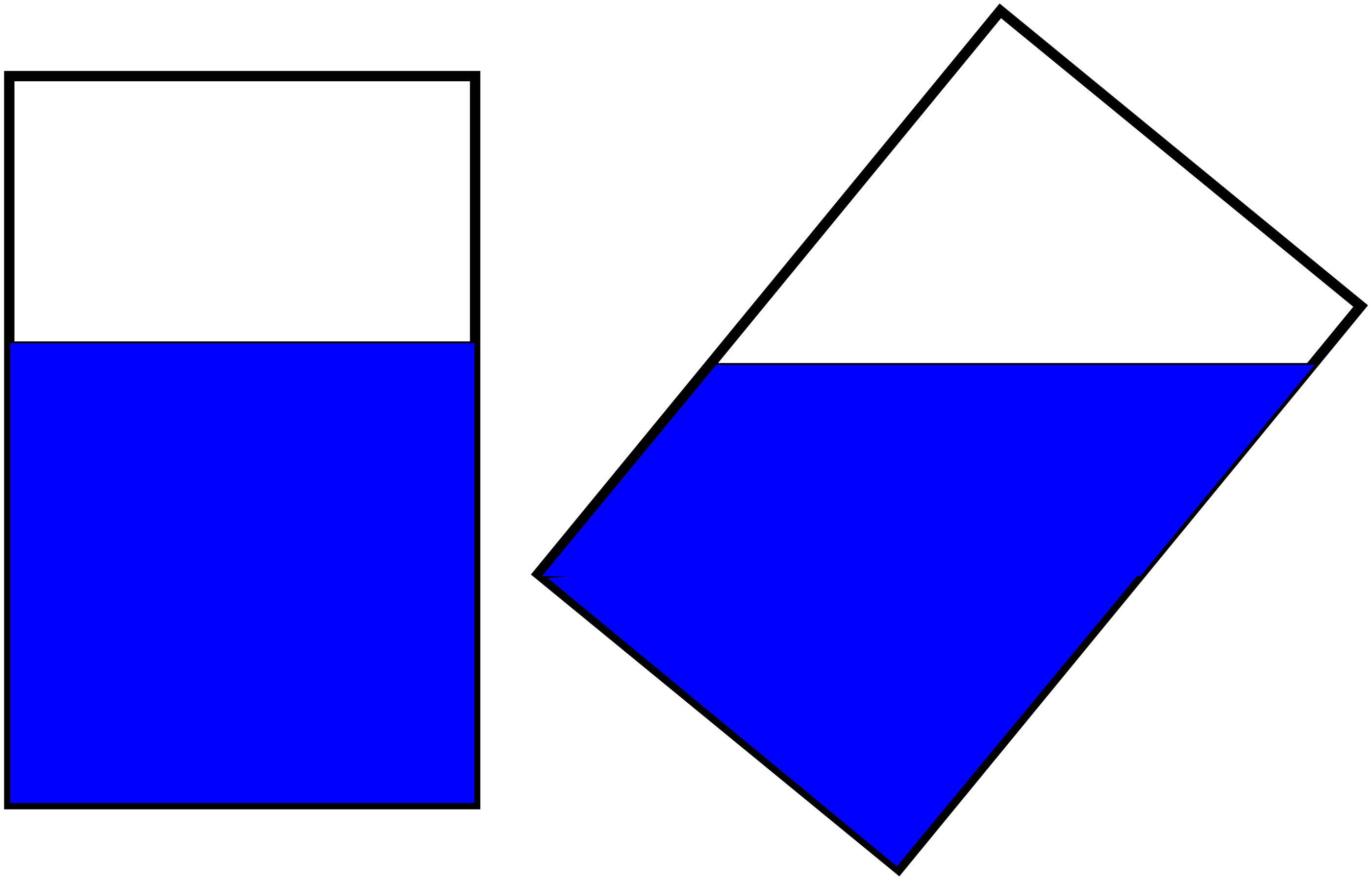
- Particles cannot completely fill a space
- Particles occupy a physical volume (and displace fluid)

Particles Are NOT Fluids



- Particles ***can*** support a shear stress

Particles Are NOT Fluids

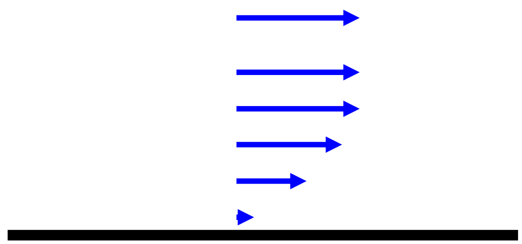


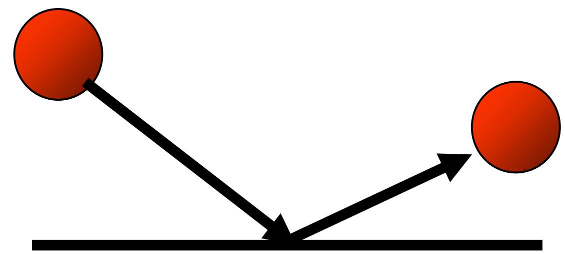
- Fluids ***cannot*** support a shear stress

Particles Are NOT Fluids

Other considerations

- Coupling between particles and fluids
- Wall treatment



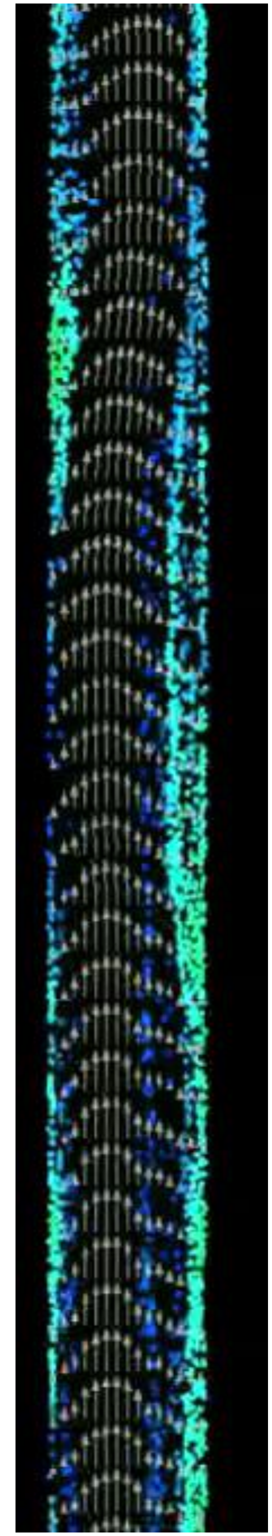


- Boundary treatment
- Thermal, chemistry, …

Modeling Fluid - Particle Flows

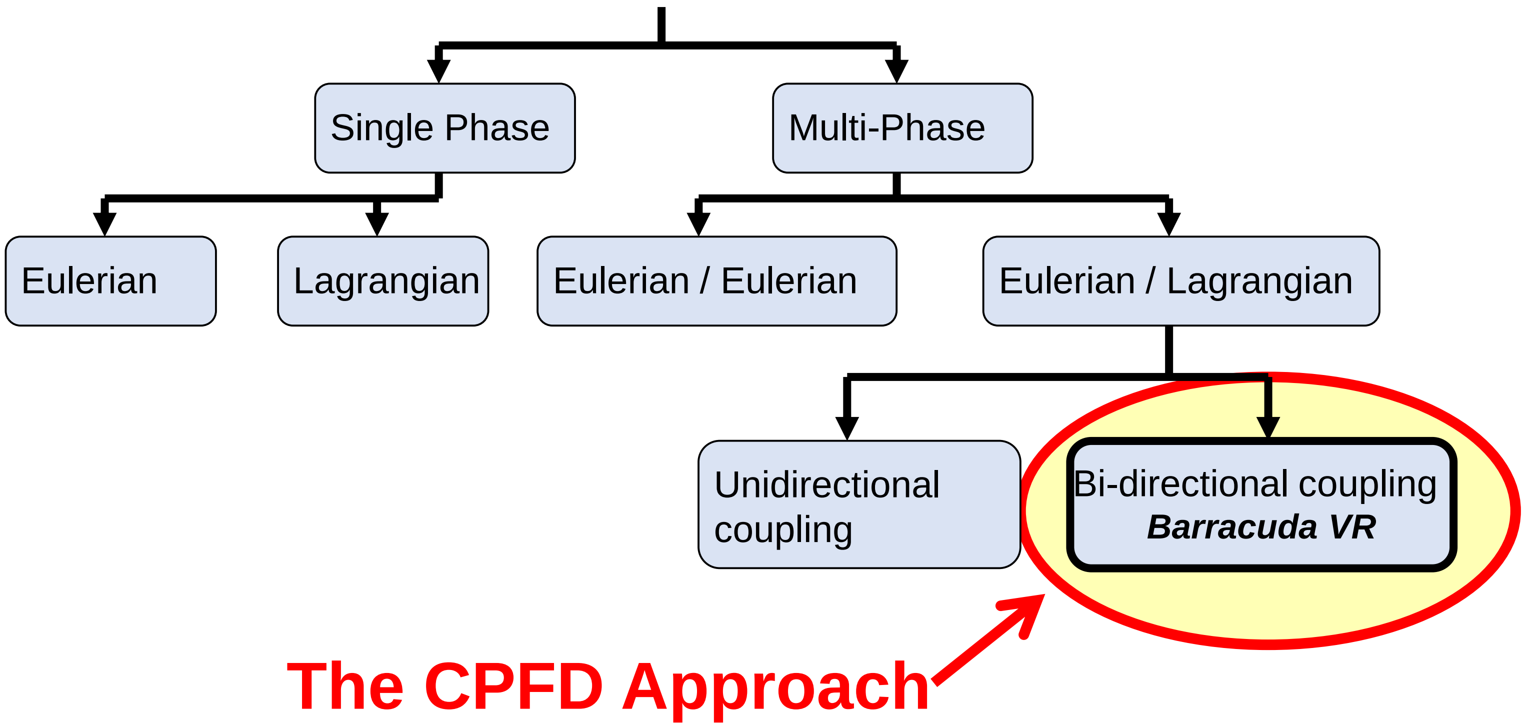
- To accurately simulate fluid-particle flows, one must model the effects of:
  - Drag and coupling
    - Dilute flows (< 1% by volume)
    - Dense flows (up to close pack)
  - Many particle sizes or size distribution
  - Multiple types of particles (size, density, composition)
  - Particle interactions (walls, other particles)
  - Heat transfer
  - Chemical reactions
    - Gas-phase (homogeneous)
    - Gas + particles (heterogeneous)
    - Changing particle composition

- What approaches can be used?

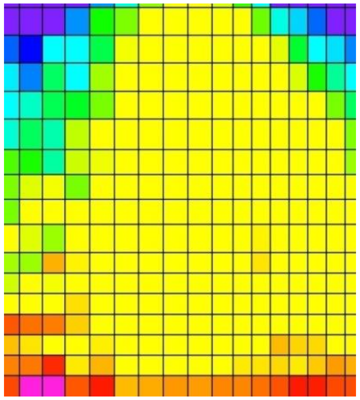


Approaches to Particle Flow Modeling

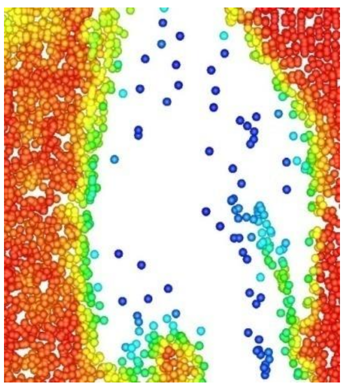
- There are different approaches to modeling particle flows (non-exhaustive listing)



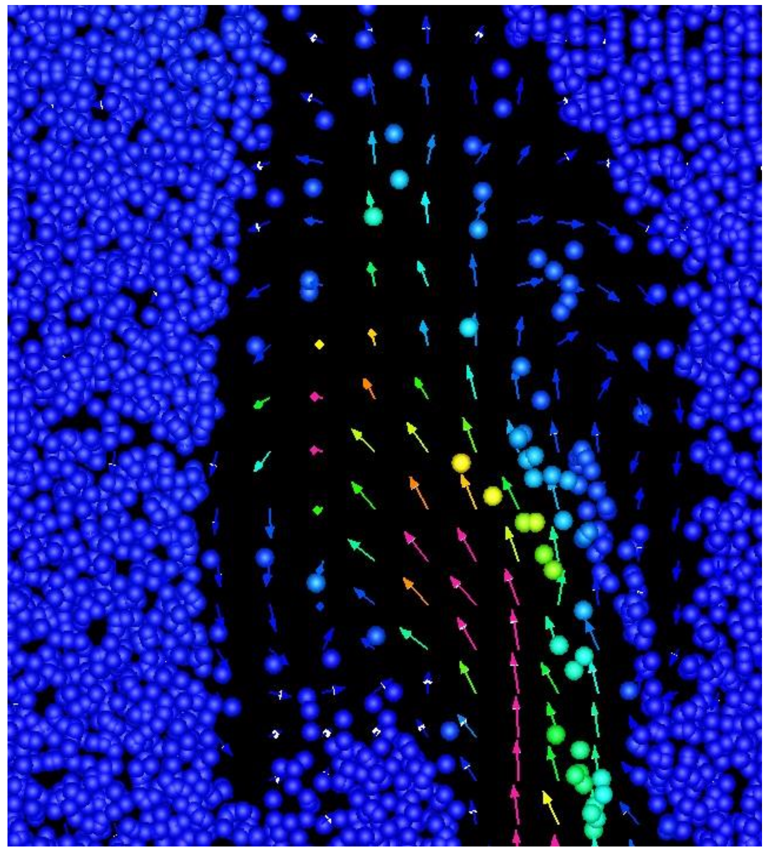
The CPFD Approach



Fluid equations
Continuous
Solved on the grid



Particle equations
Discrete
Gridless



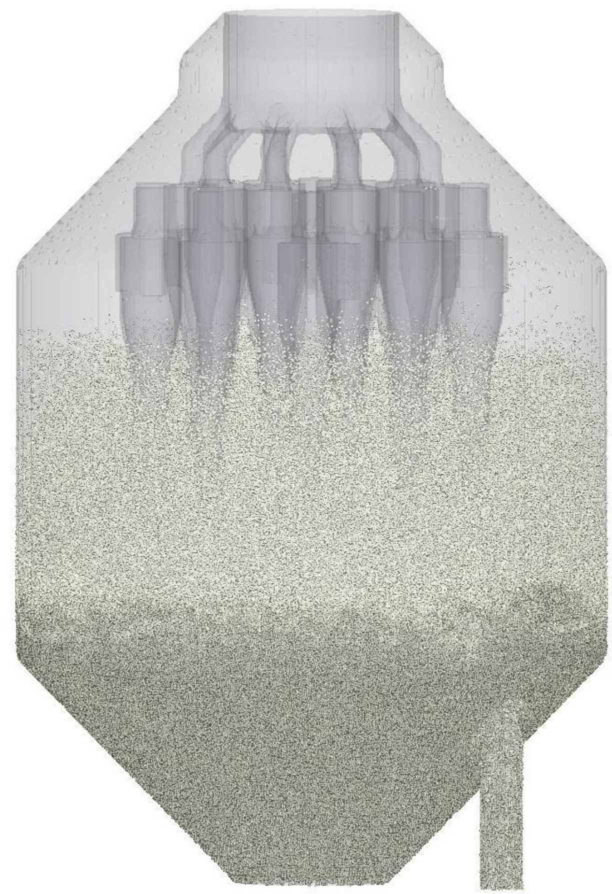
Fluid affects particles (aerodynamic / hydrodynamic drag)

