Introduction to Barracuda Virtual Reactor®

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Outline

Introduction to CPFD Software and Barracuda Virtual Reactor®

Fluid-Particle flows

- Examples
- What is different than single phase flows?

The CPFD® modeling approach

- Overview
- Advantages and disadvantages

Validation

Industrial application examples

- Biomass CFB combustor
- FCC regenerator

Deployment of Barracuda Virtual Reactor

CPFD Software

Inventors of the CPFD technology and 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

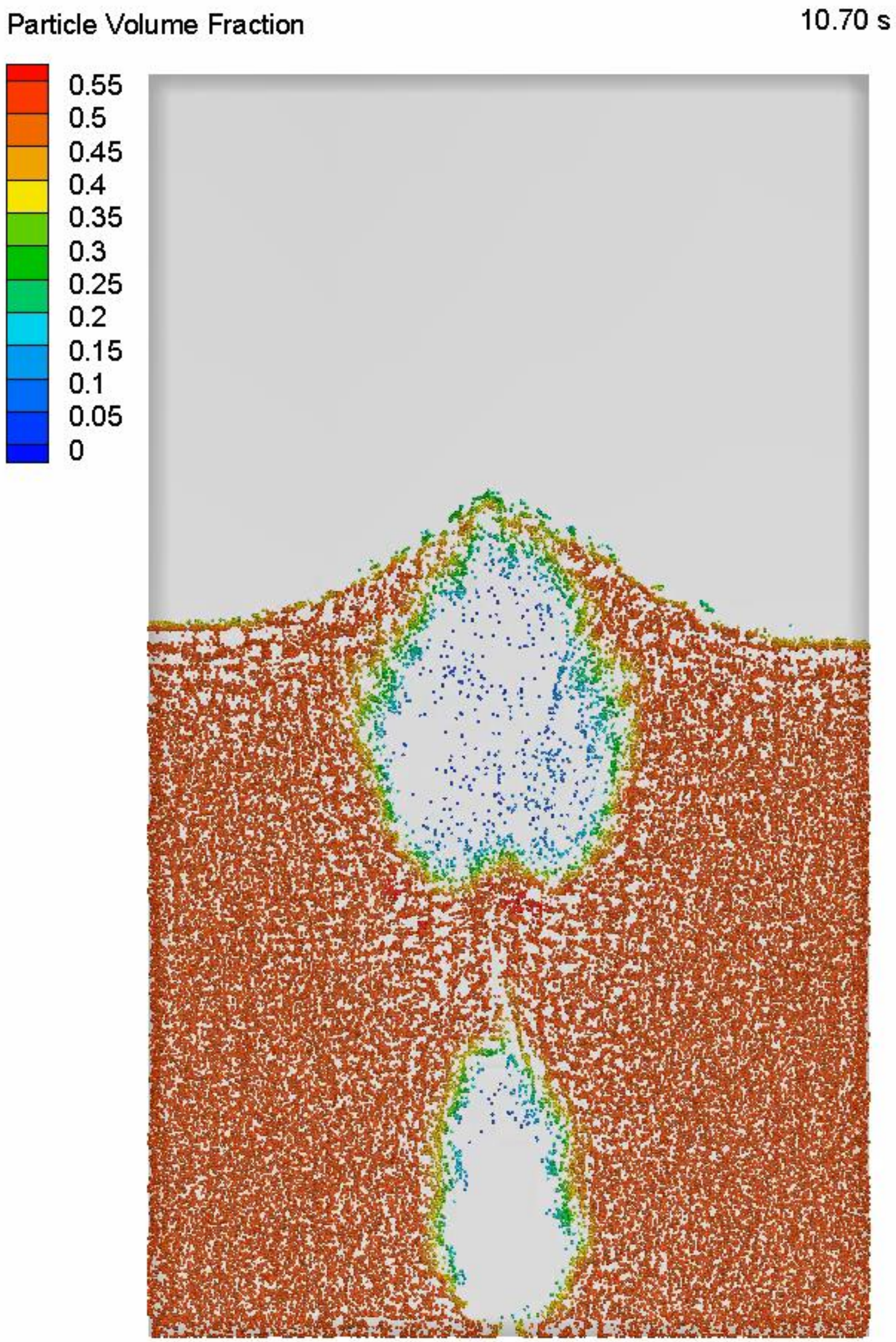
- Software licensing
- Engineering services
- Training
- Collaborative programs

CPFD Software Headquarters Office
Houston, TX, USA

Particle Flow Examples

Fluidized Beds (Experiments)

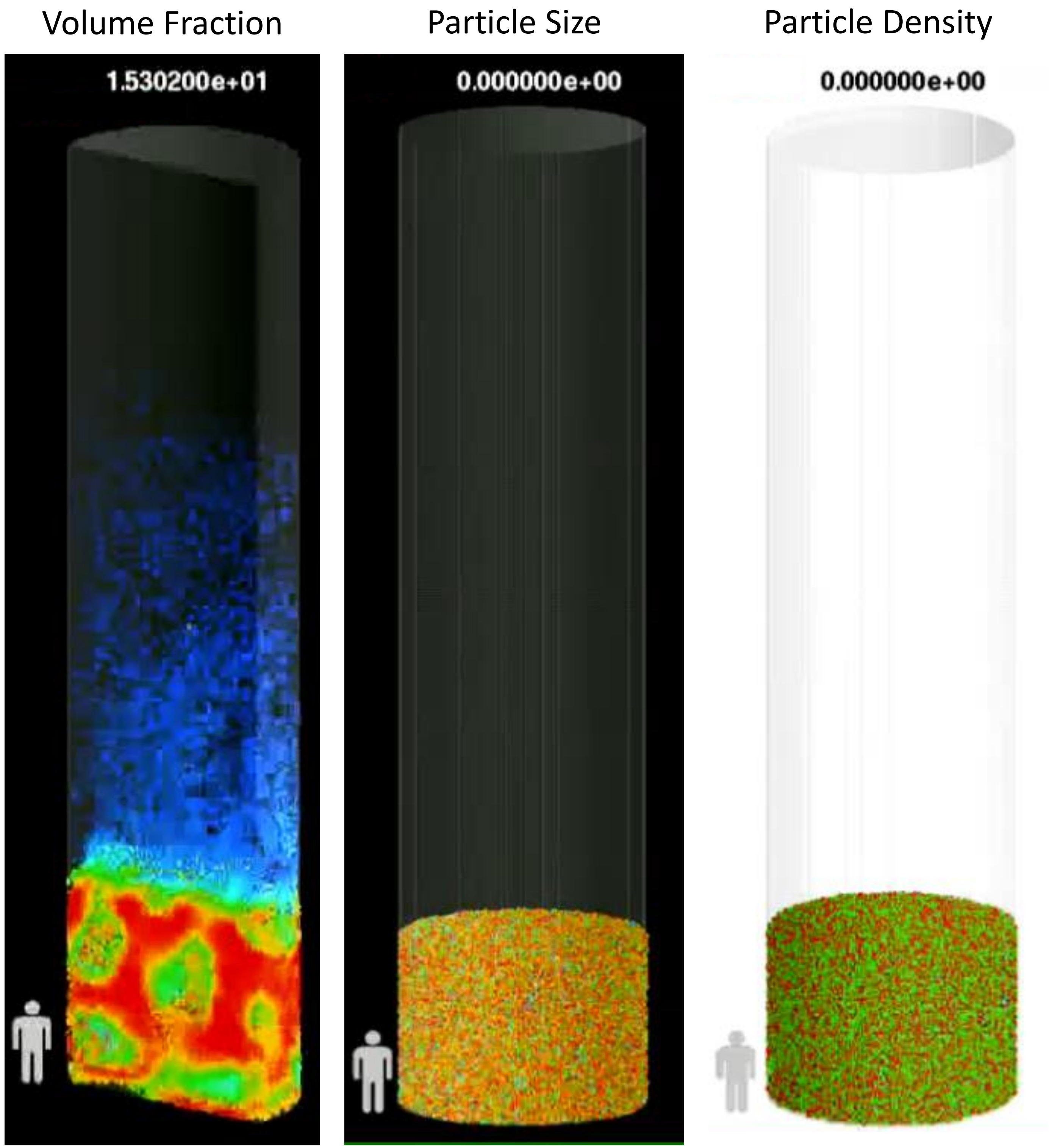
- Air (fluid) field important
- Particle field important
  - Dilute to dense
- Particle properties important
  - Size
  - Density



Particle Flow Examples

Ore Reactors (Industrial)

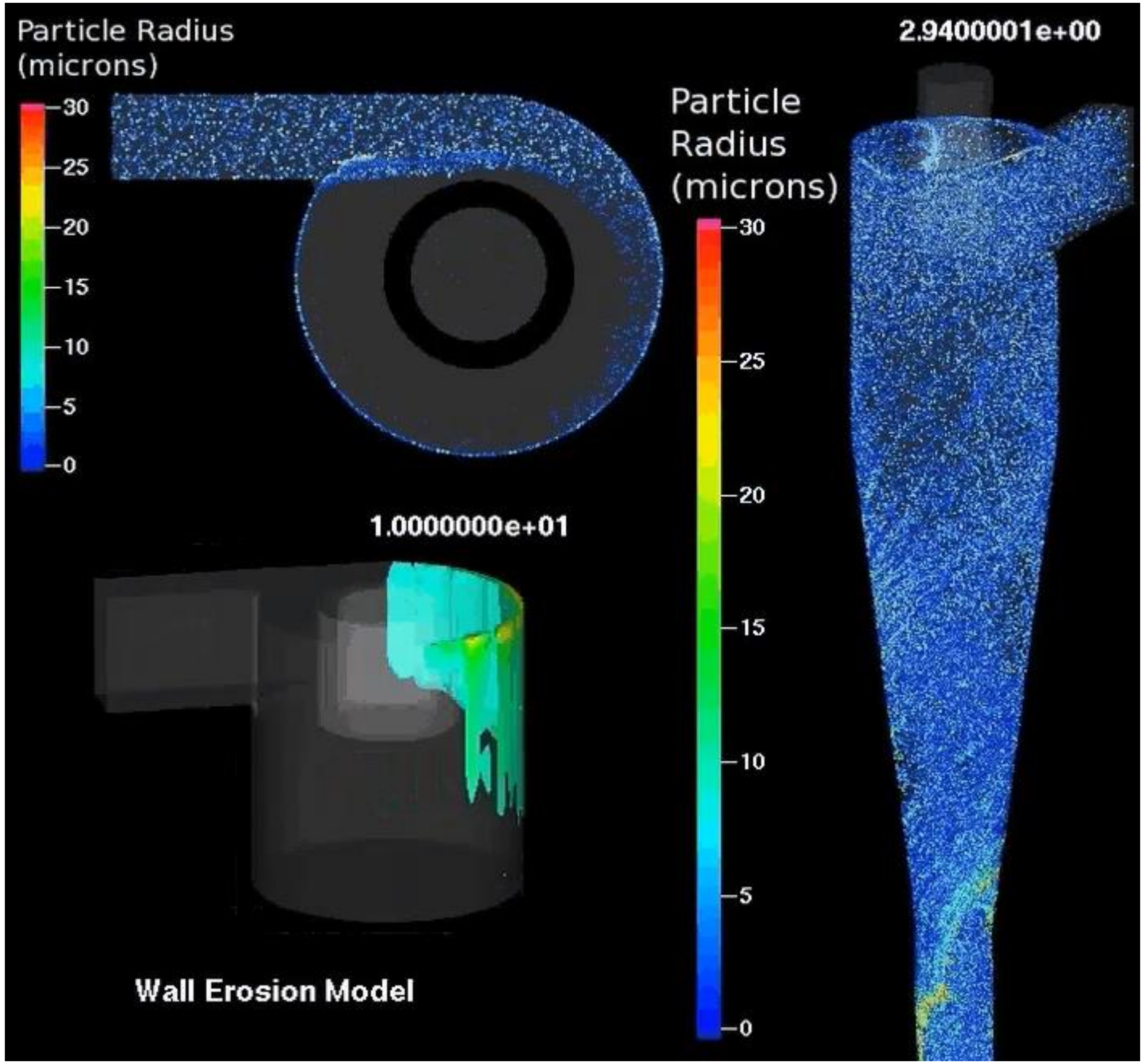
- Gas (fluid) field important
- Particle field important
  - Dilute to dense
- Particle properties important
  - Particle size distribution (PSD)
  - Different materials with different densities



