Towards a comprehensive strategy for modeling gas-solid flows

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2010 Workshop on Multiphase Flow Science
Pittsburgh, PA, May 4-6, 2010

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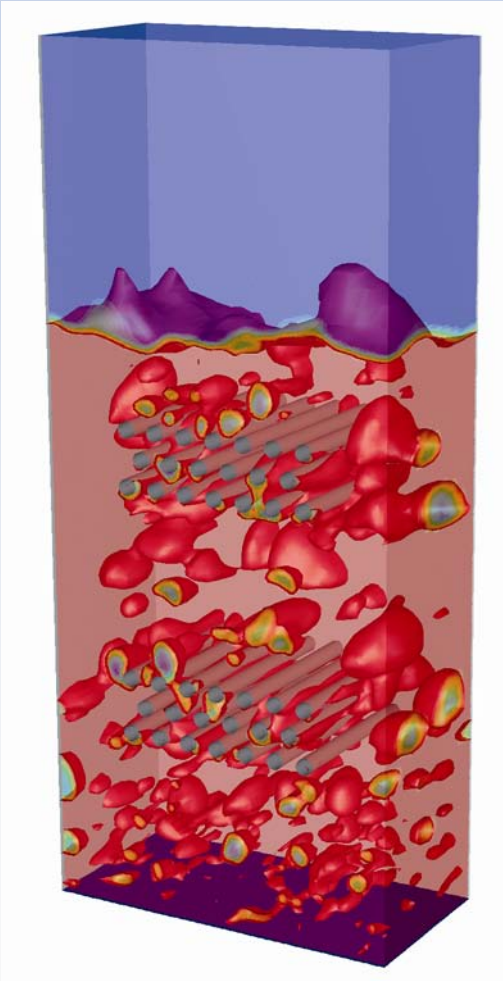
Overview

- Introduction/motivation
- Applications of gas-solid flows
- Modeling particulate flow approaches
  - Two fluid models
  - Eulerian–Lagrangian
  - Hybrid methods
- Modeling Dense phase flow using Lagrangian models
  - Volume fraction of particles
  - Particle-particle interaction
  - Particle collision
- Recap and conclusions



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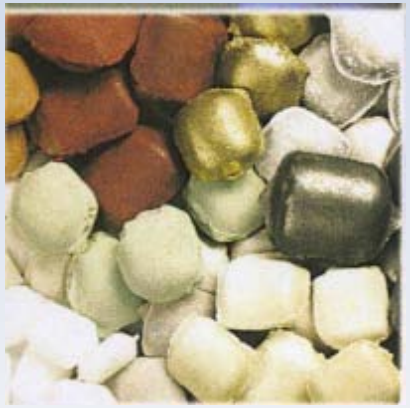
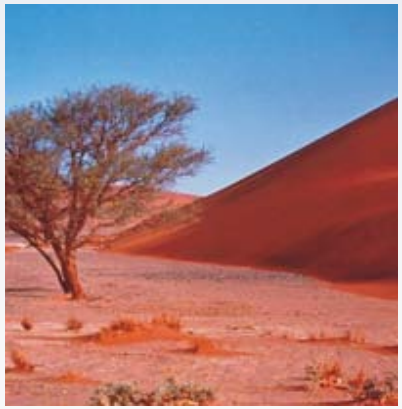
Motivation

- **Develop a modeling platform for a range of industrial applications using multiple modeling approaches:**
  - for multi-physics,
  - multi-component
  - multi-scale requirements for a range of industrial applications
- Applications include
  - Particle Products
    - Powders, granules
    - Crystals
    - Flakes, pellets
    - Pastes, emulsions
- Matrix material
    - Filled fibers
    - Filled polymers
    - Building materials
- Non-particulate
  - Droplets and bubbles





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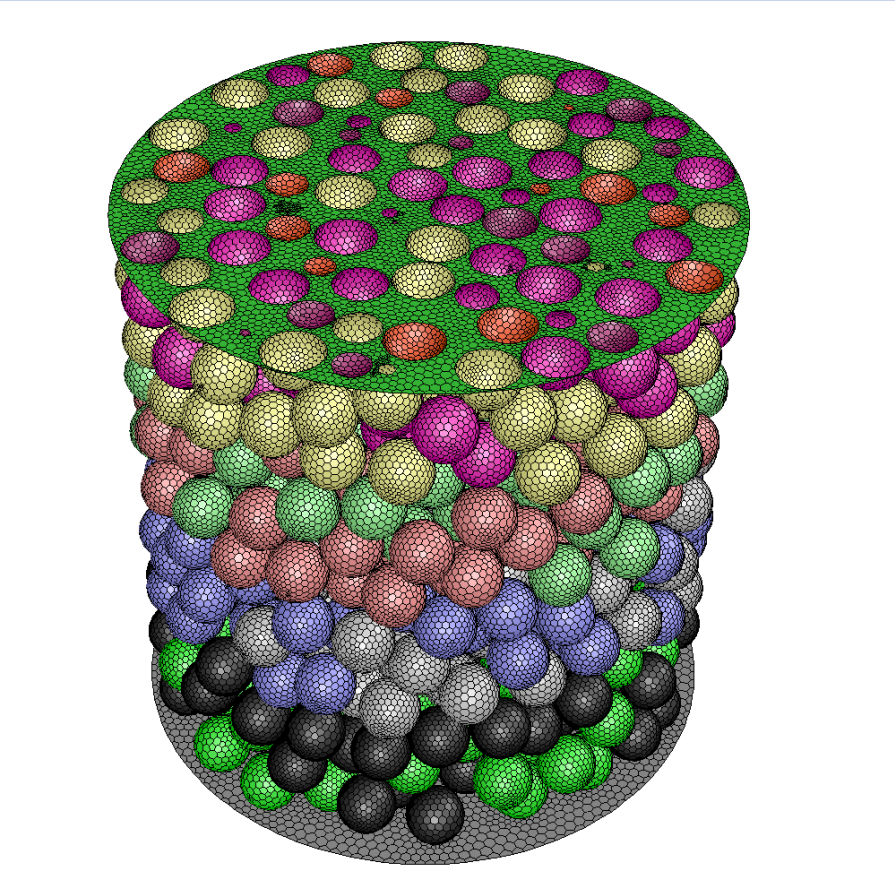
Focus on Particulate flows