Particles affect fluid (displacement, pressure drop)

Bi-directionally coupled (tight / implicit coupling)

The CPFD Approach

- Major Challenges and Solutions
    1. **What about the large number of particles?**
        - **Lesser number of computational particles**
        - The particle field is resolved by using a reasonable number of computational particles
        - Each computational particle represents one or more actual particle(s) with identical physical properties
        - The physics are computed on the individual particle (e.g. drag based on size, chemistry, etc.)
        - All changes experienced by the computational particle are applied to all actual particles represented by that computational particle (proper fluid displacement)
        - Many CPFD calculations utilize between 500,000 and 5,000,000 computational particles

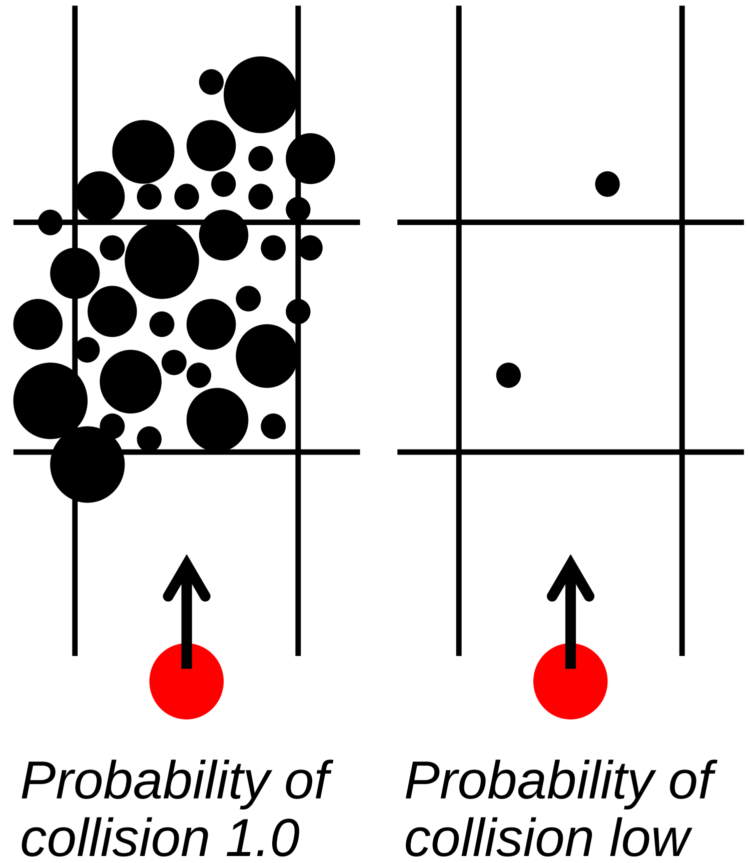


Example: Commercial regenerator:
2e+15 real particles
2.6e+6 computational particles

The CPFD Approach

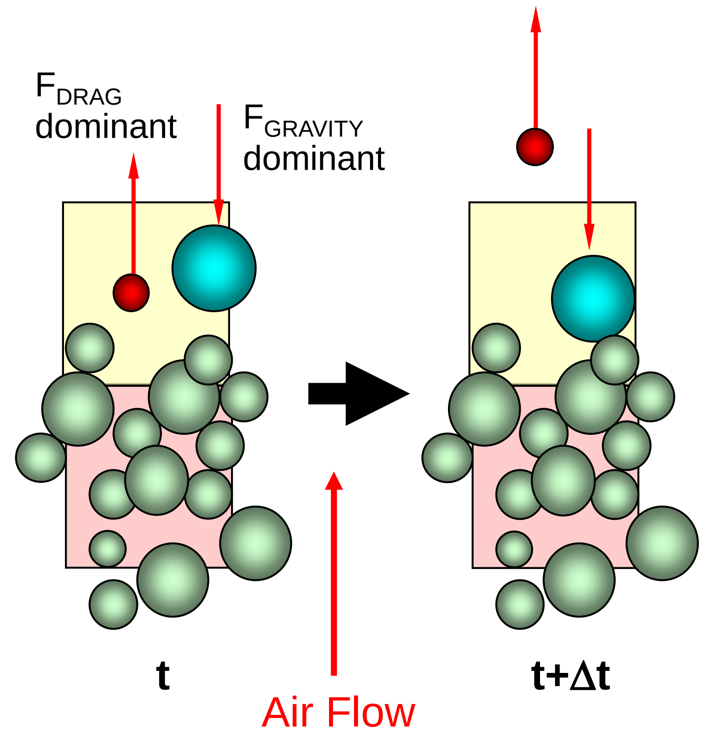
- Major Challenges and Solutions
  1. **What about the large number of particles?**
     - **Lesser number of computational particles**
  2. **What about particle contact and collision?**
     - **Modeled, rather than directly computed**

  - Collision detection can be prohibitive with millions of computational particles
  - Rather than computing **which particle** a given computational particle will impact, the CPFD method is more concerned with the question **“is a collision likely to occur?”**
  - The collisions are then subjected to various models
    - Enduring contact at close-pack handled via a non-linear stress tensor
    - BGK-type collisional damping



The CPFD Approach

- Major Challenges and Solutions
  1. **What about the large number of particles?**
     - **Lesser number of computational particles**
  2. **What about particle contact and collision?**
     - **Modeled, rather than directly computed**
  3. **What about inter-phase coupling?**
     - **Inter-phase interpolation operators, and tight, bi-directional coupling**



- Different particles experience different motion, even though both are in the same cell
- All sub-grid particle motion is coupled back to the fluid phase momentum equation

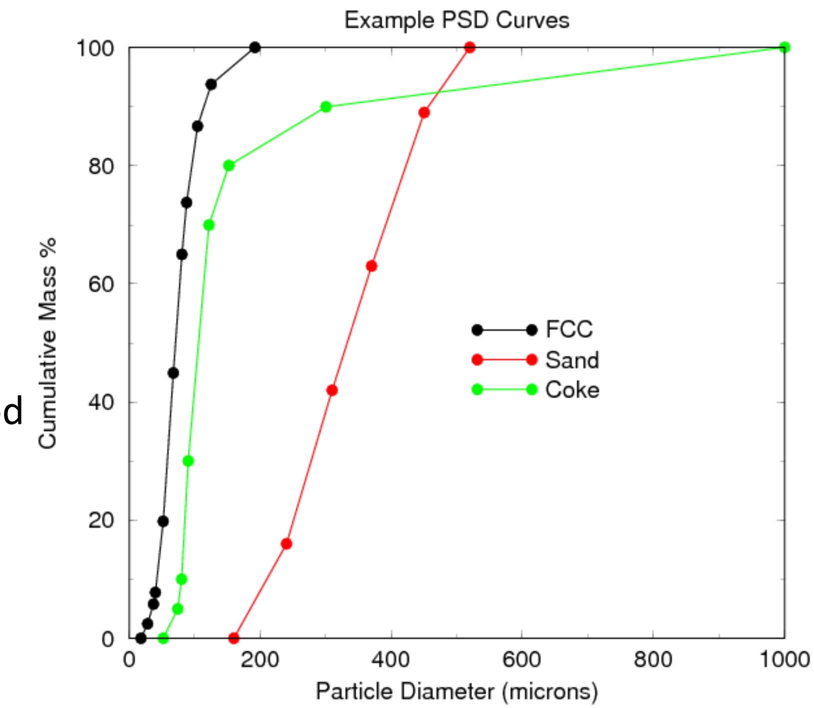
Advantages and Disadvantages

Advantages

PSD

Disadvantages

- Barracuda accepts full Particle Size Distribution (PSD) information for each particle species, since each Lagrangian particle inherently has its own size.
- Particle size is very important in fluidization behavior.
- The entire PSD, not just the d_{50} or d_{sv}, can be important.
- This is a distinct advantage of the CPFD method compared with an Eulerian multiphase approach.



Advantages and Disadvantages

Advantages	PSD **Erosion**
Disadvantages	

- Because each computational particle is a Lagrangian entity, it is known when a particle hits a wall surface.
- The erosion on the wall due to the particle impact can be estimated.
- An erosion index calculation is dependent on the particle mass, speed and impact angle.
- Typical functional form: $C_\alpha m_p u_p^{3.5}$
- Angle coefficient, C_α, is dependent upon the surface material (steel, refractory, etc.).
- This is a distinct advantage of the CPFD method compared with an Eulerian multiphase approach.

Isovolume of regions with high predicted erosion on a cyclone barrel.

Advantages and Disadvantages

Advantages

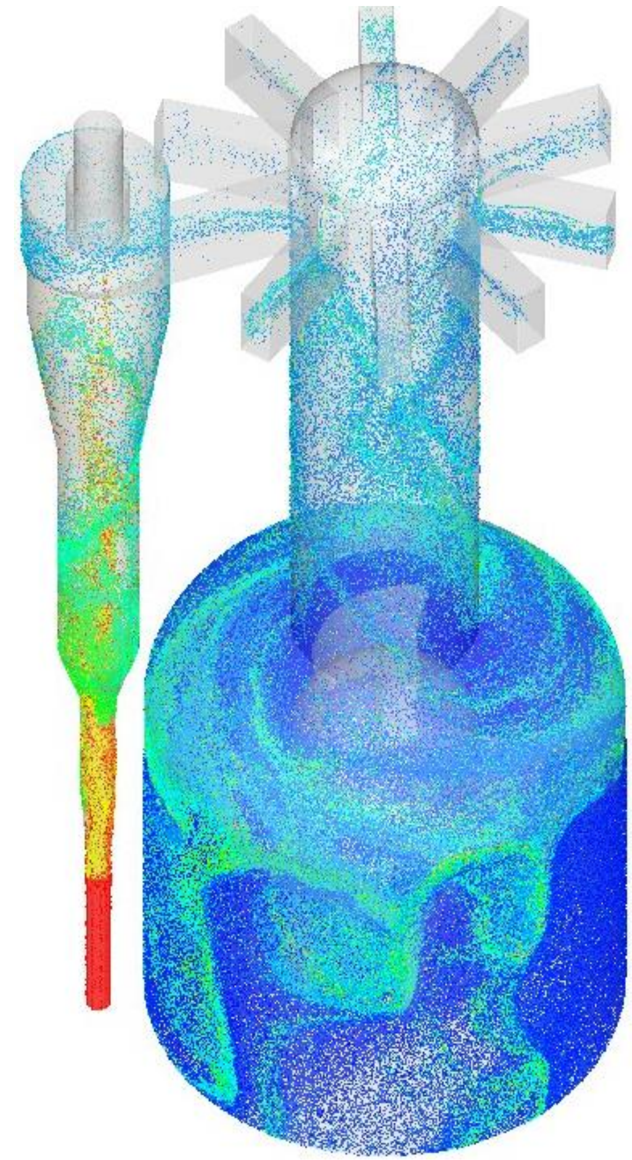
PSD

Erosion

Number of particles

Disadvantages

- An industrial reactor could have 10^{16} or more particles in it at a given time.
- With today's computing power, it is not feasible to track the motion, energy, and composition of every individual particle.
- The CPFD method, with its computational particle approximation, is able to simulate real systems with reasonable speed and accuracy.
- This is a distinct advantage of the CPFD method compared with both CFD-DEM or Lattice-Boltzman approaches.

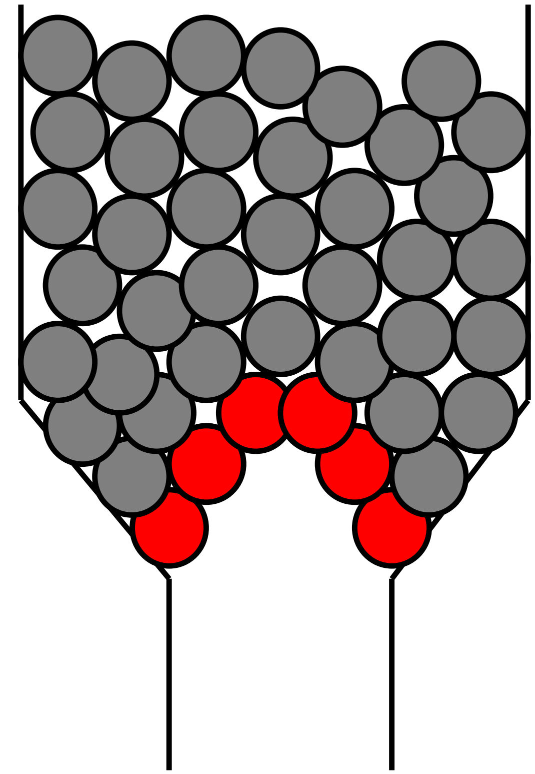


FCC Reactor Separation Unit
3e+12 real particles
1.6e+6 computational particles

Advantages and Disadvantages

Advantages	PSD Erosion Number of particles
Disadvantages	**Direct particle contact**

- Direct particle collisions and inter-particle contacts are not explicitly computed using the CPFD method.
- The use of contact and collisional models, allows Barracuda VR to simulate real systems with large numbers of particles with reasonable speed and accuracy.
- However, this means that Barracuda is not well suited for situations where the direct contact of specific particles is critical to the problem (e.g. particle bridging, defluidized beds, non-aerated hopper flows, etc.).
- Perhaps a DEM or CFD-DEM solution would be better-suited for these classes of problems.