Particle Flow Examples

Cyclones

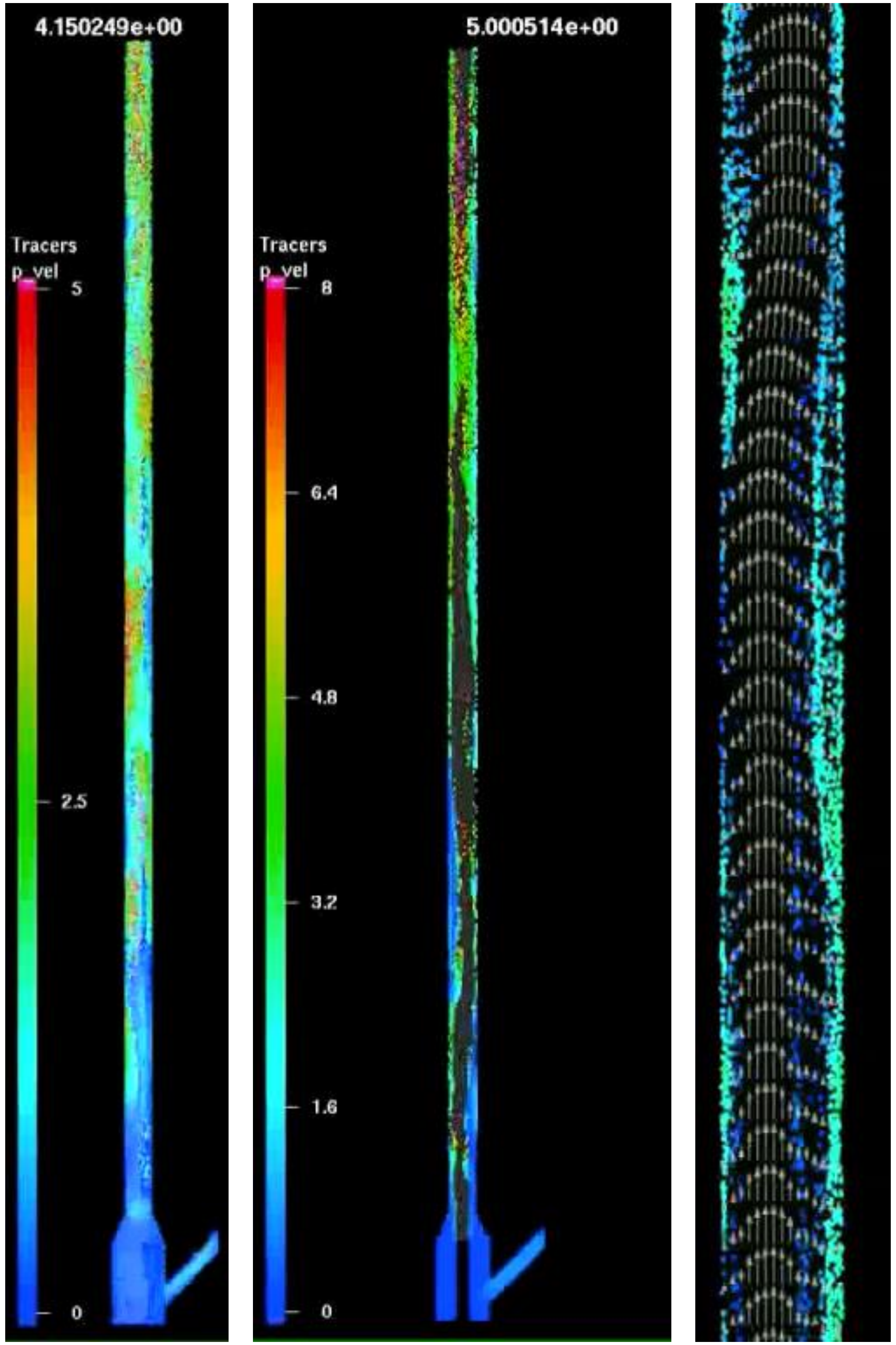
- Gas field important
- Particle field important
  - Typically dilute
- Particle properties important
  - Size and size distribution
  - Density
- Areas of interest:
  - Overall efficiency
  - Efficiency vs. size
  - Erosion
  - Pressure drop



Particle Flow Examples

Risers

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



Left: 3D view from outer surface of riser

Center: thin slice near central plan of riser

Right: thin slice zoomed in to see fluid flow vectors and particle motion

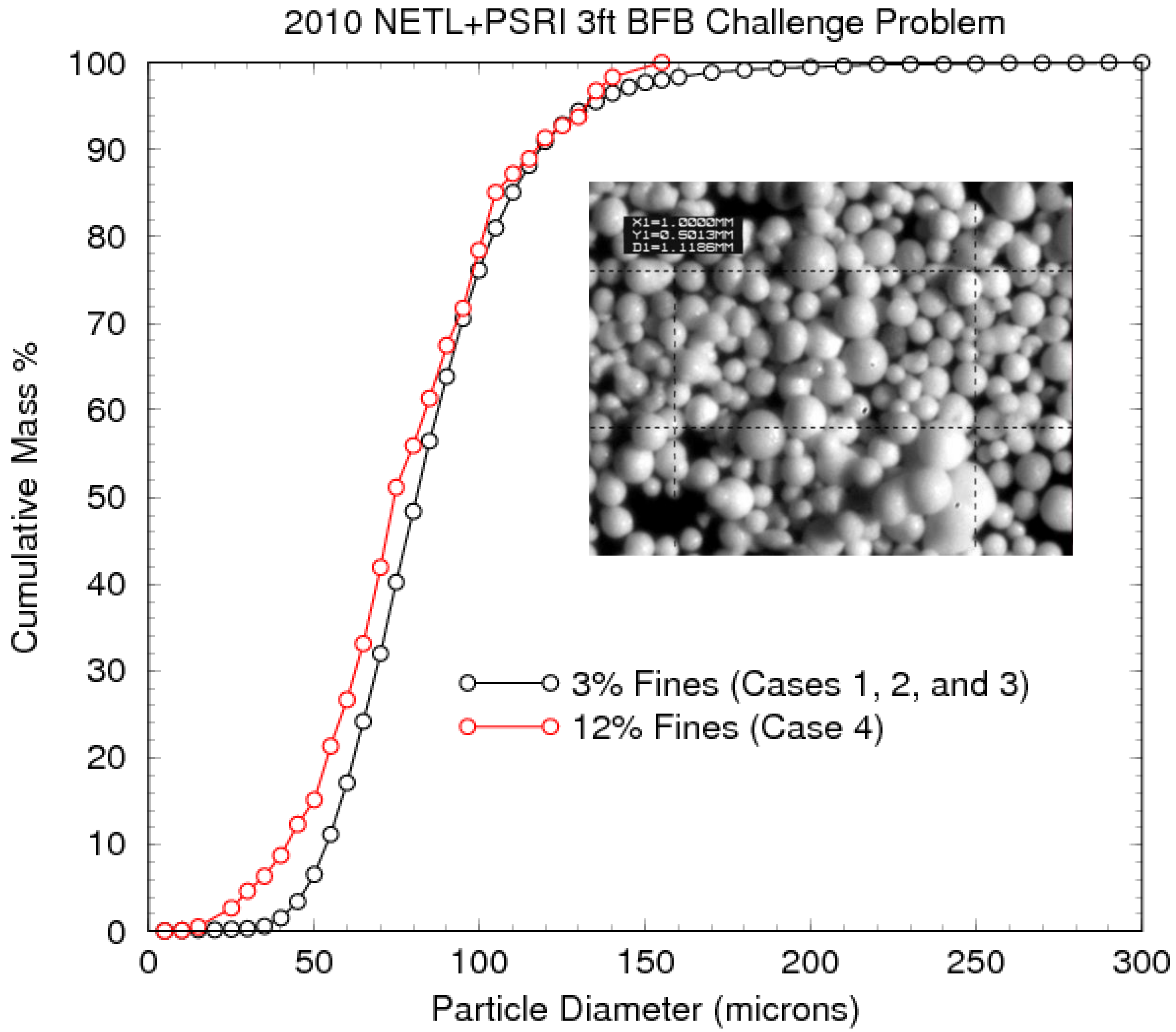
What’s Different About Modeling Fluid-Particle Flows?

Particles are discrete entities

- Cannot be subdivided like a fluid

Particles have a size distribution

Particle Size Distributions



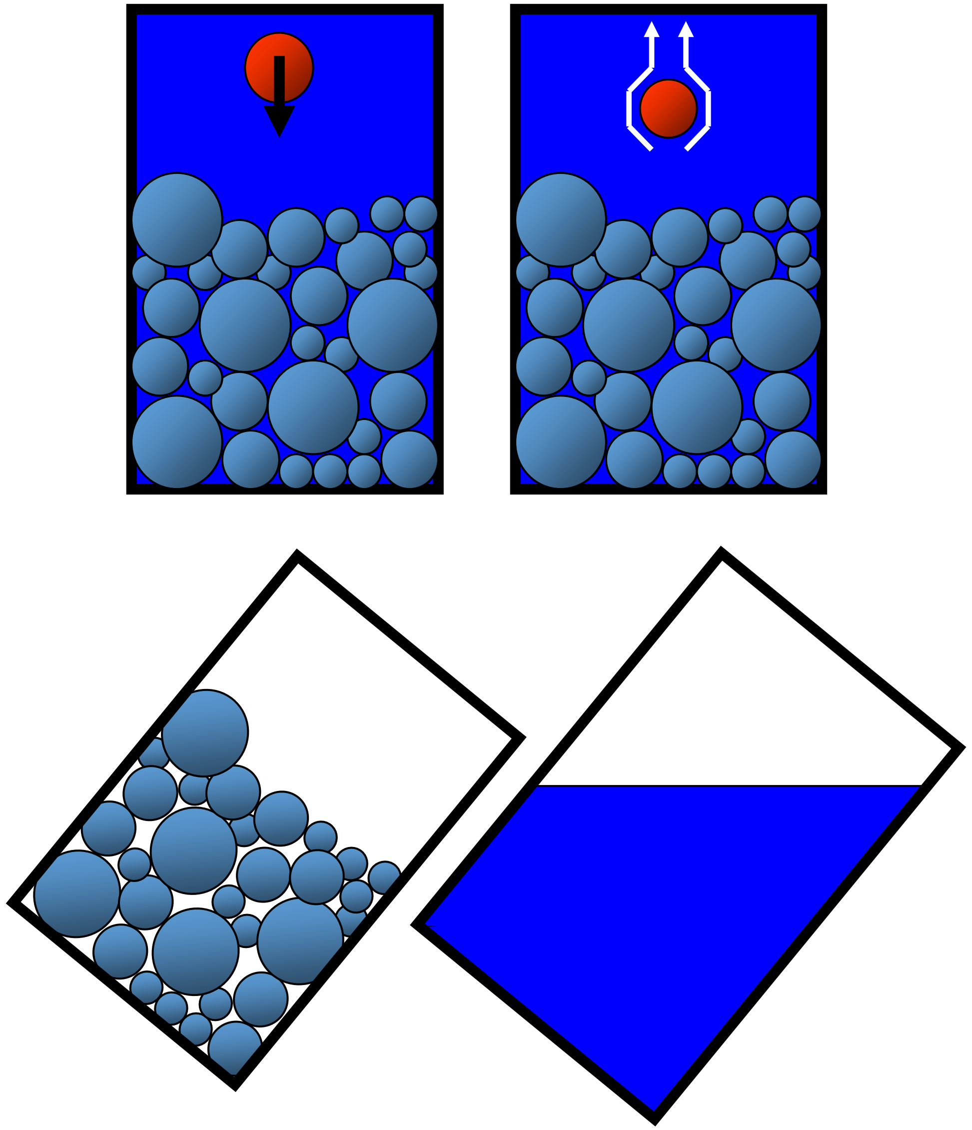
What’s Different About Modeling Fluid-Particle Flows?