Particle bridges are dependent upon precise inter-particle contact points. This is not a good problem for a CPFD code.

Advantages and Disadvantages

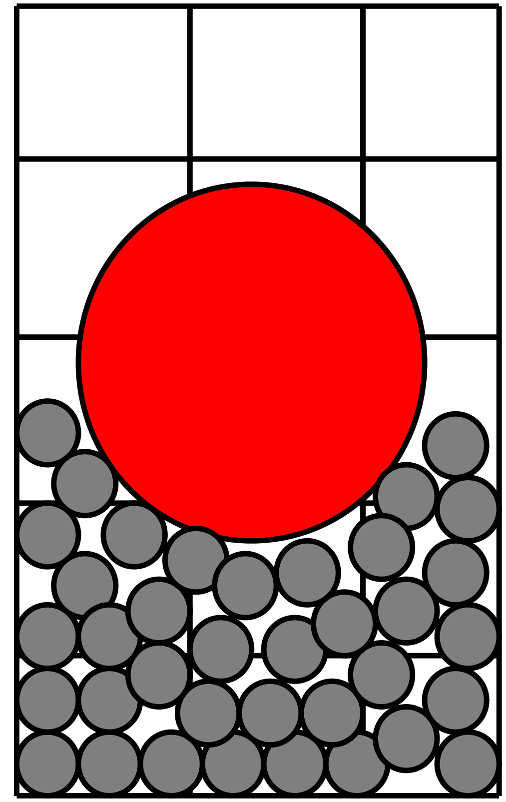
Advantages

- PSD
- Erosion
- Number of particles

Disadvantages

- Direct particle contact
- **Multiple particles must fit in cells**

- The CPFD method presupposes that a statistically-significant number of computational particles fit within a computational cell.
- This means that Barracuda is not well suited for situations where the particles are large compared with the geometry. Examples include:
  - Cases with very few particles
  - Cases with very large particles
- Perhaps a CFD code with fluid-structure interaction, or a Lattice-Boltzman approach would be better-suited for these classes of problems.



The particles are large compared with the computational cells. This is not a good problem for a CPFD code.

More Information & Publications

- This introductory presentation is meant to provide a general overview of the CPFD implementation of the MP-PIC method.

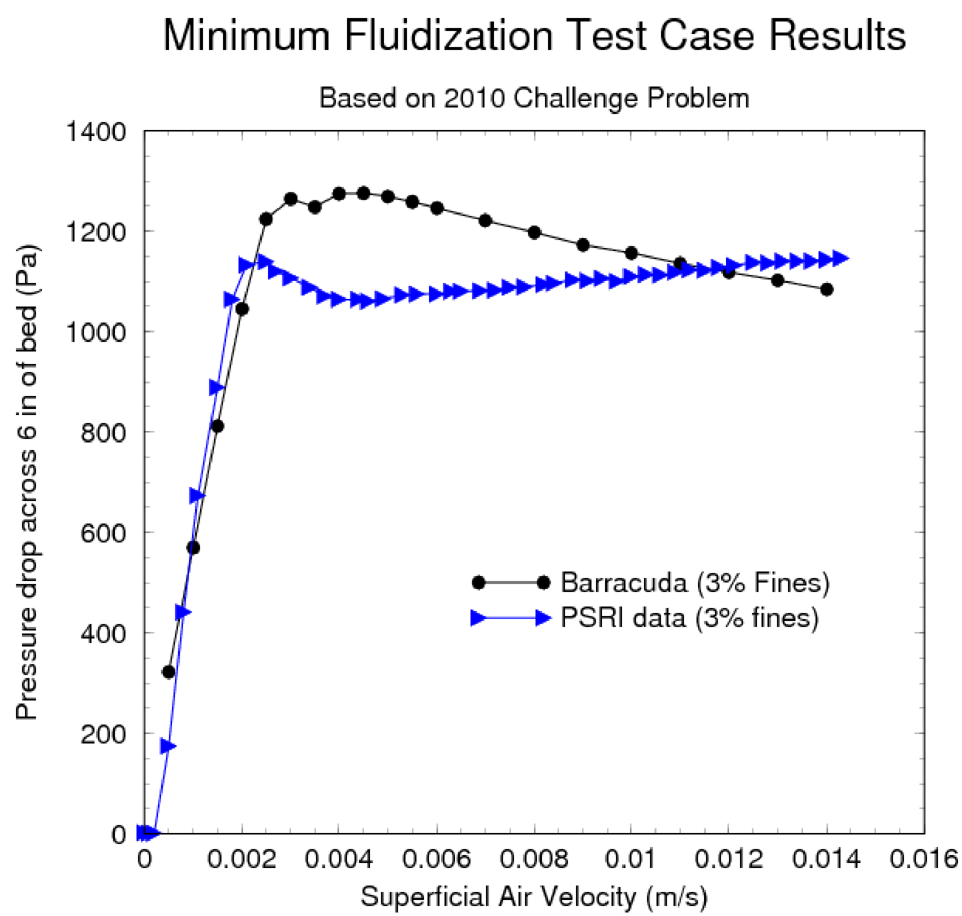
  - Detailed CPFD theory has been intentionally avoided, since the Barracuda new user training course is focused on practical application of Barracuda to solve industrial problems.

- For detailed discussions of the mathematics behind CPFD, please refer to our published journal and conference papers. These can be downloaded from our customer support site at:

http://cpfd-software.com/customer-support/downloads/category/publications-and-documentation

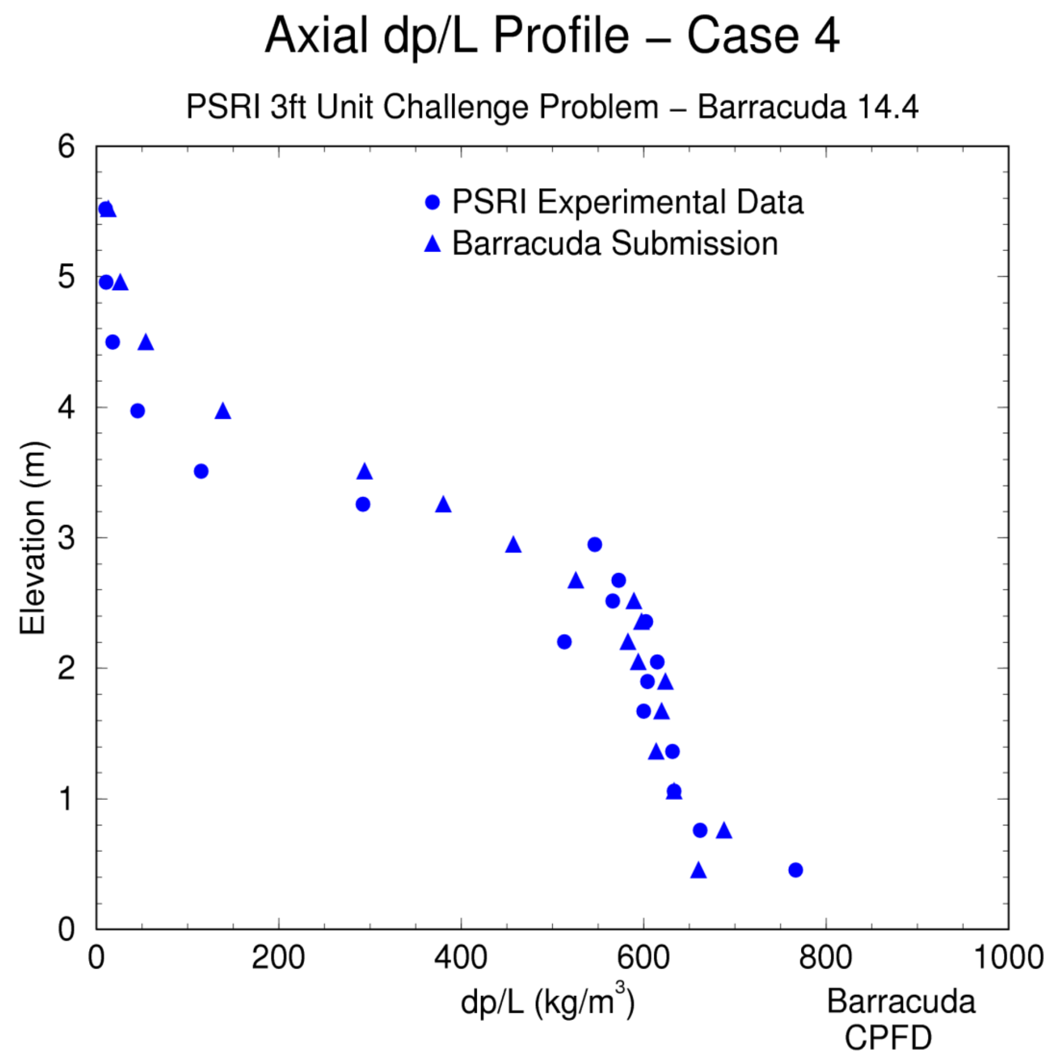
Validation: U_{mf}

- The minimum fluidization velocity, U_{mf}, curve of a particle species can be experimentally measured.
- As part of the 2010 NETL/PSRI Challenge Problem, U_{mf} data was provided as a validation point for modelers.
- Barracuda was able to match the U_{mf} curve reasonably well.
- Different boundary conditions might help to further improve agreement.

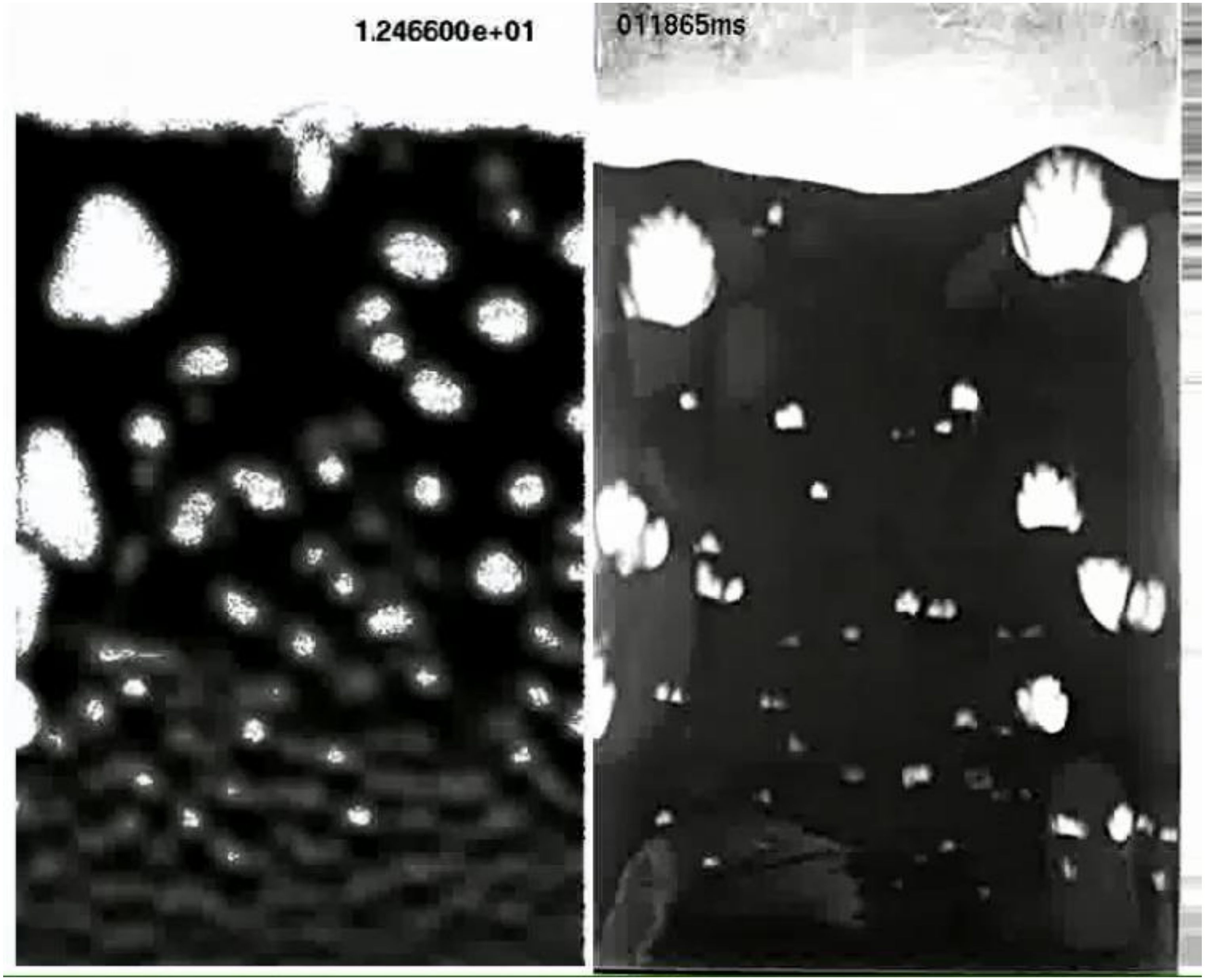


Validation: dP/dz

- 2010 NETL/PSRI Challenge Problem



Validation: 2D Bed



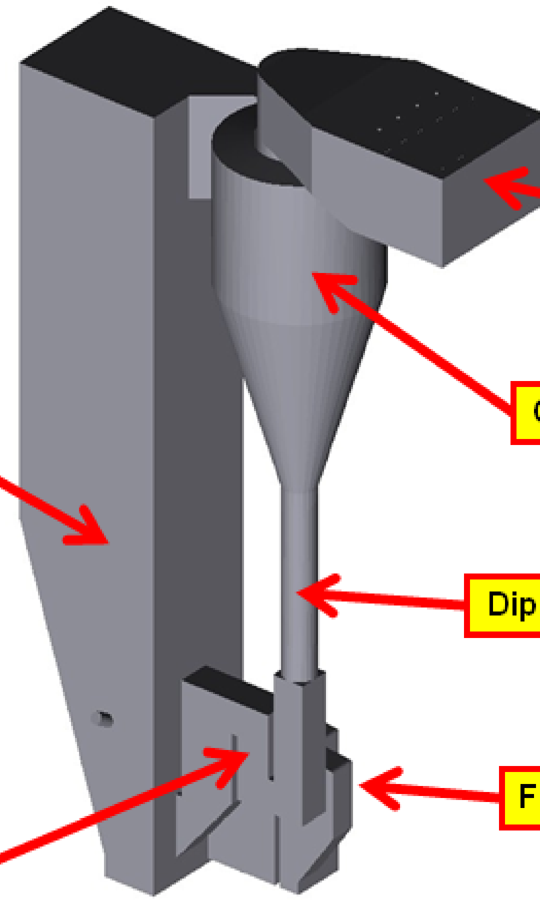
Validation: PSRI Jet Cup

- Unexpected validation due to non-intuitive particle-fluid flow behavior.