Particles cannot completely fill a space

Particles occupy a physical volume (and displace fluid)

Particles can support a shear stress

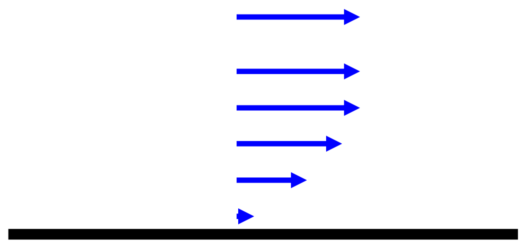
Fluids cannot support a shear stress

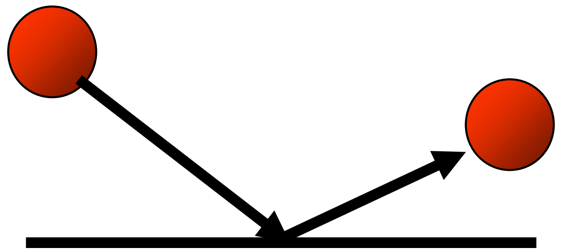


What’s Different About Modeling Fluid-Particle Flows?

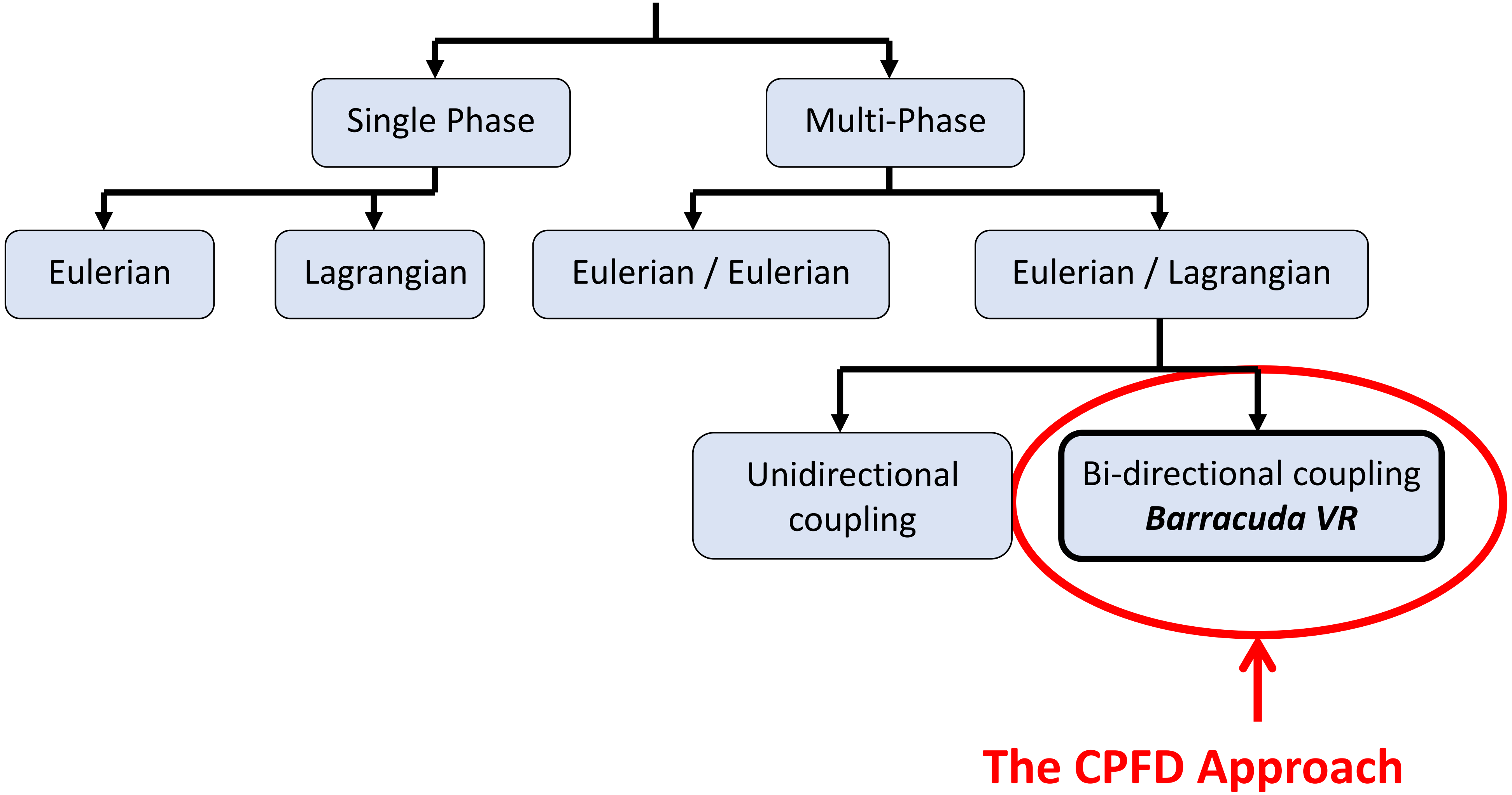
Other considerations

- Coupling between particles and fluids
- Wall treatment
- Boundary treatment
- Thermal
- Chemistry

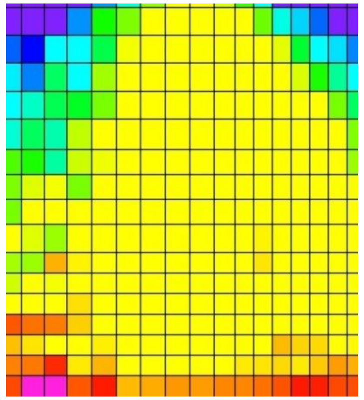




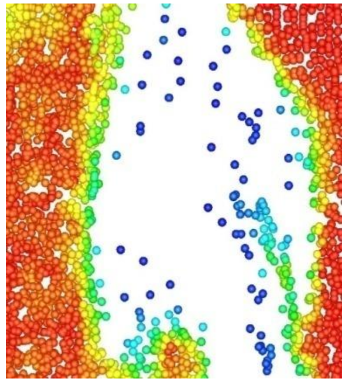
Approaches to Particle Flow Modeling



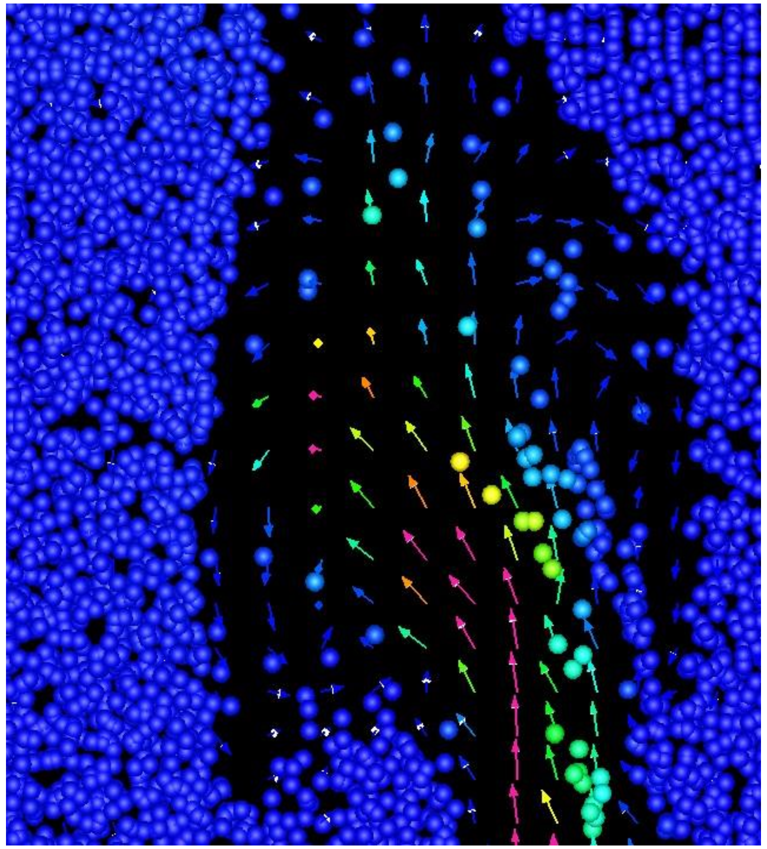
The CPFD Approach



Fluid equations
Continuous
Solved on the grid



Particle equations
Discrete
Gridless



Fluid affects particles (aerodynamic / hydrodynamic drag)

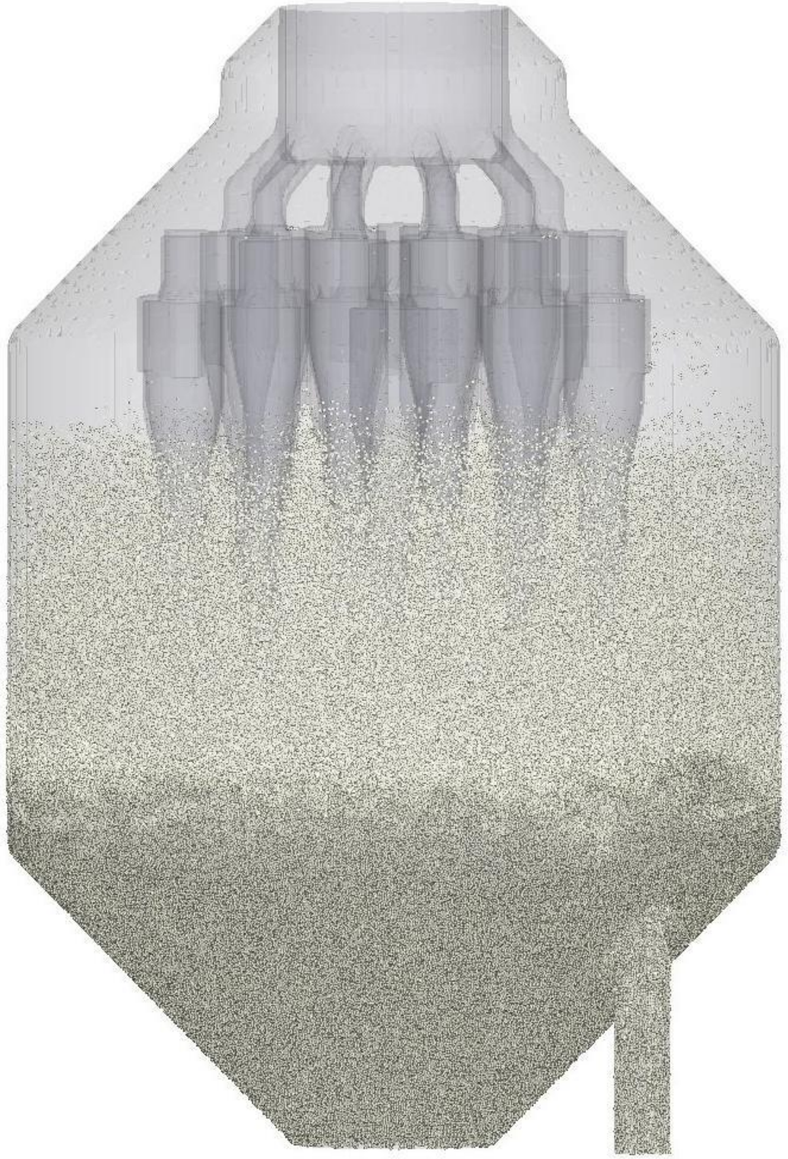
Particles affect fluid (displacement, pressure drop)

Bi-directionally coupled (tight / implicit coupling)

The CPFD Approach

What about the large number of physical particles?