Example 1:
Circulating Fluidized Bed Biomass Combustor

Introduction

30 m high

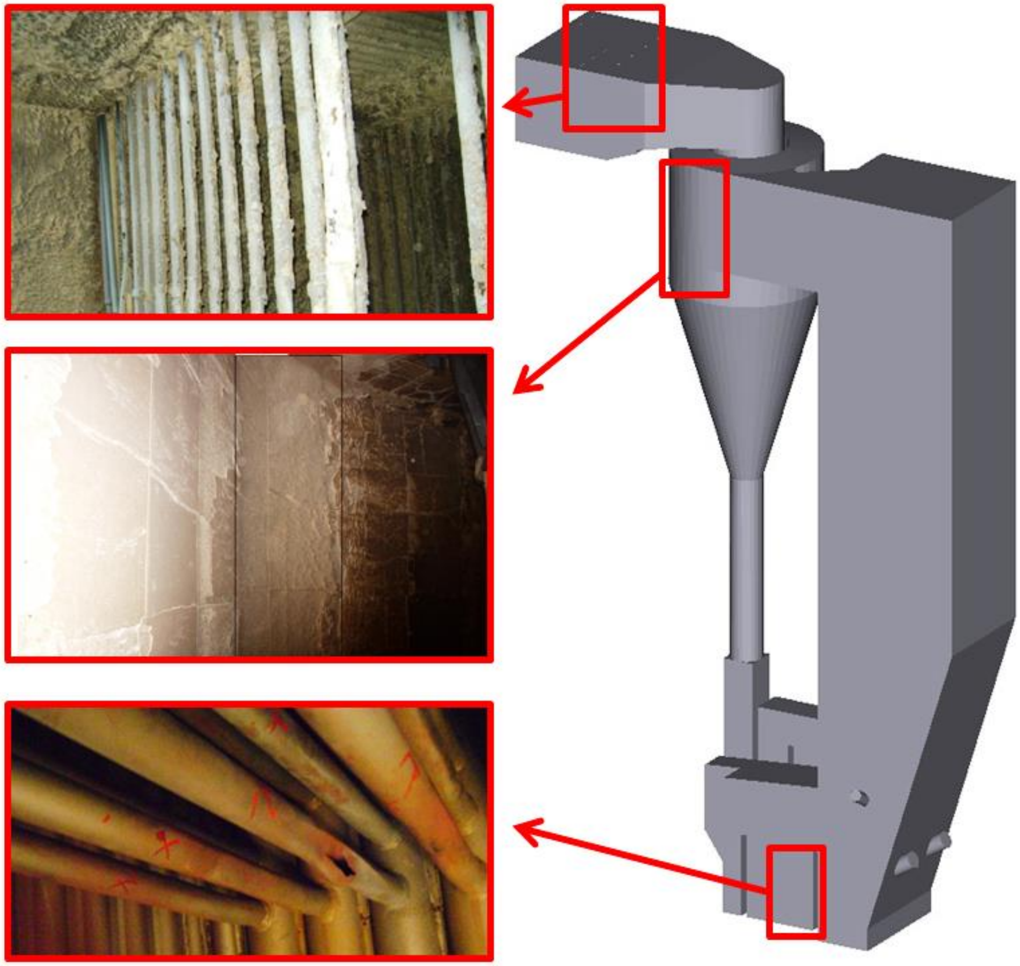


- The 40 MW Strongoli power plant, located in the Calabria region of Italy, is fueled by 100% biomass sources
  - Wood biomass
  - Exhausted olive residues
  - Palm kernel shells
- Case study courtesy of

BiomasseItalia
Energy today, Blue tomorrow

Erosion Case Study

- The plant operator, Biomasse Italia S.p.A., experienced excessive erosion in several locations
- The erosion in the cyclone inlet and suspension tube regions is the subject of this presentation
- This work was undertaken in 3 phases:
  - **Baseline assessment**. Understand the current and historic erosion, and the 3D, multiphase flow patterns causing the surface wear.
  - **Design alternatives assessment**. Model several alternatives for each component, to understand the effects of each proposed change on erosion and unit performance.
  - **Redesign assessment**. Evaluate the candidate final redesign, which may include several components of different design alternatives



Computational Grid

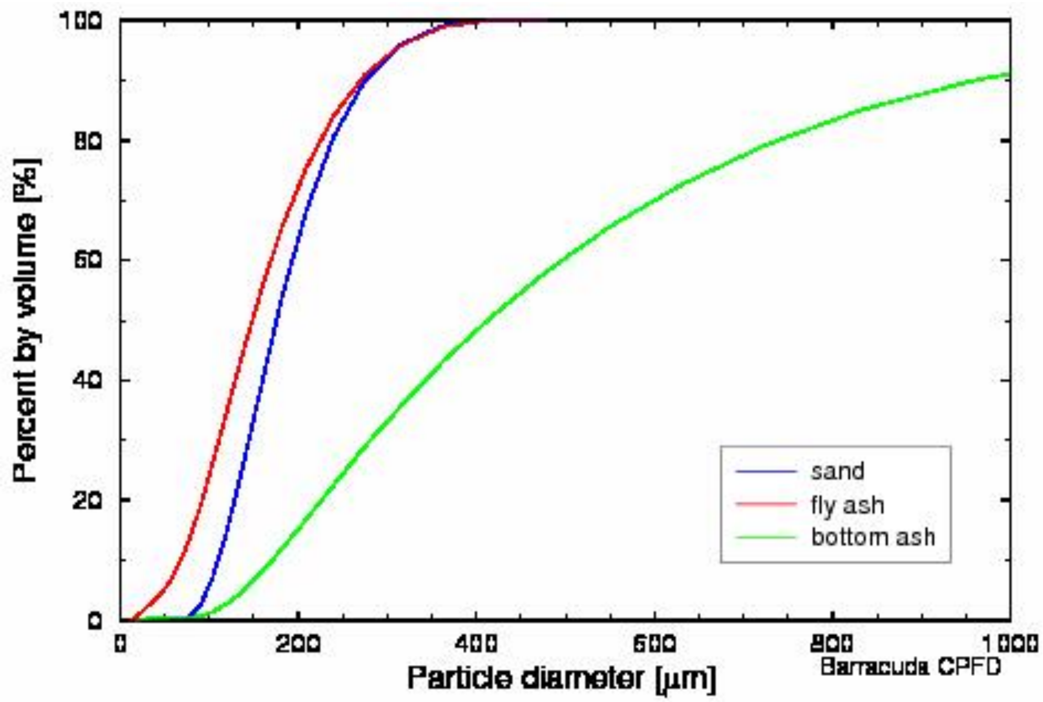
- A computational grid was cut from a 580,000 cell Cartesian mesh. The resulting numerical model included:
  - 172,000 computational cells (for scalar calculations, e.g. pressure)
  - 570,000 computational faces for vector calculations (e.g. gas velocities)
  - 1.5 million computational particles

- A grid generator methodology appropriate to Computational Particle Fluid Dynamics (CPFD)[1] calculations was used. CPFD grid walls act as:
  – boundaries of fluid control volumes
  – obstacles for particle bounce models

- The CPFD method computes:
  – The gas phase in an Eulerian frame of reference (i.e. on the grid)
  – The solids phase as discrete (Lagrangian, gridless)
  – The bidirectional coupling of the phases (aerodynamic drag, sub-grid solids displacement of the fluid)

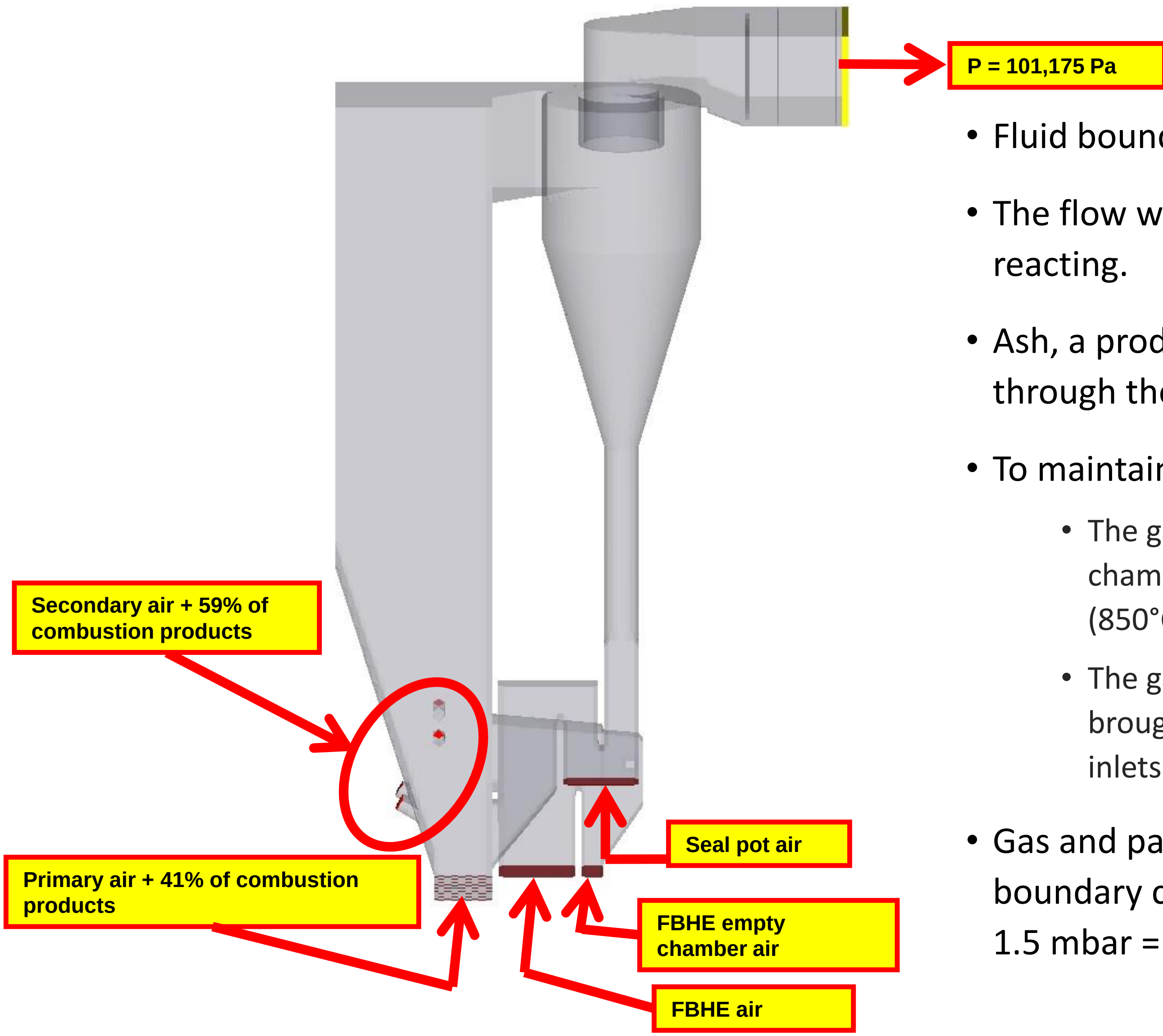
[1] The computational particle fluid dynamic (CPFD) numerical method was developed by D. Snider at CPFD Software, LLC

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 plot)
- PSD taken from plant data
- 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/m^3
  - Ash: 1500 kg/m^3
- Up to 1.5 million computational particles were used to represent the solids phase

Flows and Assumptions

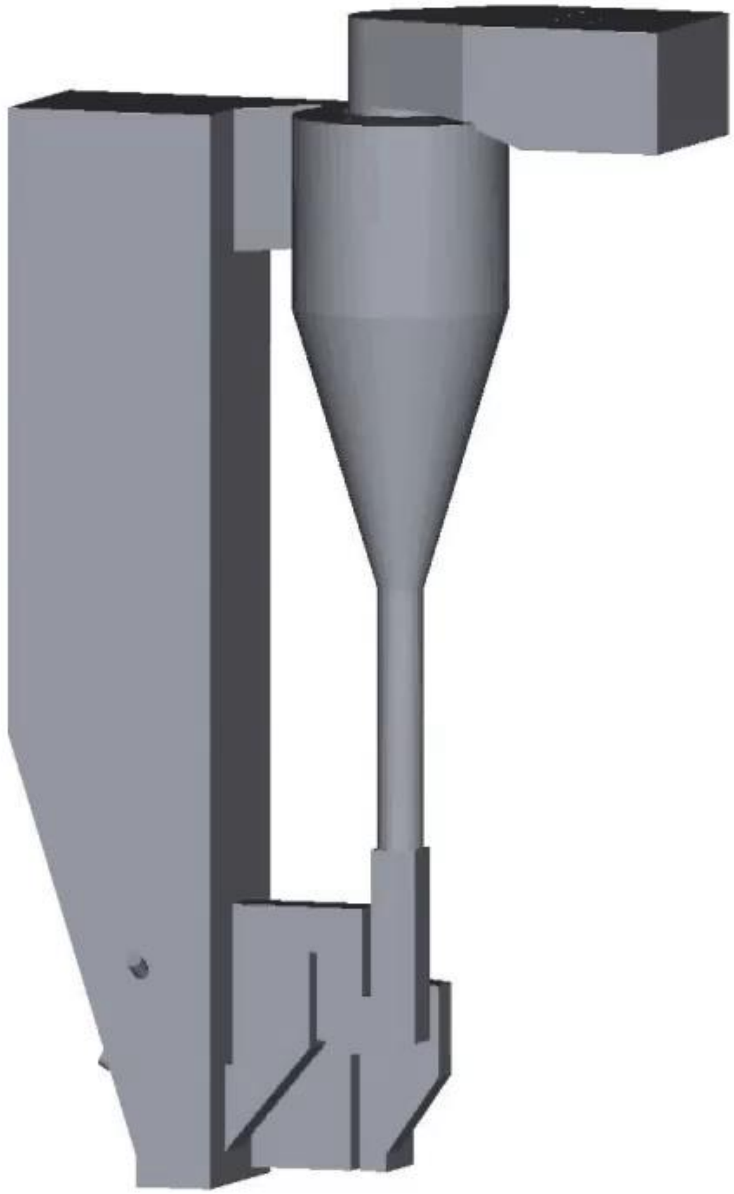


- Fluid boundary conditions were applied as shown
- The flow was modeled as isothermal and non-reacting.
- Ash, a product of combustion, was brought in through the secondary air inlets
- To maintain proper cyclone inlet velocities:
    - The gas temperature in the upper combustion chamber was used as the isothermal temperature (850°C)
    - The gas flow resulting from combustion products was brought in through the primary and secondary air inlets
- Gas and particles exit the domain at the pressure boundary condition defined on the cyclone outlet: 1.5 mbar = 101,175 Pa (absolute)

Example Courtesy of BiomasseItalia

CFB Simulation

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

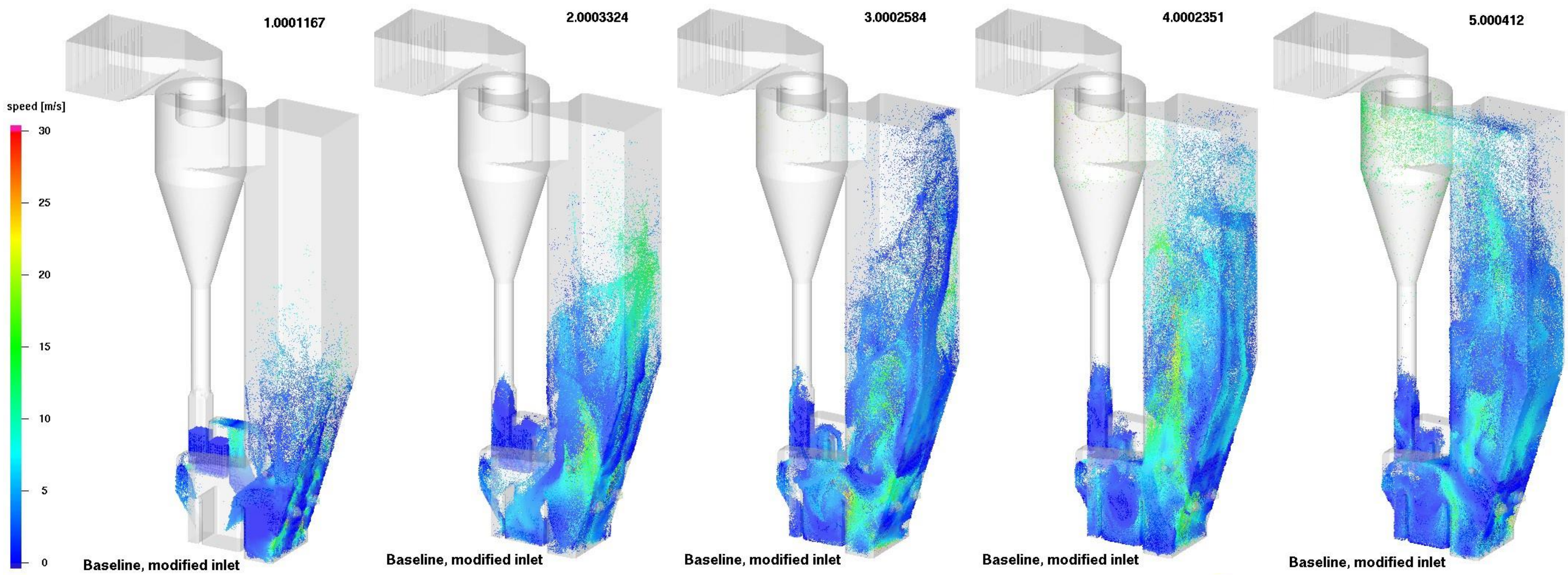


BARRACUDA

cpfd COMPUTATIONAL PARTICLE FLUID DYNAMICS

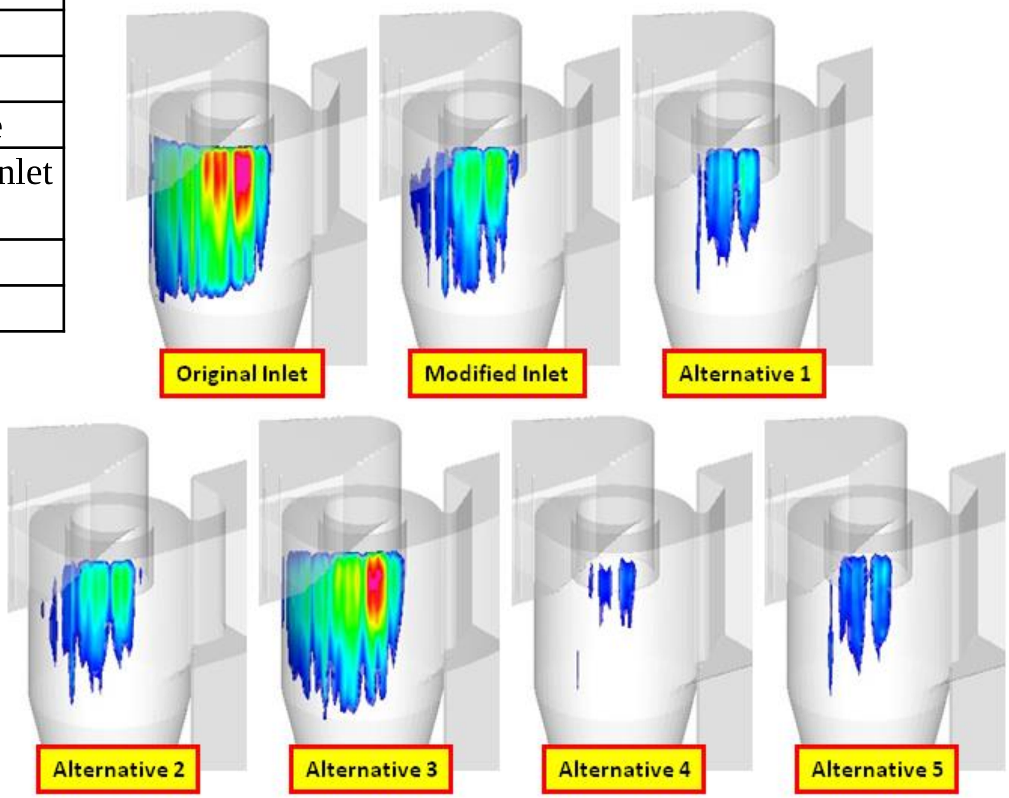
Calculation Runtime

- Approximately 20 seconds were required to ensure a quasi-steady-state solution. Time-averaging and erosion tracking were activated after 20 seconds
- The calculations took approximately 5 weeks to reach 80 seconds on a single-CPU workstation computer in 2010
- The same calculation could be completed today in a few days



Erosion Validation and Optimization

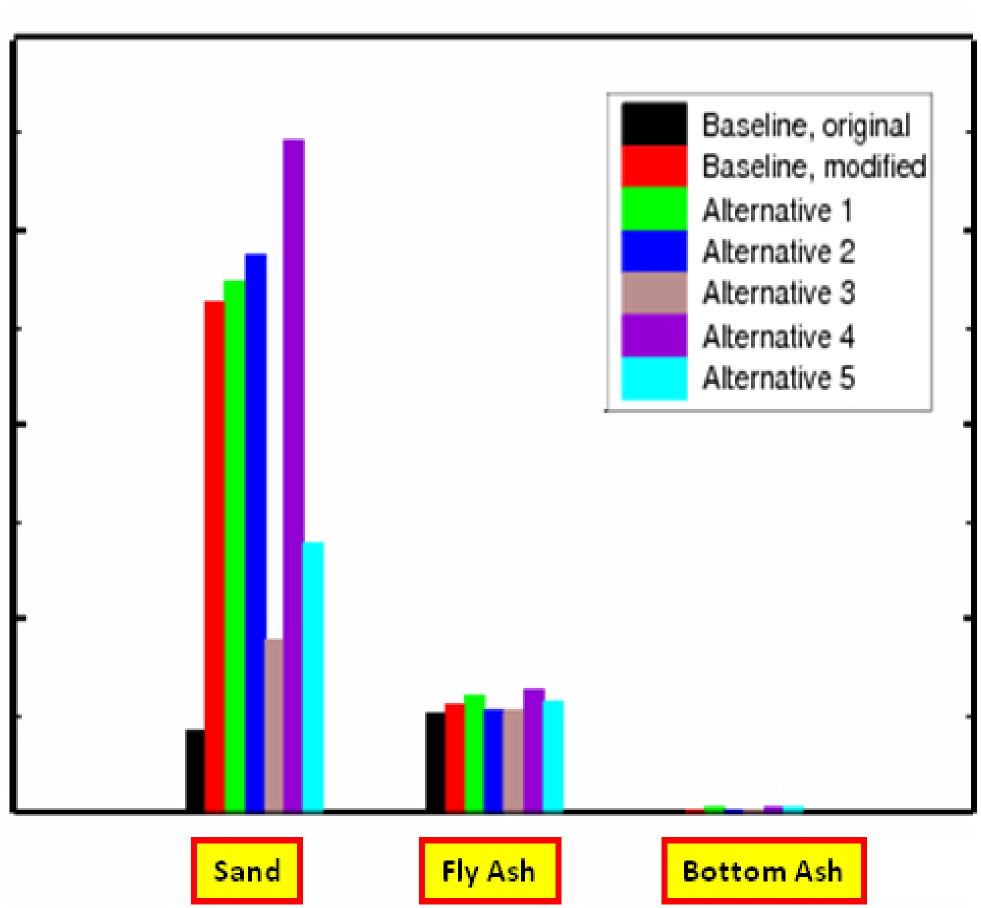
Inlet Design	Inlet area (percent increase from current design)	How the design differs from the current design
Original	-15%	Narrower inlet
Modified	no change	
Alternative 1	9%	Taller
Alternative 2	no change	Varied inside inlet curvature
Alternative 3	9%	Taller and varied outside inlet shape
Alternative 4	18%	Taller
Alternative 5	9%	Taller and narrower



- The baseline models verified that the calculation was able to predict the reduction in cyclone inlet erosion in the modified inlet case, compared with the original inlet geometry.
- The validated model was then used to compare the various alternatives with respect to cyclone inlet erosion.
- Alternatives 1, 4 and 5 predict a further reduction in erosion, compared with the current design

Erosion Validation and Optimization

- The modifications to the cyclone inlet also affected the cyclone efficiency
- The mass flow rates of particles through the suspension tube region was also studied
- Significant differences in the sand flow through the suspension tube regions was noted for the different designs
  - Alternatives 3 and 5 were predicted to have reduced erosion characteristics in the suspension tube region



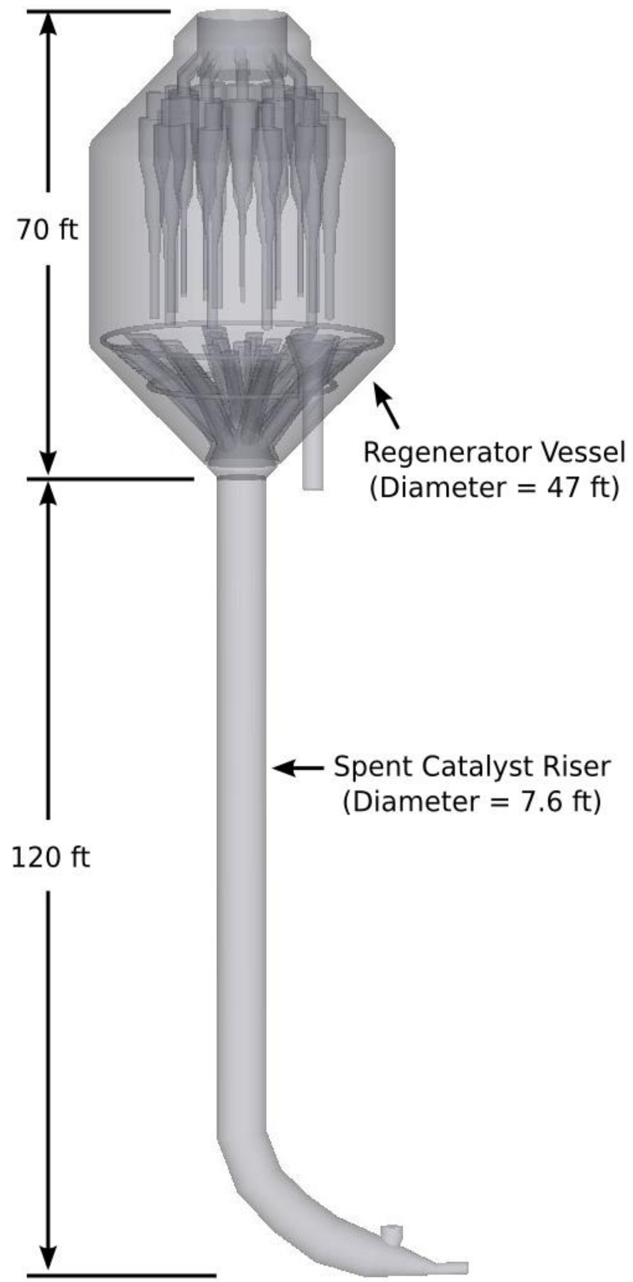
Conclusions

- The Barracuda model is capable of predicting the transient, multiphase flow and erosion characteristics for a full-scale CFB combustor