- The particle field is resolved by using a reasonable number of clouds
- Each cloud represents one or more physical particles with identical properties
- The physics are computed based on the properties of a single physical particle represented by the cloud (drag based on particle size, chemistry, etc.)
- All changes experienced by the cloud are applied to all physical particles represented by that cloud

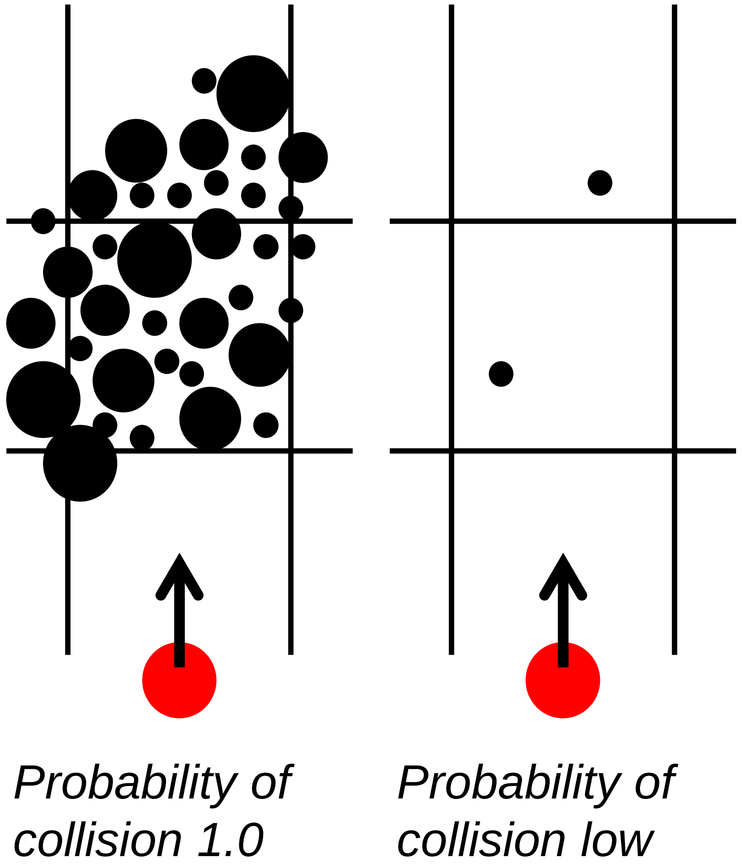


Commercial FCC Regenerator
2e+15 physical particles
2e+6 clouds in simulation

The CPFD Approach

What about particle contact and collision?

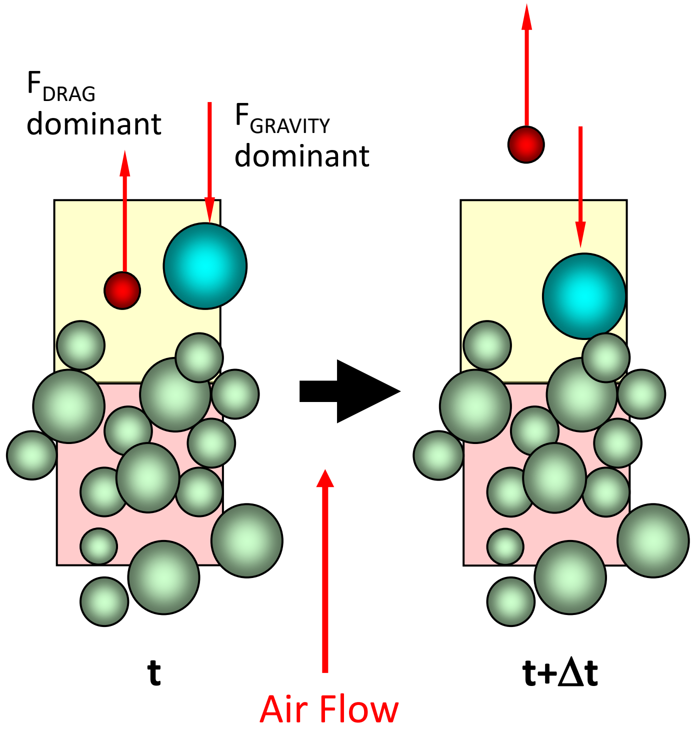
- Modeled, rather than directly computed
- Collision detection is prohibitive with millions of clouds
- Rather than computing which specific clouds will collide, the CPFD method is more concerned with the question **“is a collision likely to occur?”**
- The collisions are then subjected to various models
  - Enduring contact at close-pack handled via a non-linear stress tensor
  - BGK-type collisional damping



The CPFD Approach

What about inter-phase coupling?

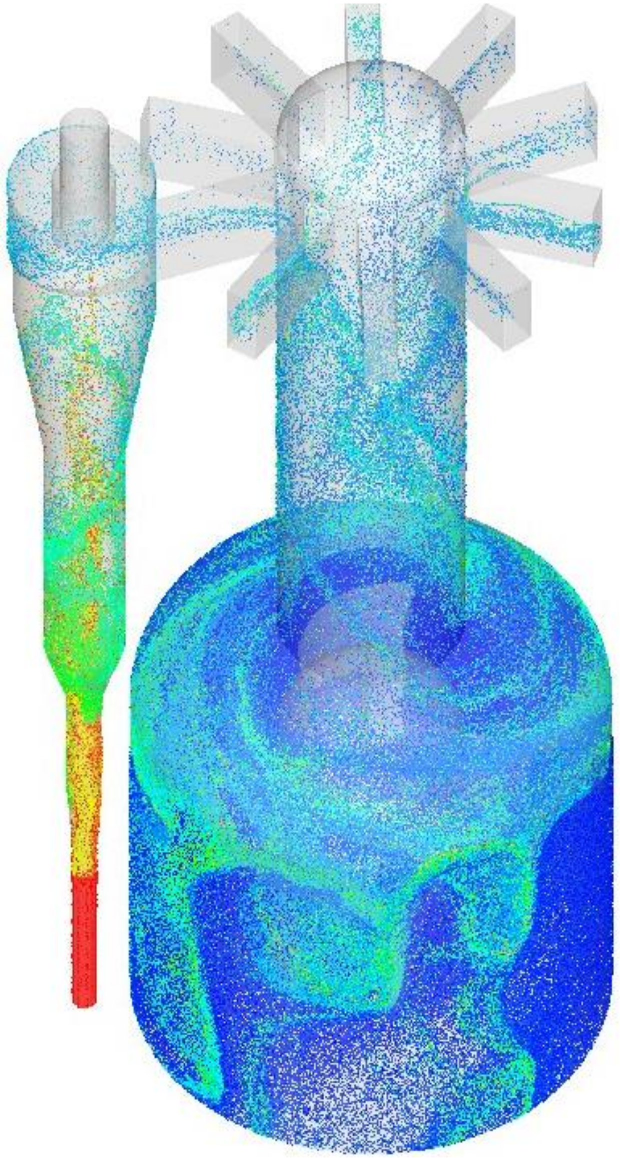
- Inter-phase interpolation operators, and tight, bi-directional coupling
- Different particles experience different motion, even though both are in the same cell
- All sub-grid particle motion is coupled back to the fluid phase momentum equation



Advantage 1: High Physical Particle Counts

An industrial reactor can have 10^{16} or more particles

- 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 cloud 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.

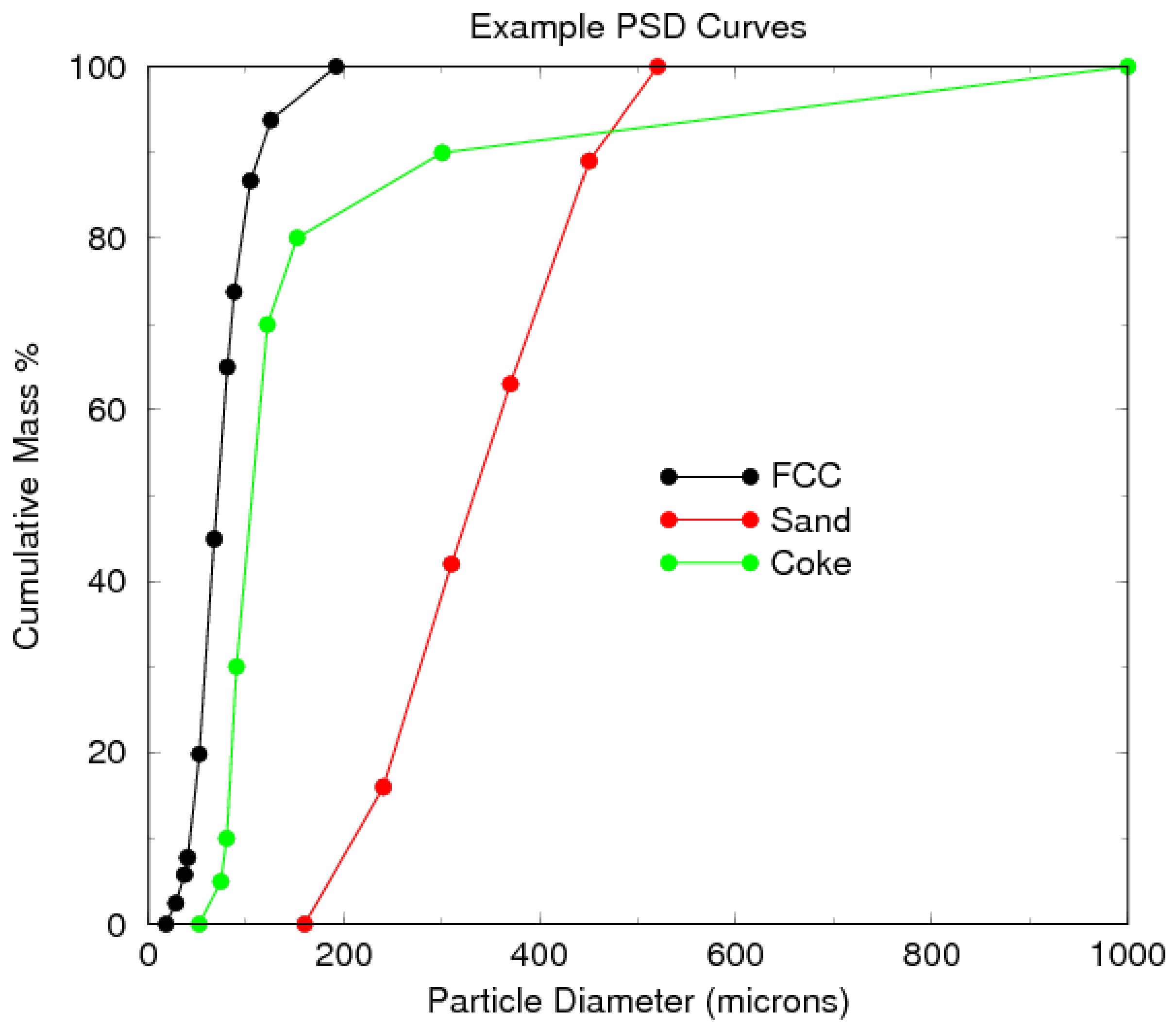


FCC Reactor Separation Unit
3e+12 real particles
1.6e+6 clouds

Advantage 2: Particle Size Distribution

Particle size is very important in fluidization behavior

- Barracuda accepts full Particle Size Distribution (PSD) information for each particle species, since each Lagrangian particle inherently has its own size.
- The entire PSD, not just the d_{50} or d_{32}, can be important.
- This is a distinct advantage of the CPFD method compared with an Eulerian multiphase approach.



Advantage 3: Tracking Wall Impacts

Because each cloud is a Lagrangian entity, it is known when a particle hits a wall surface.

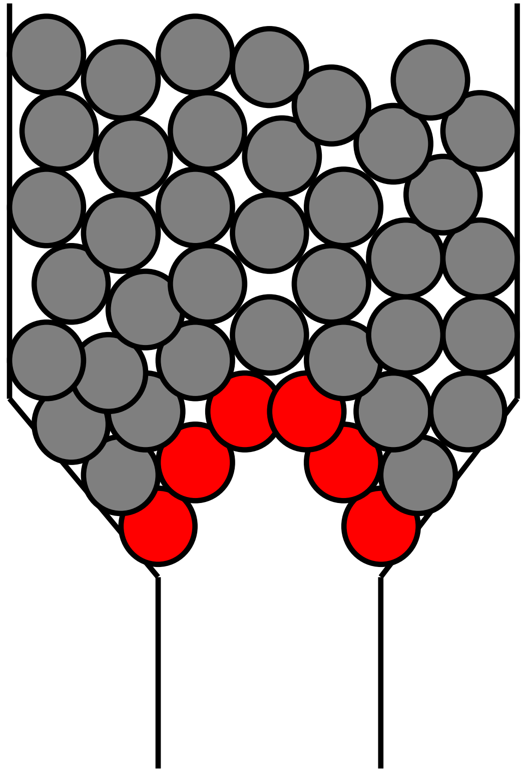
- The erosion on the wall due to the particle impact can be estimated.
- An erosion index calculation is dependent on the particle mass, speed and impact angle.
- Typical functional form: $C_\alpha m_p u_p^{3.5}$
- Angle coefficient, C_α, is dependent upon the surface material (steel, refractory, etc.).
- 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.

Disadvantage 1: Direct Particle Contact not Computed

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.).
- A DEM or CFD-DEM solution is often better-suited for these classes of problems.