- The model was validated based on historical operational experience at the plant. At the last turn-around prior to this study:
    - Cyclone inlet erosion was decreased (captured by the model)
    - Suspension tube erosion was increased (captured by the model)

- The validated model was then used to assess various alternate designs, and compare predicted performance for multiple objectives:
    - minimize cyclone inlet erosion
    - minimize suspension tube erosion
    - minimize cyclone pressure drop
    - ensure modifications do not degrade performance elsewhere in the complex circulating system

Example 2:
Commercial FCC Regenerator



Introduction

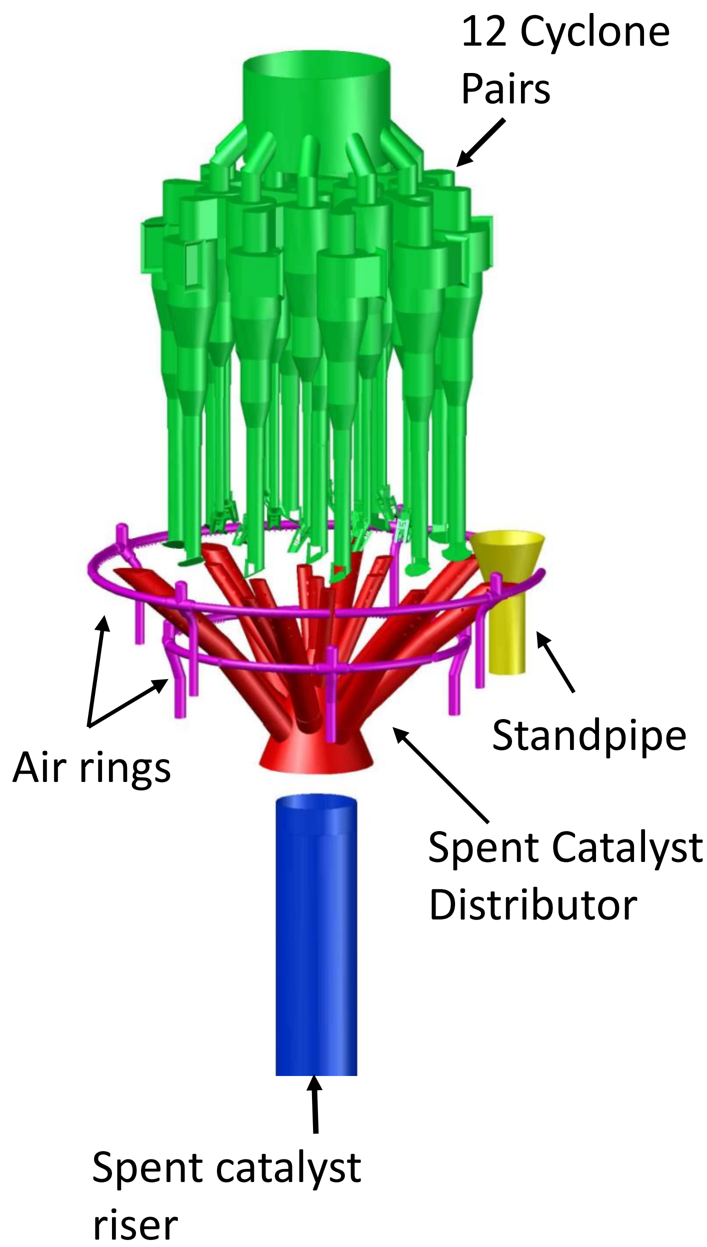
- The Barracuda Virtual Reactor was used to simulate an operating FCC regenerator unit.

- The regenerator has known afterburn problems (~100°F).

- The purposes of the simulation were to:
    - Understand the root cause of the afterburn (primary)
    - Act as the basis for future studies to minimize afterburn (primary)
    - Act as the basis for future work aimed at minimizing SOx and NOx emissions (secondary)

Challenges

- Complex geometry
  - Vessel internals
  - Widely varying length scales
- Thermal, reacting, multiphase system
  - Afterburn (thermal)
  - Emissions (reactions)
  - All multiphase and multi-component
- Boundary and initial conditions
  - Scope of model
  - Particle withdrawal from standpipe
  - Initial conditions
    - Temperatures, particle compositions, etc.
  - Specification of coke composition



Multiple Model Strategy for Simulation

- The regenerator problem was broken down into three sub-models

Model 1. Spent cat riser

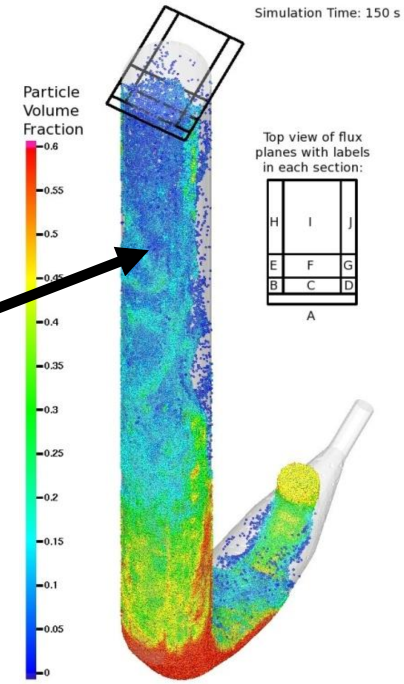
- To get boundary conditions for catalyst distributor

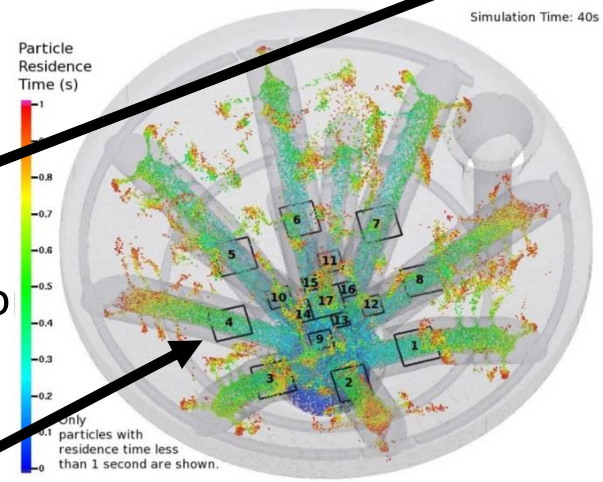
Model 2. Distributor arms

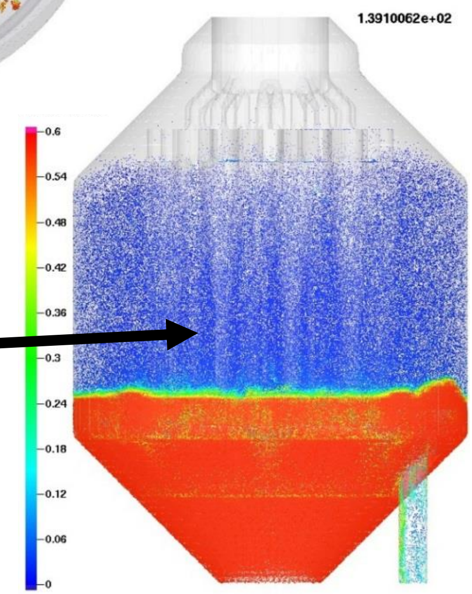
- To get boundary conditions for regenerator

Model 3. Full regenerator

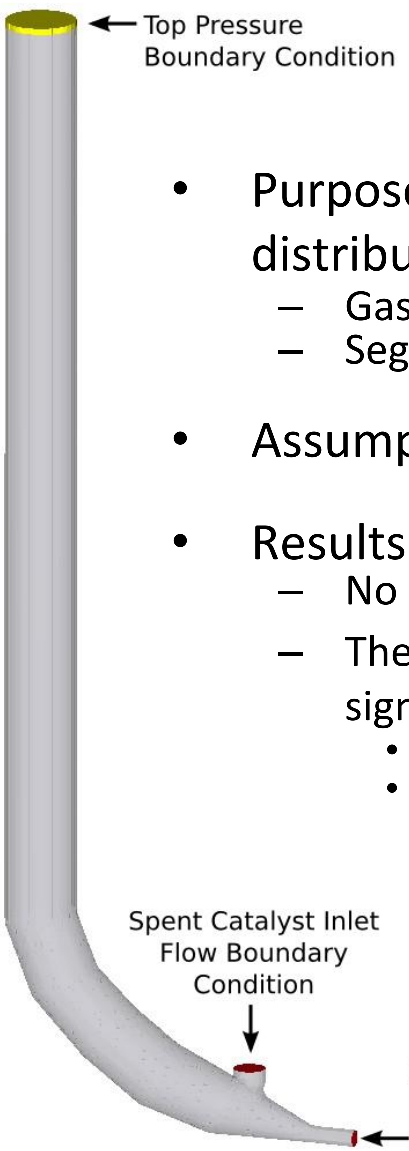
- To address afterburn and emissions questions



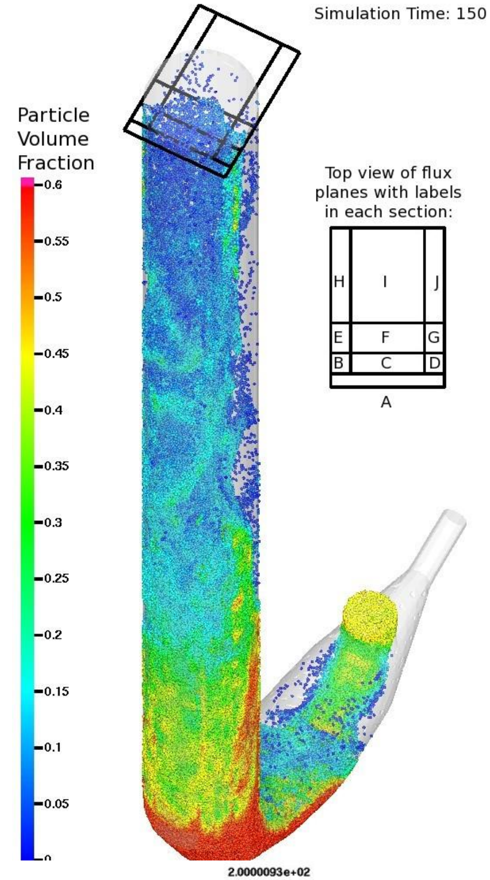


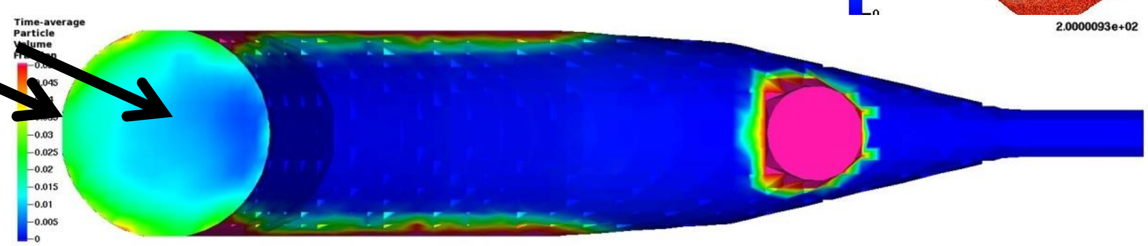


Model 1: Spent Catalyst Riser



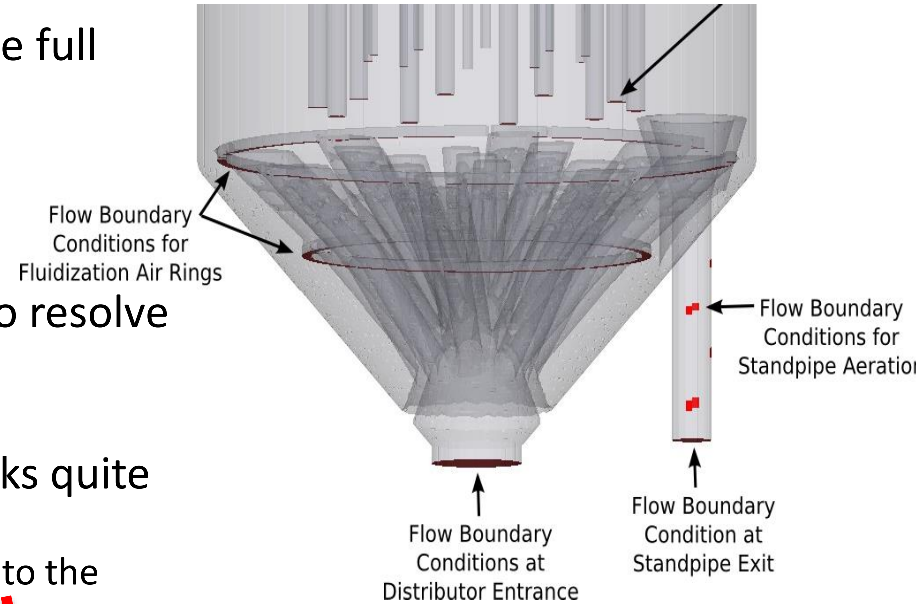
- Purpose: To get boundary conditions to catalyst distributor model
  - Gas and particle spatial distributions
  - Segregation by particle size, if any
- Assumptions: Isothermal, non-reacting
- Results:
  - No catalyst segregation by size was observed
  - The gas and particle mass fluxes were found to be significantly non-uniform upon exiting the top of the riser
    - **Near outer edge**: 275 kg/m²/s solids, 9.4 kg/m²/s gas
    - **Near center**: 170 kg/m²/s solids, 17 kg/m²/s gas

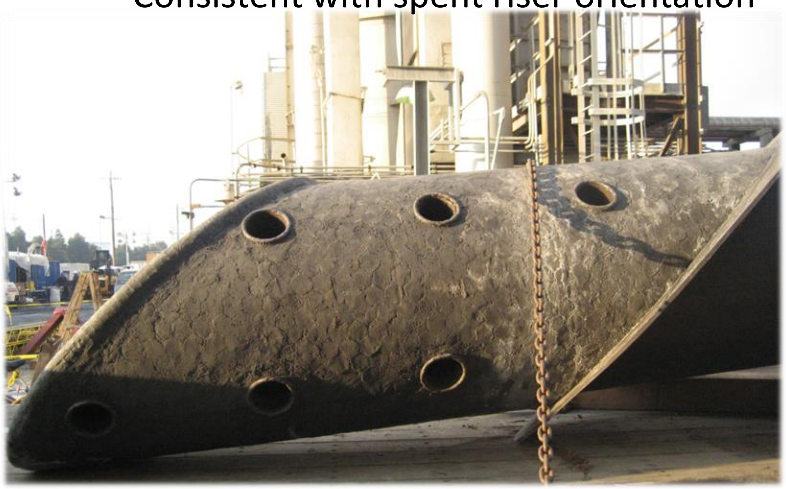


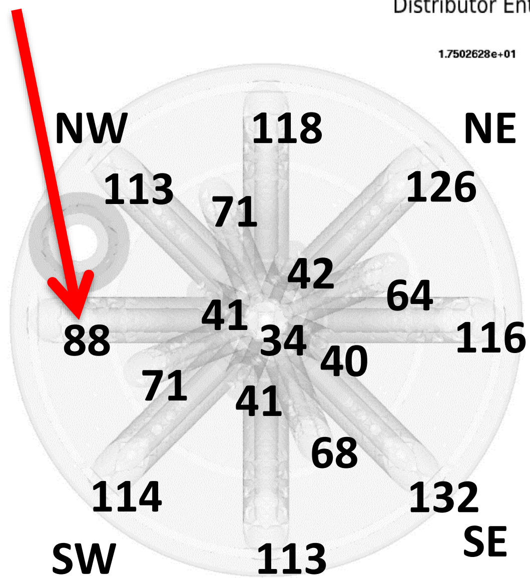


Model 2: Full Model Focused on Spent Catalyst Distributor Arms

- Purpose: To get boundary conditions to the full regenerator model
- Assumptions: Thermal + reacting
- Challenge: Relatively fine mesh required to resolve holes in distributor arms
- Results: The spent catalyst distributor works quite well
  - Loadings are slightly lower on the side closest to the regenerated catalyst standpipe
  - Consistent with spent riser orientation



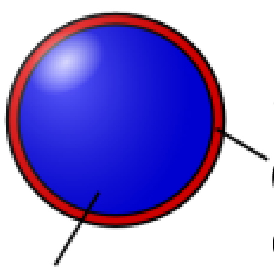




Spent catalyst loadings (lb/s)

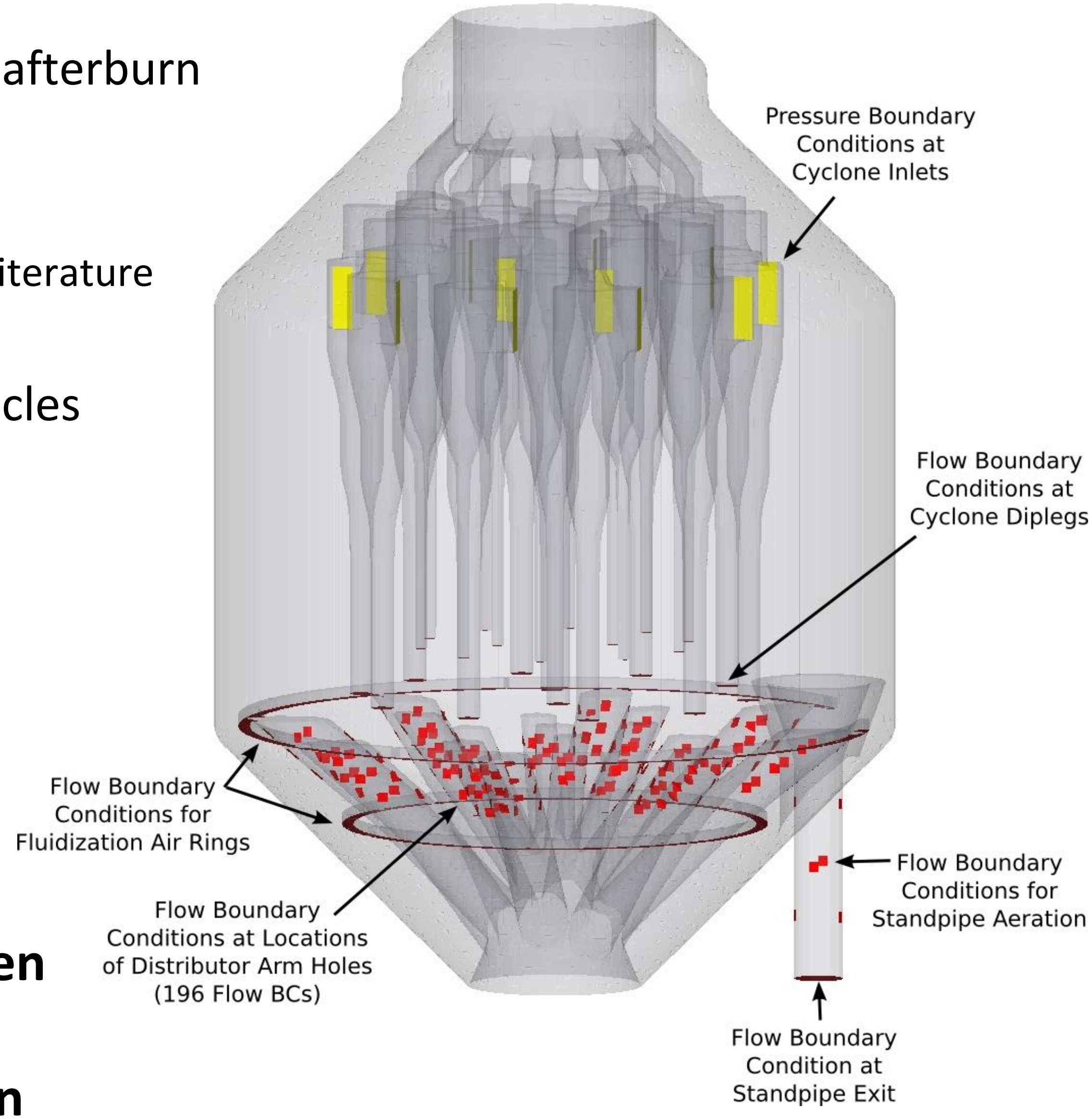
Model 3: Regenerator Vessel

- Purpose: Determine root cause of afterburn
- Assumptions: Thermal + reacting
  - Reactions and rates from the open literature
- Challenge: Discrete nature of particles
  - PSD
  - Multi-component composition
  - Temperature, etc.



Catalyst 99.3264%

Coke:
0.6048% carbon
0.0299% hydrogen
0.0003% sulfur
0.0386% nitrogen



Regenerator Chemical Reactions

Taken from Open Literature

> The chemical kinetics shown are for demonstration or education purpose only and have not been validated, nor are they recommended for any application. Development, validation, and use of chemical kinetics is the User's responsibility, and CPFD Software, LLC, does not warrant or endorse these chemical kinetics for any purpose.

- Coke combustion (Source: Kanervo, 2001)

$$C + O_2 \rightarrow CO + CO_2$$

- CO oxidation (Source: Arandes, 1999)

$$CO + \frac{1}{2}O_2 \rightarrow CO_2$$

- Nitrogen combustion (Source: Jones, 1999)

$$N + \frac{1}{2}O_2 \rightarrow NO \qquad 2C + 2NO \rightarrow 2CO + N_2$$

- Sulfur combustion (Source: Jones, 1999)

$$S + O_2 \rightarrow SO_2$$

- Hydrogen combustion (Source: Jones, 1999)

$$2H + \frac{1}{2}O_2 \rightarrow H_2O$$

- References:

  – Kanervo, et al, "Kinetics of the regeneration of a cracking catalyst derived from TPO measurements". *Chemical Engineering Science* 56 (2001): 1221-1227.
  – Arandes, et al, "Kinetics of Gaseous Product Formation in the Coke Combustion of a Fluidized Catalytic Cracking Catalyst". *Ind. Eng. Chem. Res.* 38 (1999): 3255-3260.
  – Jones, et al, "Approaches to modelling heterogeneous char NO formation / destruction during Pulverised coal combustion". *Carbon* 37 (1999): 1545-1552.

Chemical Reaction Rates (1 of 2)

$$C + O_2 \rightarrow CO + CO_2$$

$$\frac{d(C)}{dt} = 9.2\times10^{7}\exp\left(\frac{-17560}{T}\right)\theta_f[O_2]^{0.58}m_C + 2.5\times10^{5}\exp\left(\frac{-13470}{T}\right)\theta_f[O_2]^{0.64}m_C \quad \text{Units:}\frac{\text{mol}}{s}$$

$$CO + \frac{1}{2}O_2 \rightarrow CO_2$$

$$\frac{d(CO)}{dt} = 7.6\times10^{13}\exp\left(\frac{-6190}{T}\right)P_{O2}P_{CO} \quad \text{Units:}\frac{\text{mol}}{m^3\cdot s}$$

$$N + \frac{1}{2}O_2 \rightarrow NO$$

$$\frac{d(N)}{dt} = 7.9\times10^{7}\exp\left(\frac{-17560}{T}\right)\theta_f[O_2]^{0.58}m_N + 2.1\times10^{5}\exp\left(\frac{-13470}{T}\right)\theta_f[O_2]^{0.64}m_N \quad \text{Units:}\frac{\text{mol}}{s}$$

Chemical Reaction Rates (2 of 2)

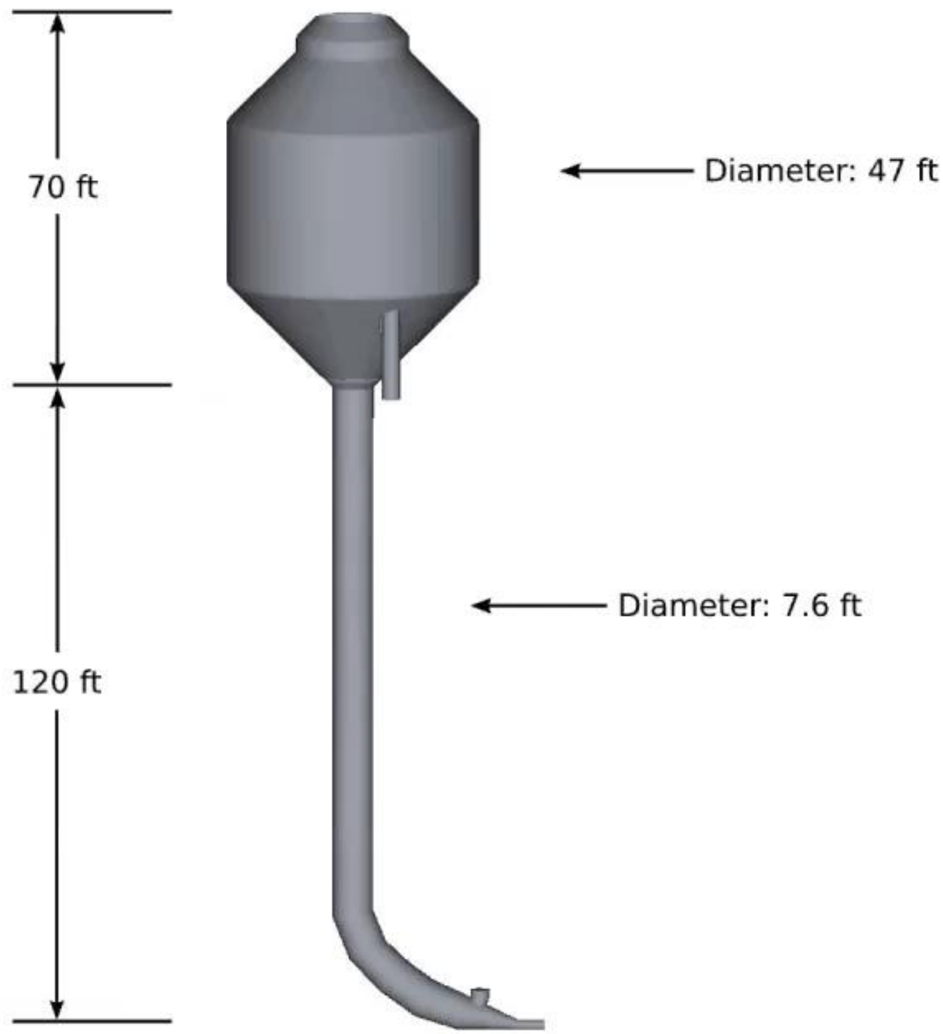
$$2C + 2NO \rightarrow 2CO + N_2 \qquad \frac{d(C)}{dt} = 2.6\times 10^{8} \exp\left(\frac{-15900}{T}\right) A_{cat}\, m_{cat}^{-1} P_{NO} \quad \text{Units:} \frac{\text{mol}}{s}$$

$$S + O_2 \rightarrow SO_2 \qquad \frac{d(S)}{dt} = 3.5\times 10^{7} \exp\left(\frac{-17560}{T}\right) \theta_f [O_2]^{0.58} m_S + 9.4\times 10^{4} \exp\left(\frac{-13470}{T}\right) \theta_f [O_2]^{0.64} m_S \quad \text{Units:} \frac{\text{mol}}{s}$$

$$2H + \frac{1}{2} O_2 \rightarrow H_2O \qquad \frac{d(H)}{dt} = 1.1\times 10^{9} \exp\left(\frac{-17560}{T}\right) \theta_f [O_2]^{0.58} m_H + 3.0\times 10^{6} \exp\left(\frac{-13470}{T}\right) \theta_f [O_2]^{0.64} m_H \quad \text{Units:} \frac{\text{mol}}{s}$$

The chemical kinetics shown are for demonstration or education purpose only and have not been validated, nor are they recommended for any application. Development, validation, and use of chemical kinetics is the User's responsibility, and CPFD Software, LLC, does not warrant or endorse these chemical kinetics for any purpose.