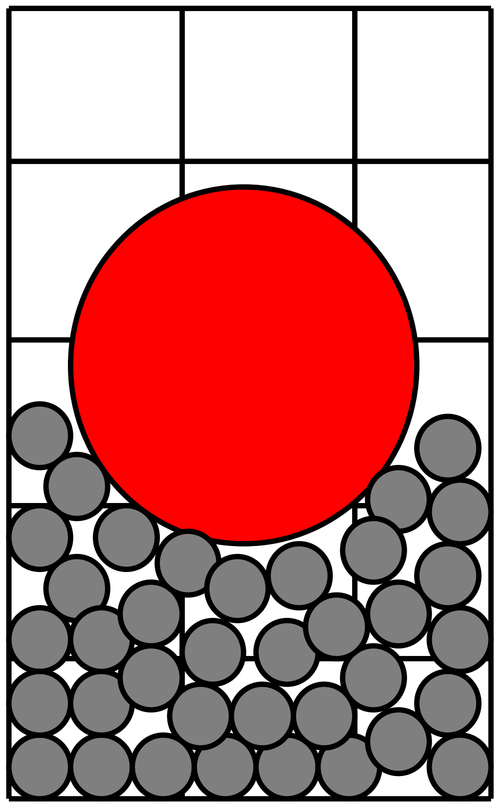


Particle bridges are dependent upon precise inter-particle contact points. This is not a good problem for a CPFD code.

Disadvantage 2: Many Particle Must Fit in Each Cell

The CPFD method presupposes that a statistically-significant number of clouds 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
- A CFD code with fluid-structure interaction, or a Lattice-Boltzman approach may be better-suited for these classes of problems.



The red particle is too 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:

https://cpfd-software.com/customer-support/knowledge-base/publications-about-barracuda-virtual-reactor

Validation: 2D Bed

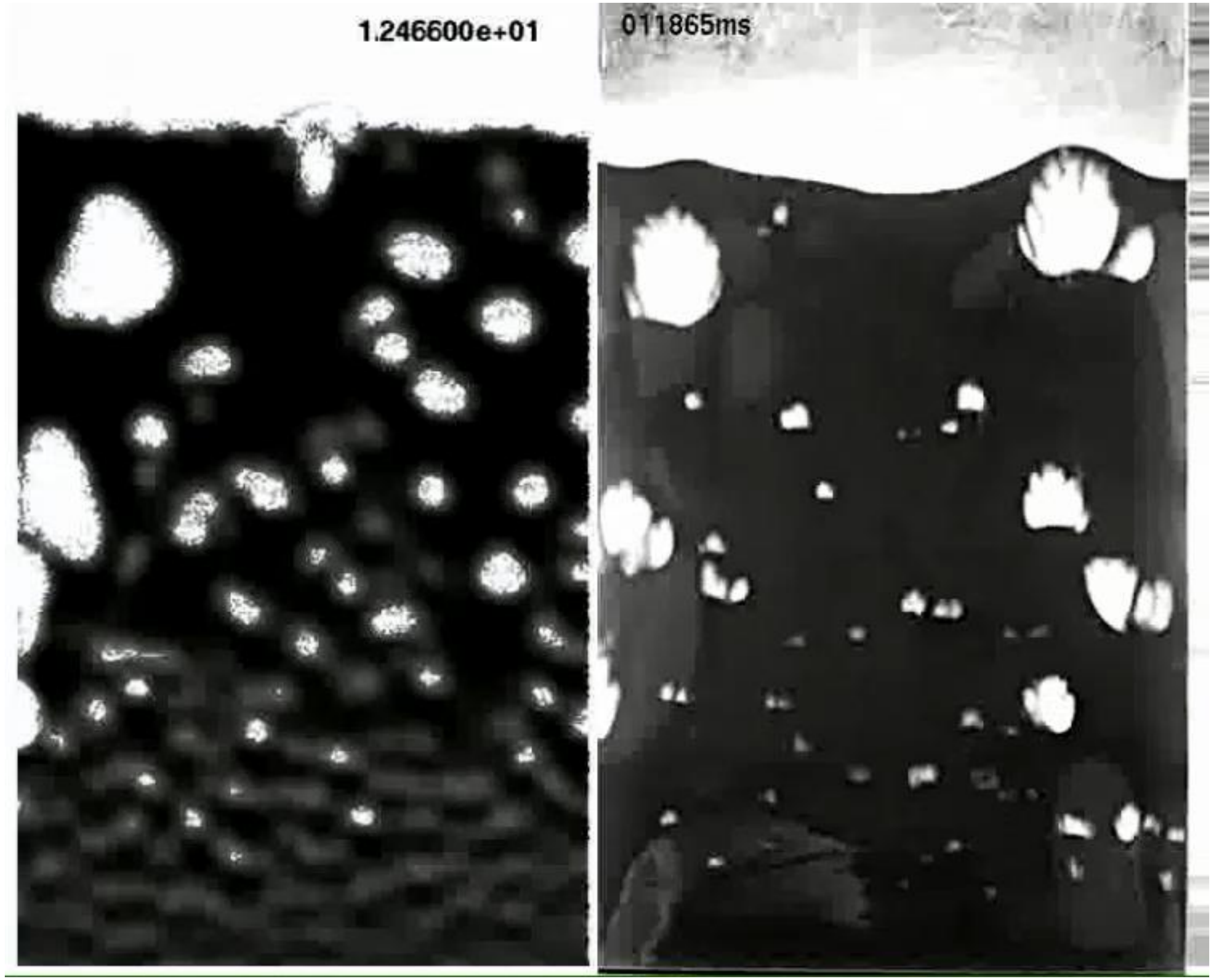
Experimental 2D bed to visualize bubble formation and motion

- Left: Barracuda simulation
- Right: Experimental video

Boundary conditions

- Fluidization gas at bottom
- High-speed jet at left (started after bed is fluidized)

Bubble size, shape, and motion are captured in the simulation



Validation: PSRI Jet Cup

Jet cups are used to measure particle attrition

- High-speed jet of gas introduced tangentially
- Particles collide at high velocity
- Change in PSD (production of fines) is measured to quantify attrition

Simulation (top video) predicted stagnant region of particles

- Predicted behavior was non-intuitive, and a problem with the simulation was suspected initially

PSRI constructed a Plexiglas jet cup (bottom video) and found that the behavior predicted by the simulation was physically realistic

- Unexpected validation due to non-intuitive particle-fluid flow behavior.
- PSRI designed a better jet cup based on this experience, and has improved the reproducibility of their attrition testing based on insights gained from jet cup simulation results

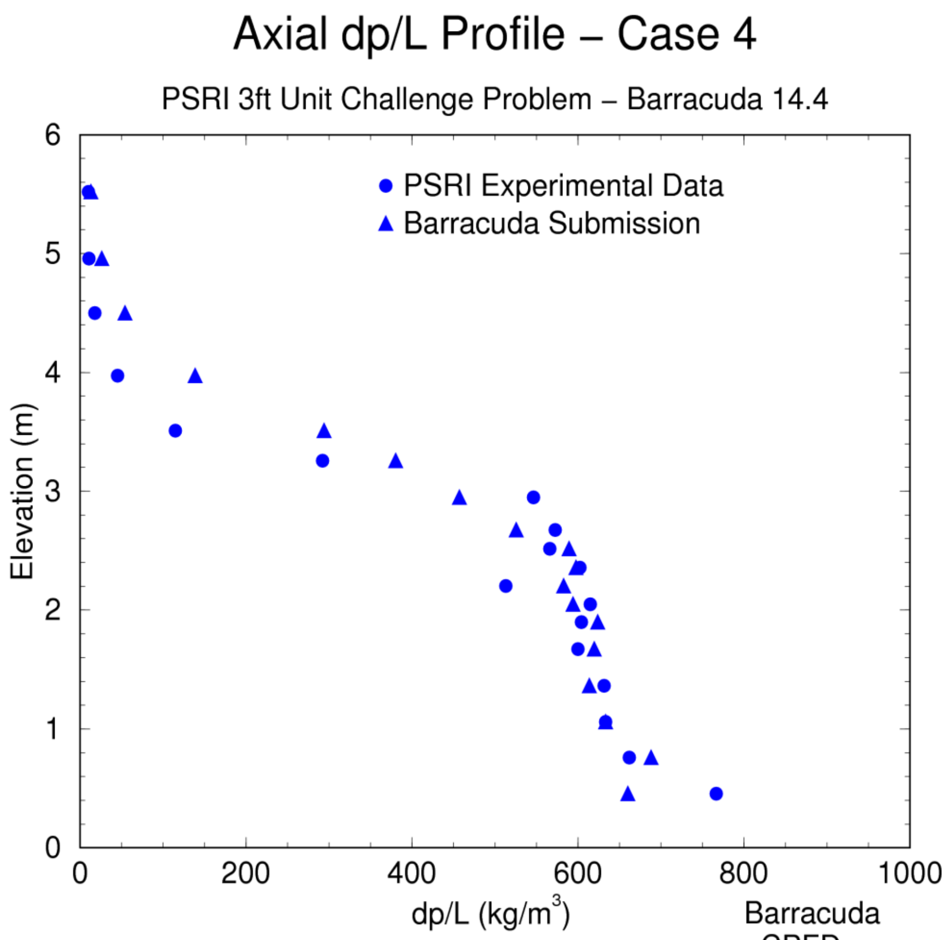
Validation: Pressure Profile in a Large-Scale Experiment

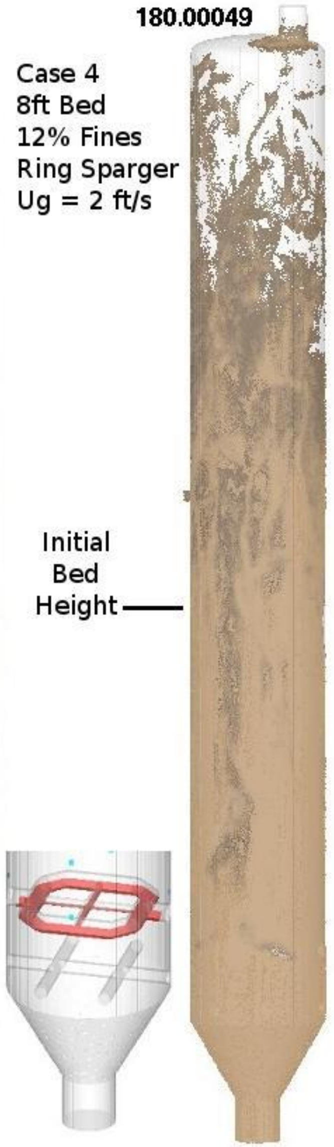
3 ft diameter bubbling fluidized bed

- [Challenge Problem III (2010)]
- Published by NETL and PSRI
- Operating conditions and geometry were made publicly available, and modelers submitted simulation results before seeing the experimental results

Figures at right show:

- Apparent bed density vs elevation
  - Dense bed results matched experimental results very closely
  - Freeboard results captured the correct trend
- Visualization of simulation results





Barracuda CPFD

Industrial Application Example 1: Circulating Fluidized Bed Biomass Combustor

Introduction

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

- Blaser, P. J.; Corina, G. Validation and Application of Computational Modeling to Reduce Erosion in a Circulating Fluidized Bed Boiler. *International Journal of Chemical Reactor Engineering* **2012**, *10* (1). https://doi.org/10.1515/1542-6580.3001.