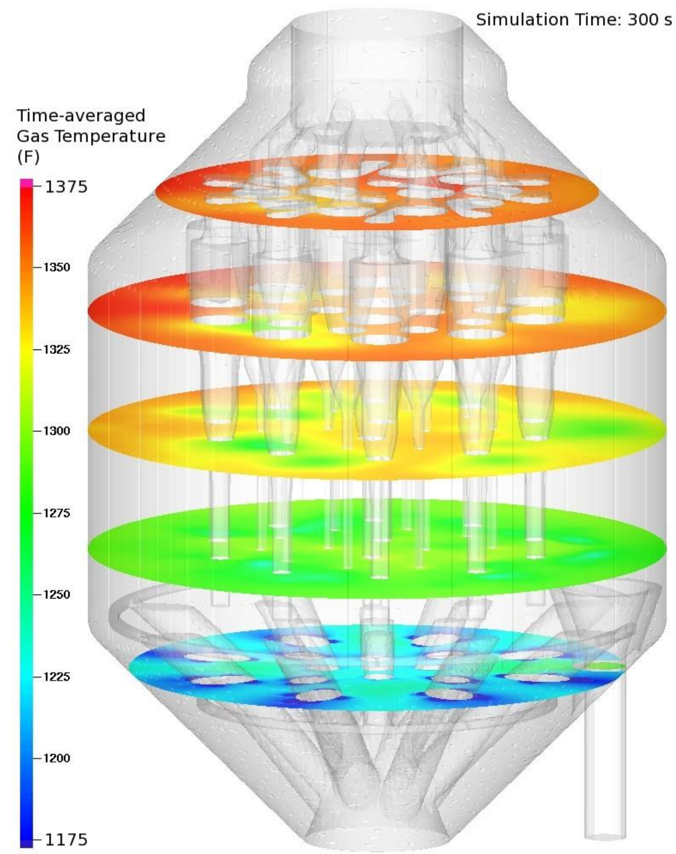
Commercial FCC Regenerator Simulation

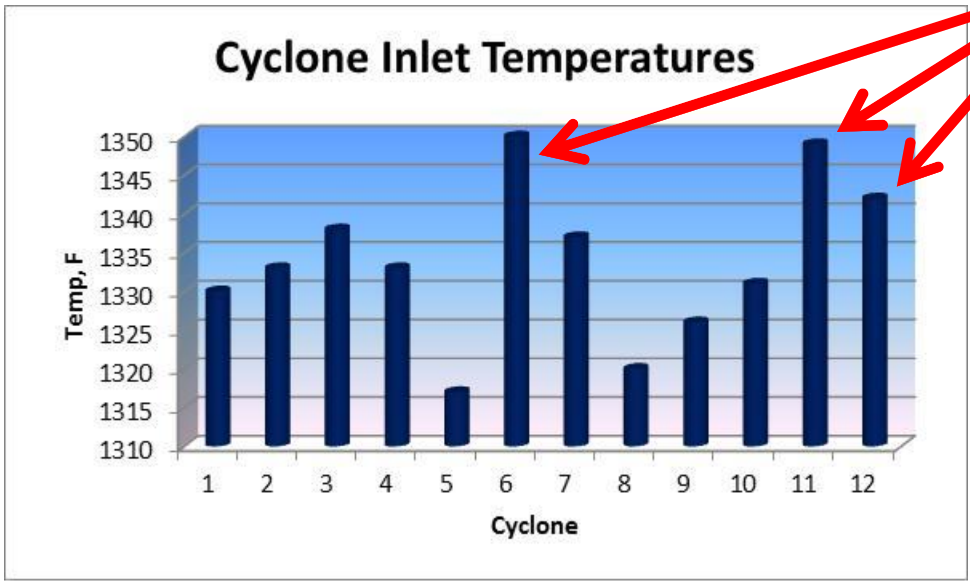


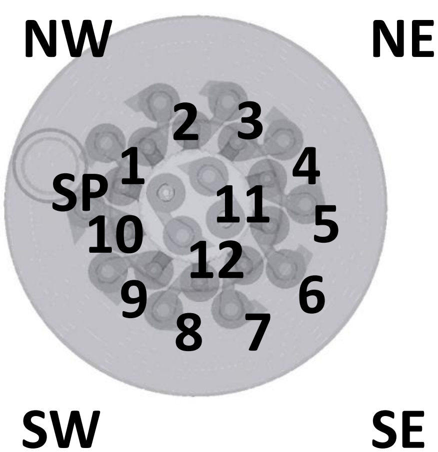
Combined Geometry: Spent Cat Riser + Regenerator

Results - Afterburn

- Afterburn was successfully predicted by the model
  - approx. 100 °F temperature difference from the dense bed to the dilute freeboard observed at the refinery
- The model predicts temperatures are highest at cyclones 6, 11 and 12
  - Highest temperatures at the refinery are observed in these cyclones

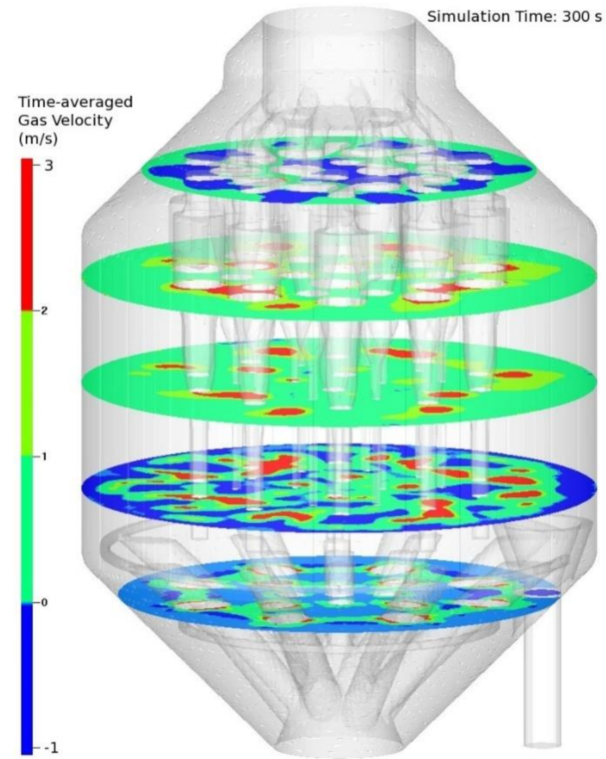


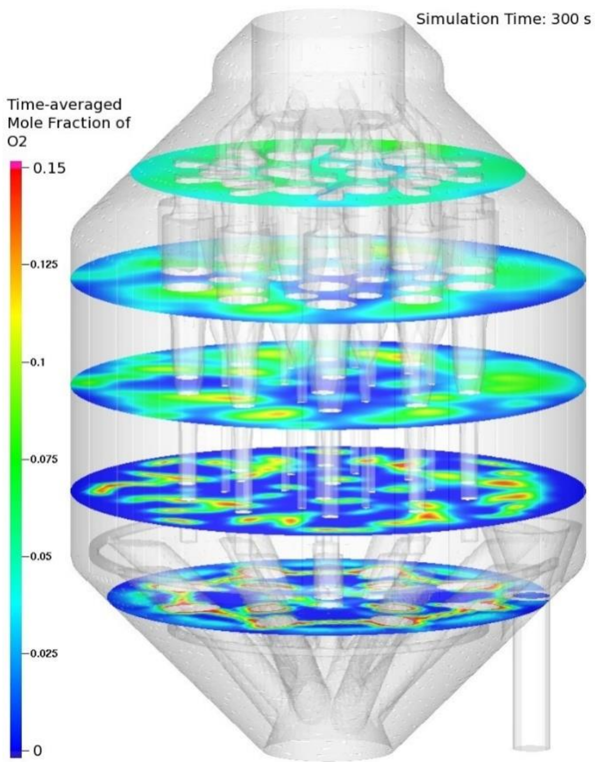




Why Afterburn?

- Average superficial velocity in regenerator is about 0.74 m/s (2.4 ft/s).
- High velocity regions of gas “bypassing” or “streaming” are seen as influenced by each of the outer-most distributor arms.

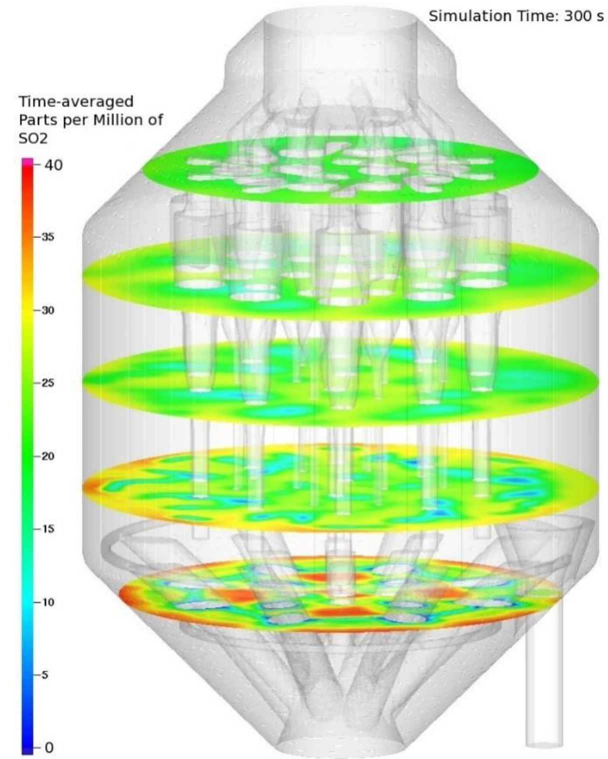


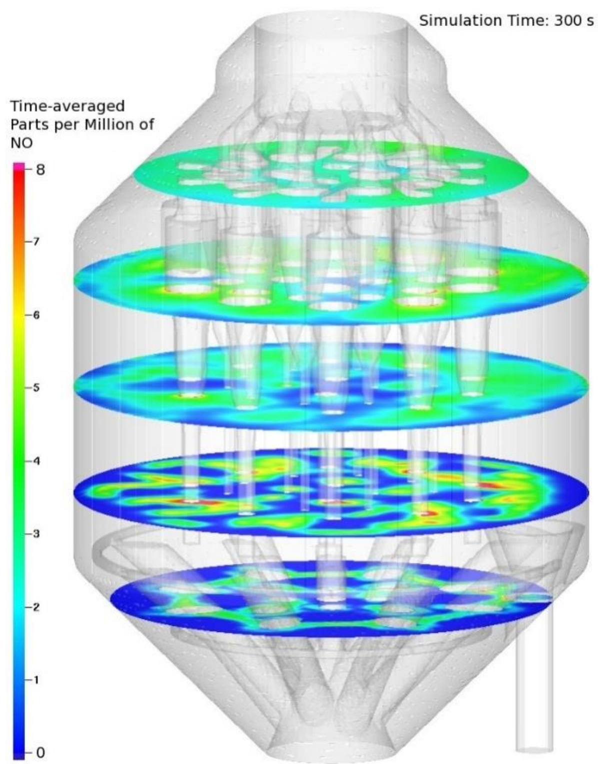


- Areas of high O_2 concentration correspond to regions of high gas velocity.
- A significant portion of the O_2 is reaching the freeboard quickly, without sufficient time for proper mixing with the bed
- Combustion in the freeboard leads to higher temperatures because less particle mass is available to absorb heat.

Emissions

- A secondary goal of the simulation was to evaluate the production of pollutants.
- The refinery operating data shows SO_2 levels leaving the regenerator to be about 30 ppm
  - Simulation results: 20 ppm
  - Agreement with data for SO_2 is reasonable





- Operational data shows NO levels to be about 40 ppm
  - Simulation results: 5 ppm at cyclone inlets
  - Agreement with data for NO is poor
- Possible causes for discrepancy:
  - Initial particle composition could have had too little nitrogen
  - Reaction rates may be inaccurate or inconsistent
  - A reaction pathway for NO formation is missing
  - NO could be formed after exiting the freeboard

Conclusions

- The model predicted the afterburn observed at the refinery
  - Magnitude (100°F) and asymmetry
  - Root cause is:
    - Not due to the performance of the spent cat riser or catalyst distributor
    - Is due to bed mixing and gas bypass as influenced by fluidization headers and internal structures
- The model predicted emissions:
  - SO_2 was captured well (20 ppm vs. 30 ppm measured)
  - NO was not captured well (5 ppm vs. 40 ppm measured)
- Challenges overcome:
  - Multiple models allowed for:
    - Complex geometry (vessel internals, widely varying length scales)
    - Inclusion of otherwise unknown boundary conditions in the regenerator model
    - Minimization of total runtime
  - The discrete, multi-component particle formulation allowed for:
    - A prediction of emissions from the lesser elements in the coke
  - The initial conditions minimized transients by starting the bed close to operating conditions (hot, some coke on catalyst reflecting ecat)
  - Standpipe catalyst exit was maintained with iteration on aeration and outflow
- Challenges outstanding:
  - Improvements in NO prediction

Runtimes of the Three Models

- Due to the different purposes and assumptions of the three models, the runtimes were quite different (note – 2011/2012 work prior to GPU code)
- Model 1: Spent Catalyst Riser
  - Isothermal, no chemistry
  - 30,361 real cells
  - 590,000 computational particles
- Model 2: Distributor Arms
  - Thermal + chemistry
  - 407,196 real cells
  - 4.6 million computational particles
- Model 3: Regenerator Vessel
  - Thermal + chemistry
  - 237,999 real cells
  - 2.6 million computational particles

Note: each simulation was run on a single core of an Intel i7 processor.