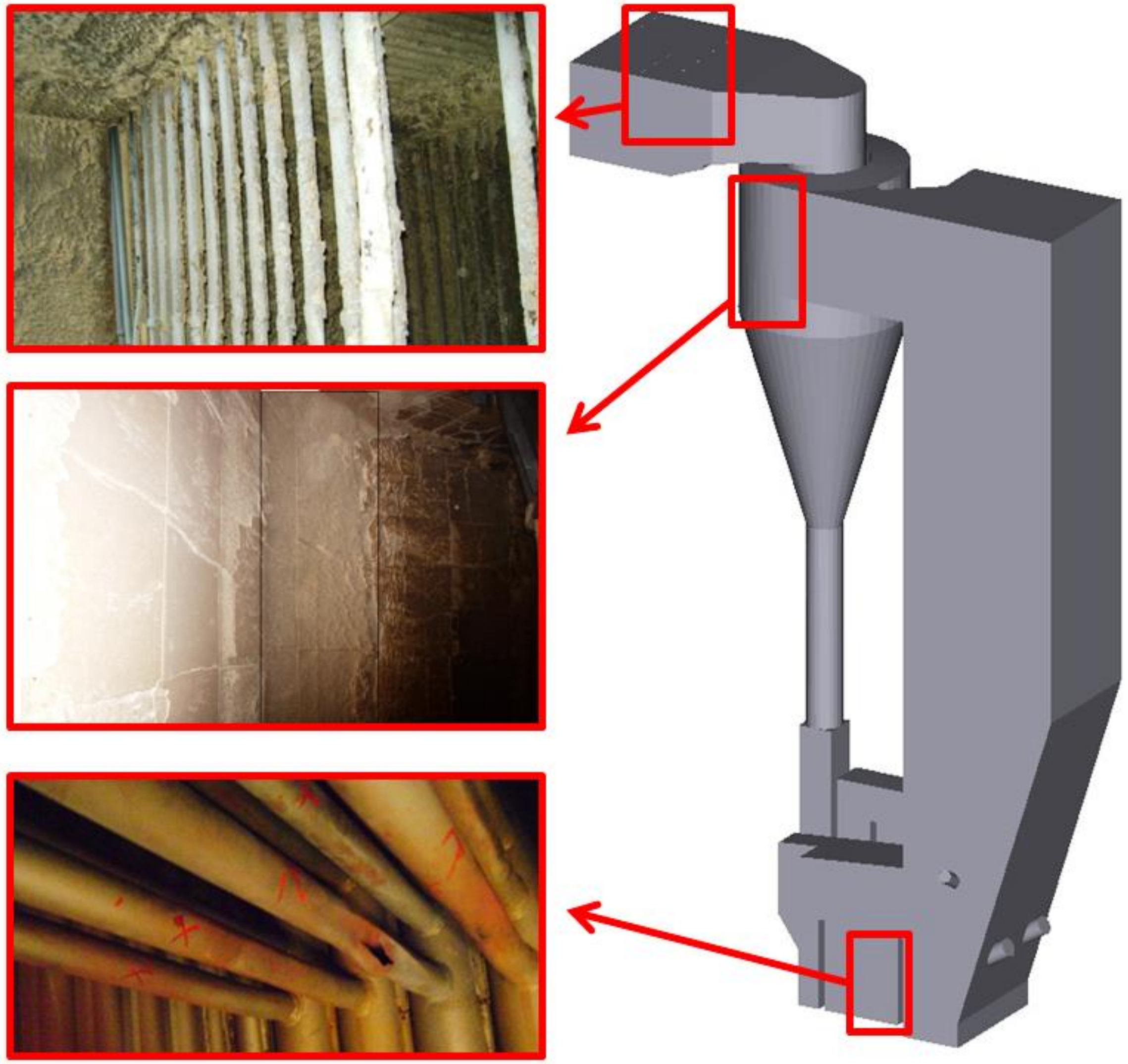
Erosion Case Study

The plant operator, Biomasse Italia S.p.A., experienced excessive erosion in several locations

The erosion in the cyclone inlet and suspension tube regions was the subject of the Barracuda Virtual Reactor simulation project

This work was undertaken in 3 phases:

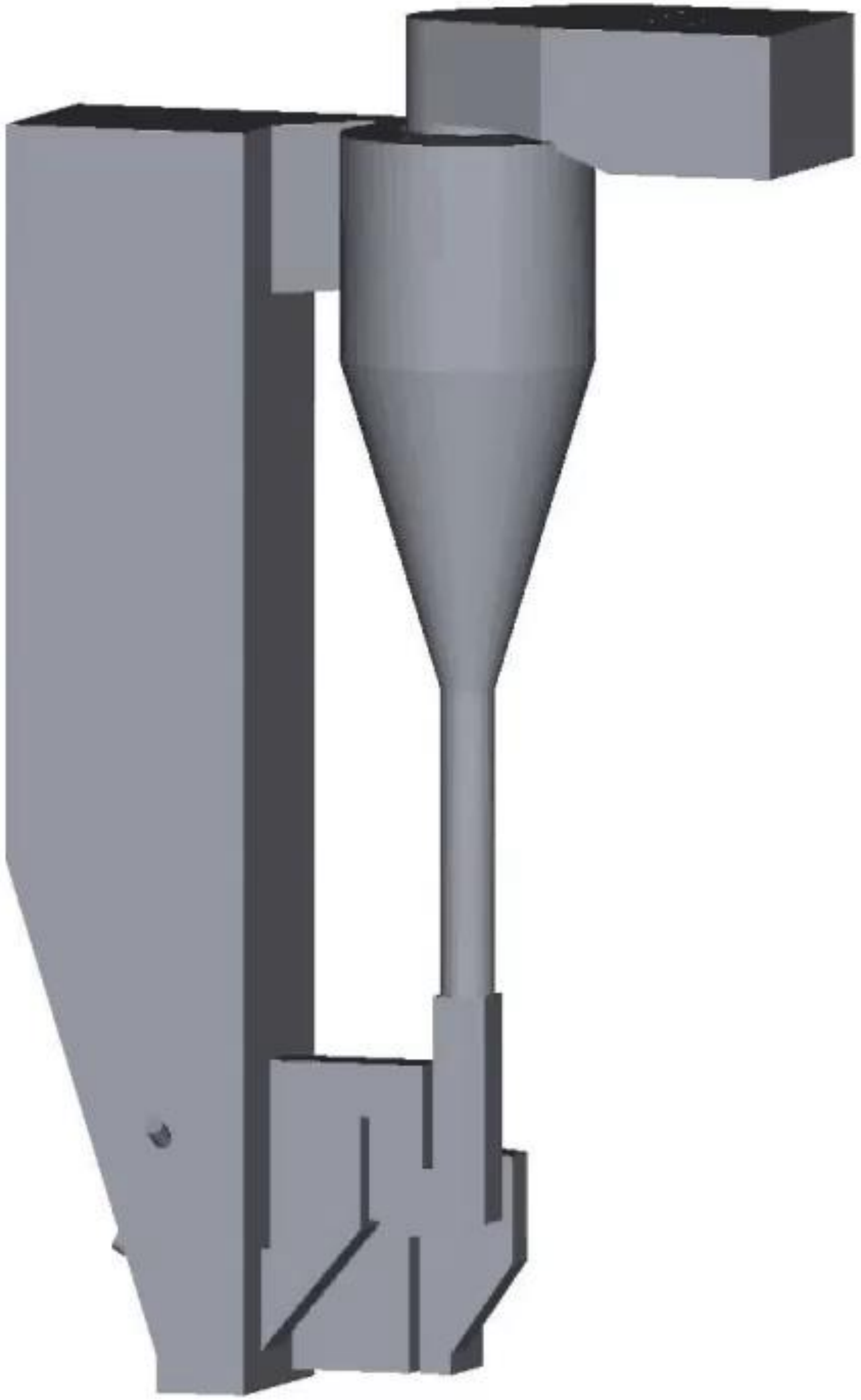
- **Baseline assessment.** Understand the current and historic erosion, and the 3D, multiphase flow patterns causing the surface wear.
- **Design alternatives assessment.** Model several alternatives for each component, to understand the effects of each proposed change on erosion and unit performance.
- **Redesign assessment.** Evaluate the candidate final redesign, which may include several components of different design alternatives



Example Courtesy of BiomasseItalia

CFB Simulation

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



BARRACUDA

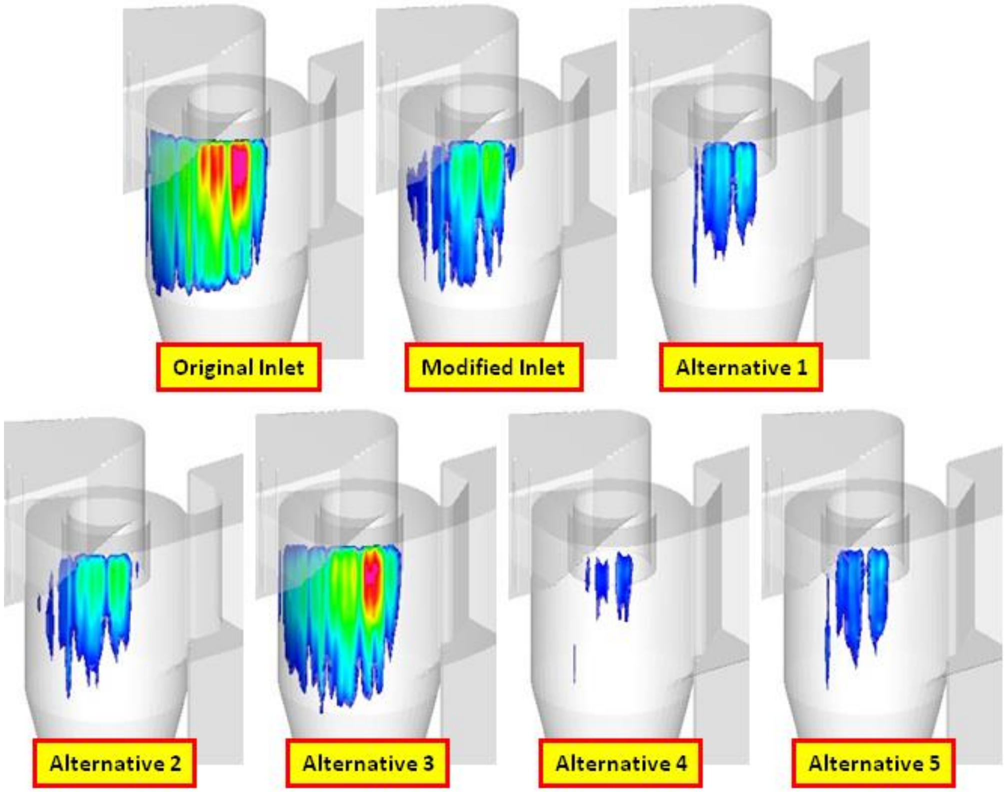
cpfd COMPUTATIONAL PARTICLE FLUID DYNAMICS

Erosion Validation and Optimization

Baseline models were used to verify that the simulations matched operational experience

Design alternative models were used to compare expected cyclone inlet erosion

Alternatives 1, 4 and 5 showed a reduction in erosion, compared with the current design



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

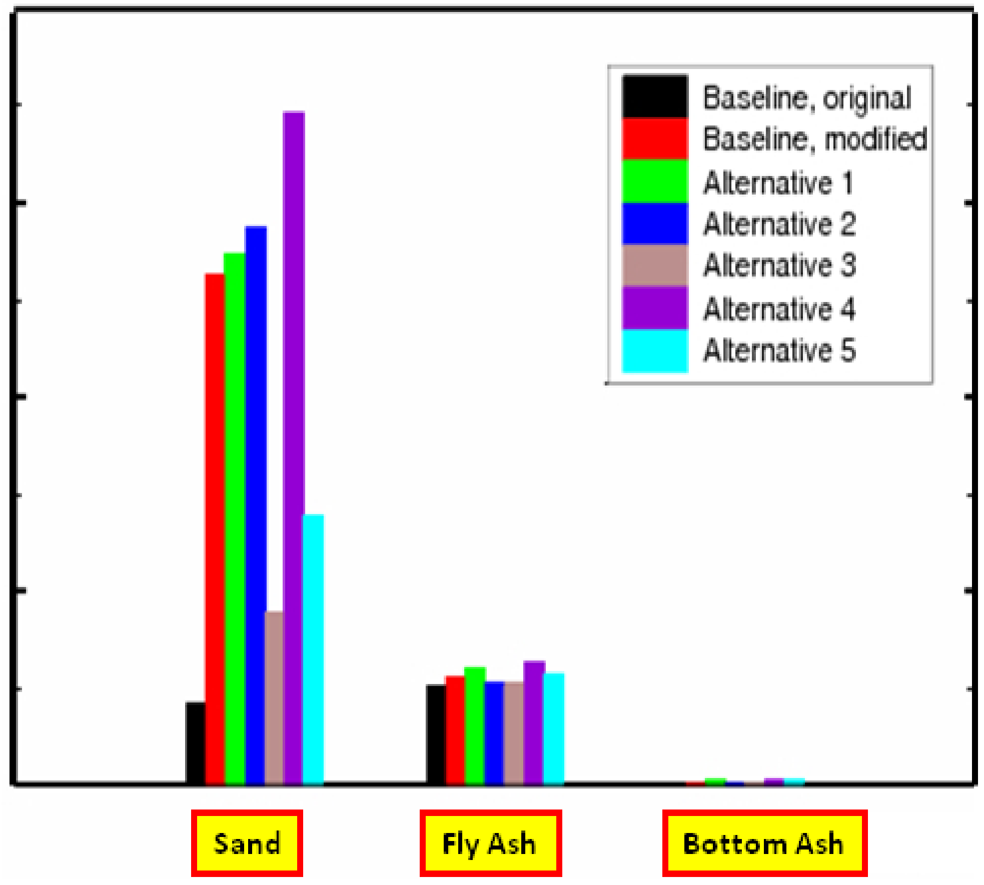
Erosion Validation and Optimization

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 from Industrial Application Example

The Barracuda model was 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

Industrial Application Example 2: Commercial FCC Regenerator

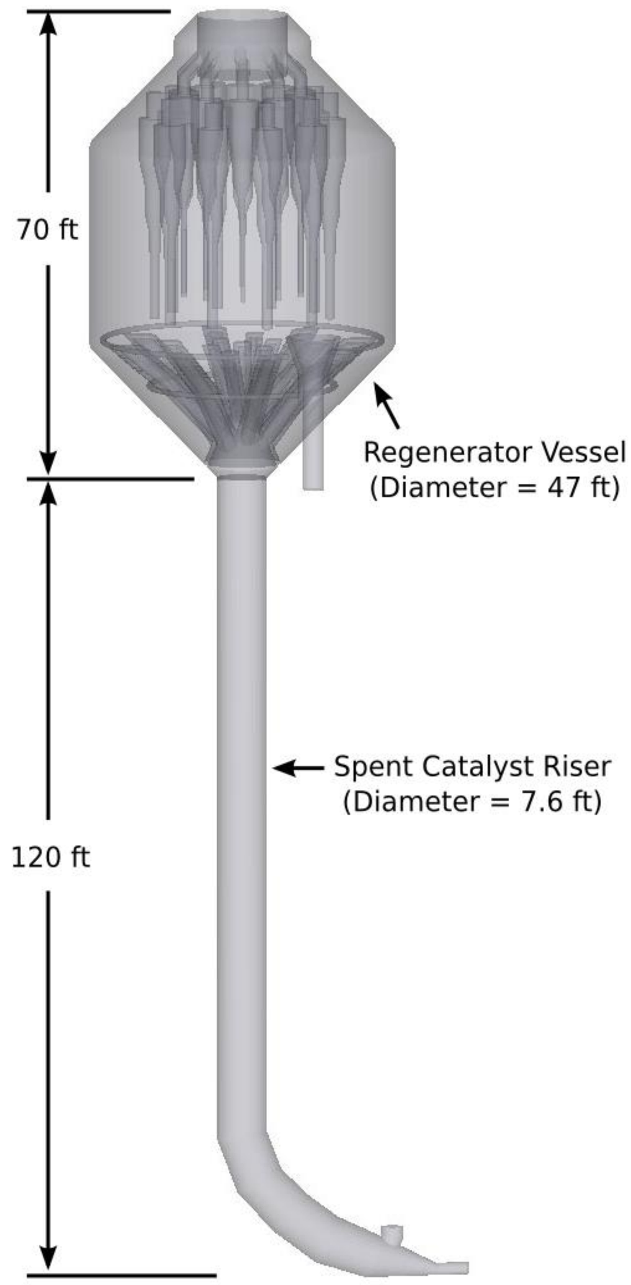
Introduction

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

The regenerator had 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)

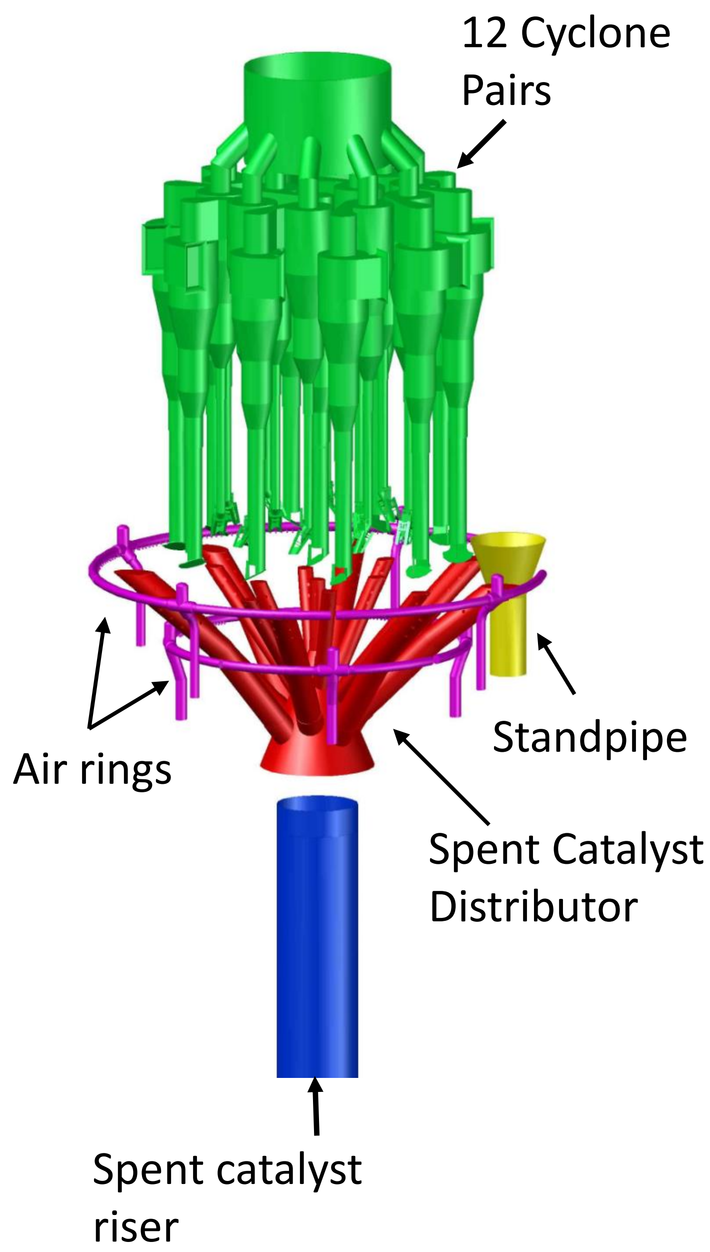


Challenges

Complex geometry
- Vessel internals
- Widely varying length scales

Thermal, reacting, multiphase system
- Afterburn (thermal)
- Emissions (reactions)
- All multiphase and multi-component

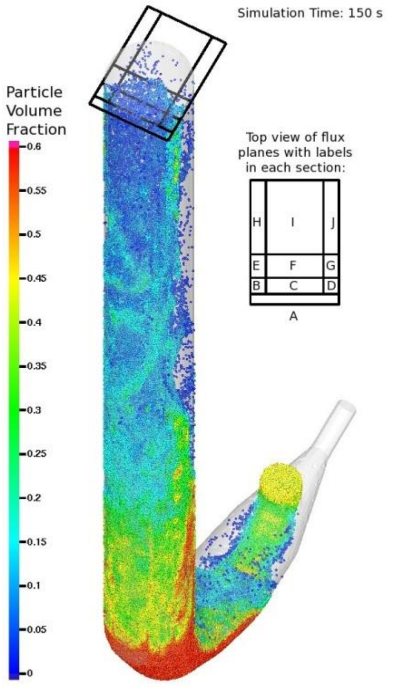
Boundary and initial conditions
- Scope of model
- Particle withdrawal from standpipe
- Initial conditions
  - Temperatures, particle compositions, etc.
- Specification of coke composition

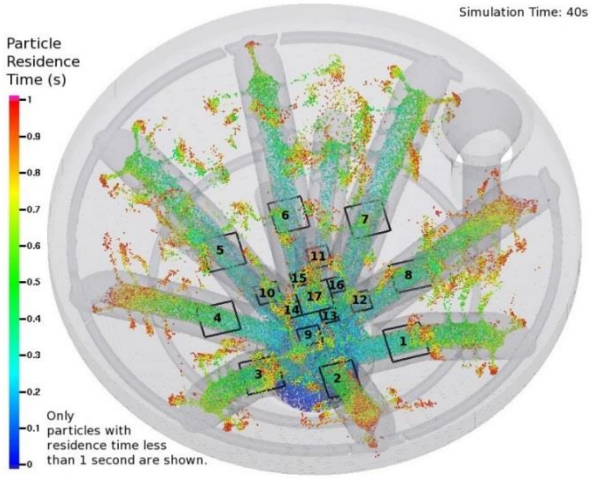


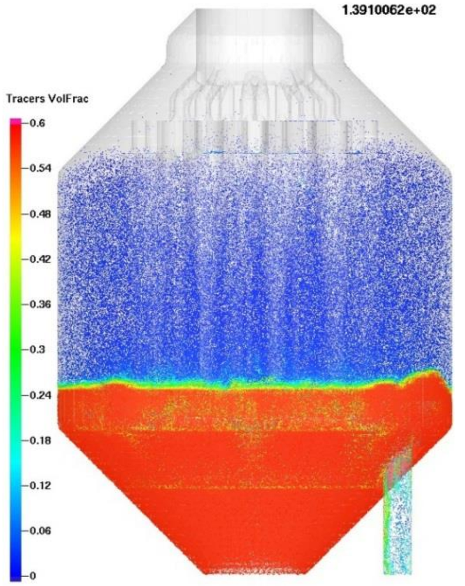
Multiple Model Strategy for Simulation

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







Chemical Reactions

Chemical reactions from open literature were used

- Kanervo, et al, “Kinetics of the regeneration of a cracking catalyst derived from TPO measurements”. *Chemical Engineering Science* 56 (2001): 1221-1227. https://doi.org/10.1016/S0009-2509(00)00343-2
- 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. https://doi.org/10.1021/ie980764b
- Jones, et al, “Approaches to modelling heterogeneous char NO formation / destruction during pulverised coal combustion”. *Carbon* 37 (1999): 1545-1552. https://doi.org/10.1016/S0008-6223(99)00034-2

Multi-material particles were used to represent complex particle compositions

$$\mathrm{C} + \mathrm{O_2} \rightarrow \mathrm{CO} + \mathrm{CO_2}$$

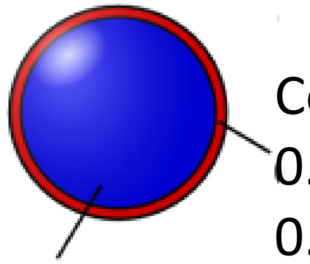
$$\mathrm{CO} + \frac{1}{2}\mathrm{O_2} \rightarrow \mathrm{CO_2}$$

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

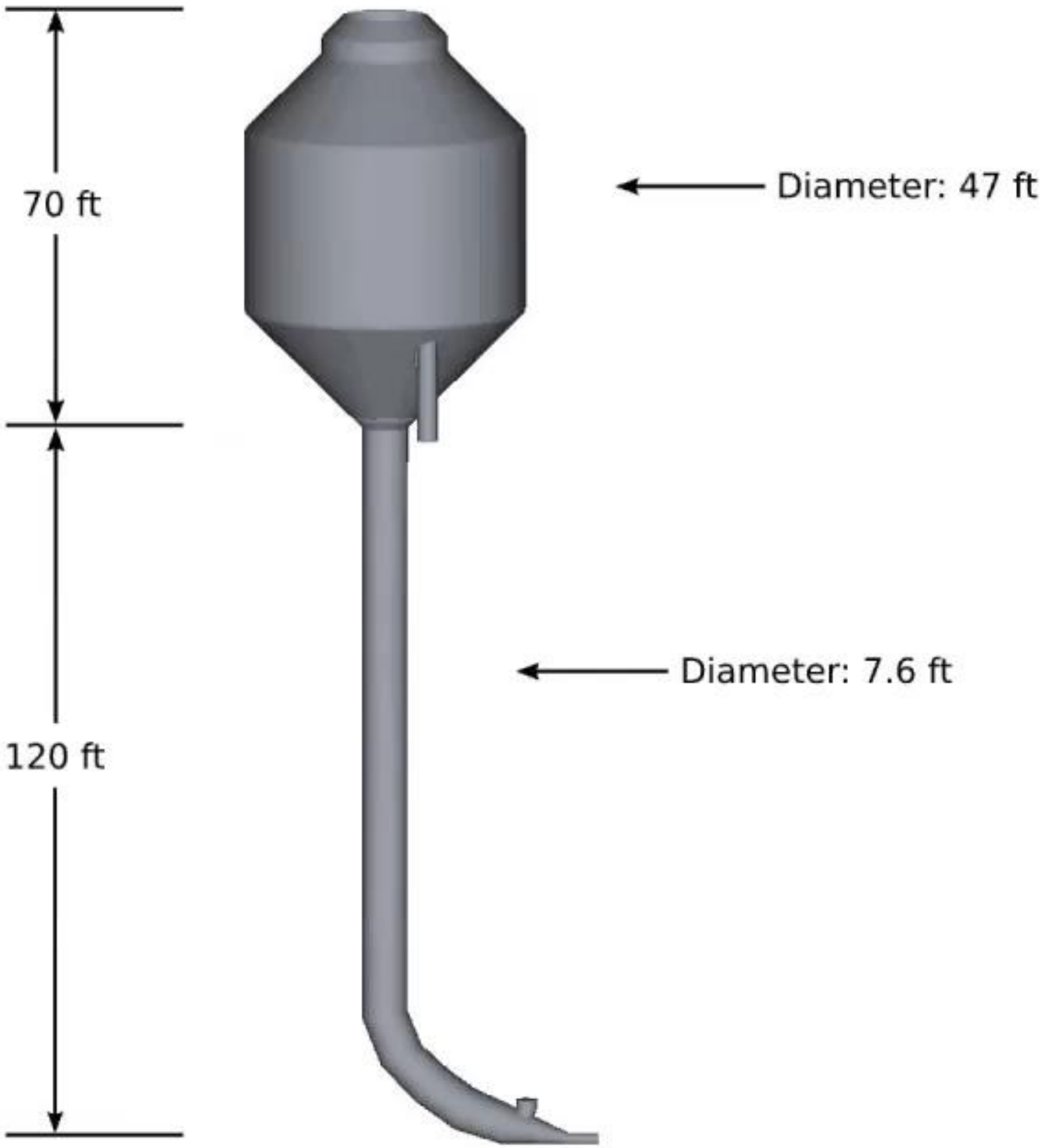
$$\mathrm{S} + \mathrm{O_2} \rightarrow \mathrm{SO_2}$$

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

$$2\mathrm{C} + 2\mathrm{NO} \rightarrow 2\mathrm{CO} + \mathrm{N_2}$$



Commercial FCC Regenerator Simulation



Combined Geometry: Spent Cat Riser + Regenerator

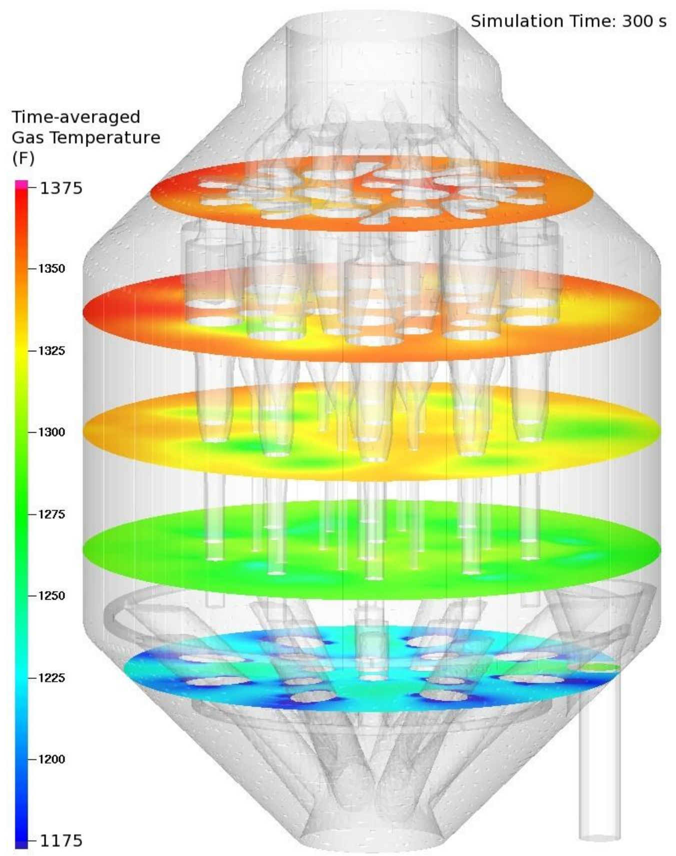
Simulation Results: Afterburn

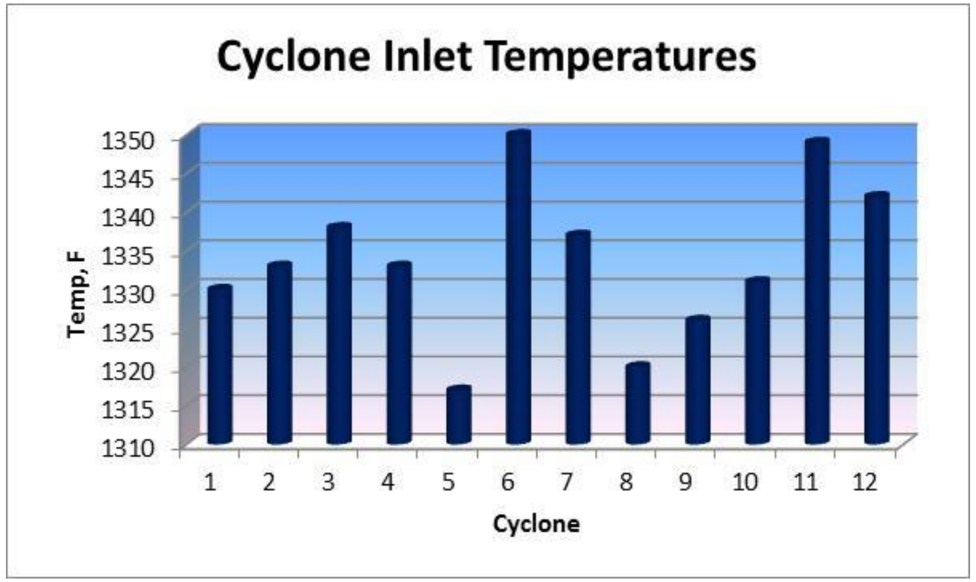
Afterburn was successfully predicted by the model

- 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





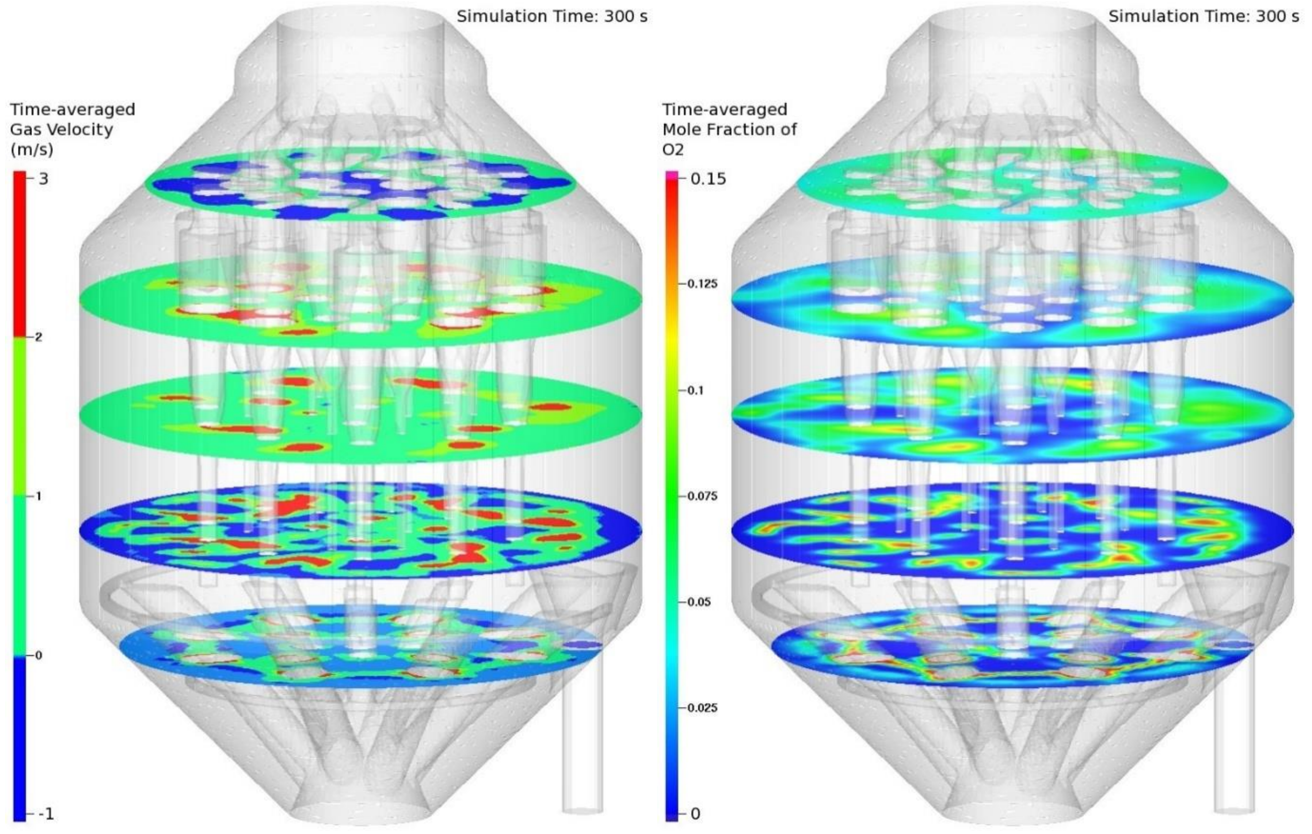
What Caused Afterburn?

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 amount of 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



Conclusions from Industrial Application Example

The model predicted the afterburn observed at the refinery

- Magnitude (100°F) and asymmetry
- Root cause was understood by examining simulation results:
  - Not due to the performance of the spent cat riser or catalyst distributor
  - Due to bed mixing and gas bypass as influenced by fluidization headers and internal structures

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 equilibrium catalyst composition)

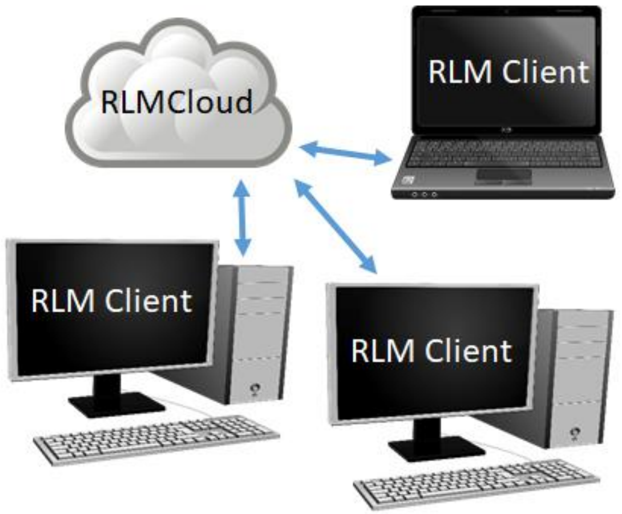
Deployment of Barracuda Virtual Reactor

Computer Hardware

- System requirements
- Recommended hardware
- GPU acceleration

How Licensing Works

- Details on CPFD website
- Number of licenses = number of solvers running
- Unlimited pre-processing and post-processing
- RLMCloud vs On-Premise RLM Server



Summary of Introduction Presentation

Barracuda Virtual Reactor uses the CPFD Method to model fluid-particle flow

- Able to model large industrial systems with high particle counts
- Able to handle full Particle Size Distribution (PSD)
- Able to track particle-to-wall impacts and predict most likely regions of erosion

Barracuda Virtual Reactor has been validated against experimental data

Barracuda Virtual Reactor has been used to model large-scale commercial systems and solve high-value problems

- Insights from simulation results help to understand root causes
- Simulating multiple design alternatives enables optimization