- **Modeling Gas –solid systems can include:**
  - **Particle flows**
  - **Particle size distribution**
  - **Particle mechanics**
  - **Surface and morphology**
  - **Particle-particle interaction**
  - **Turbulence and dispersion**
  - **Geometry effects**
  - **Particle attrition**
  - **Homogenous and hydrogenous reaction**
  - **Fluid forces and drag**
  - **Cohesion**
  - **Electrostatic**



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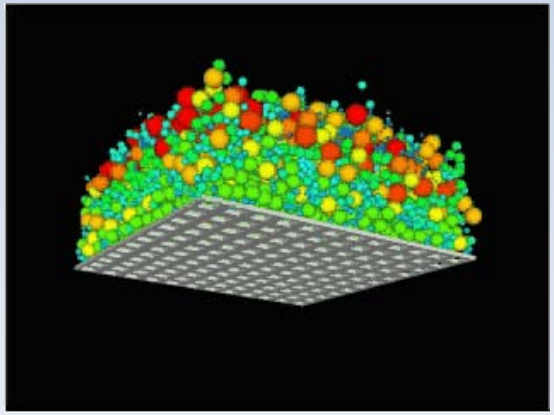
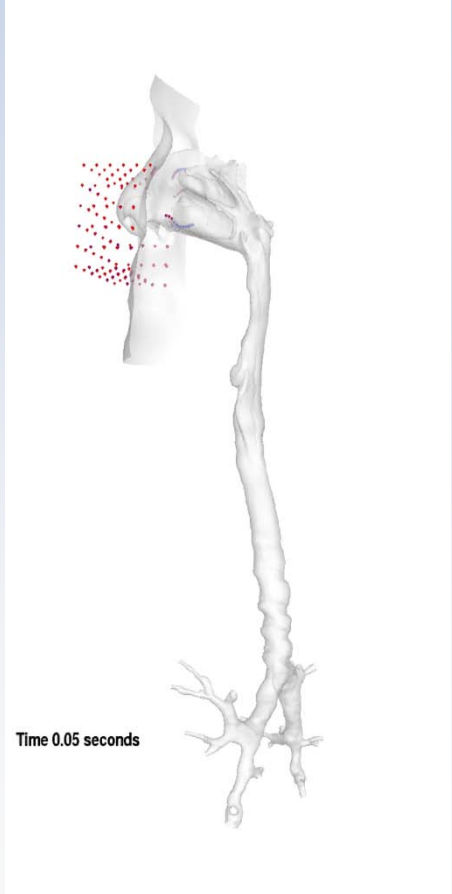
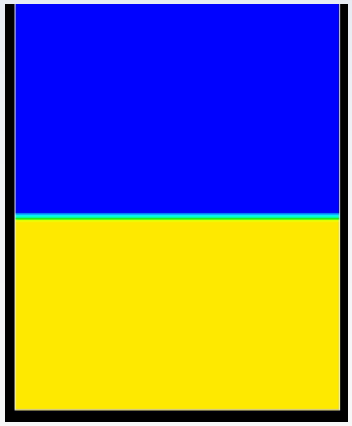
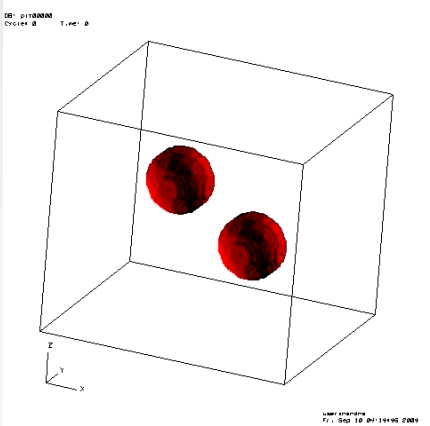
Modeling Multiphase Flows

- **Ability to model Multiphase flows expanding**









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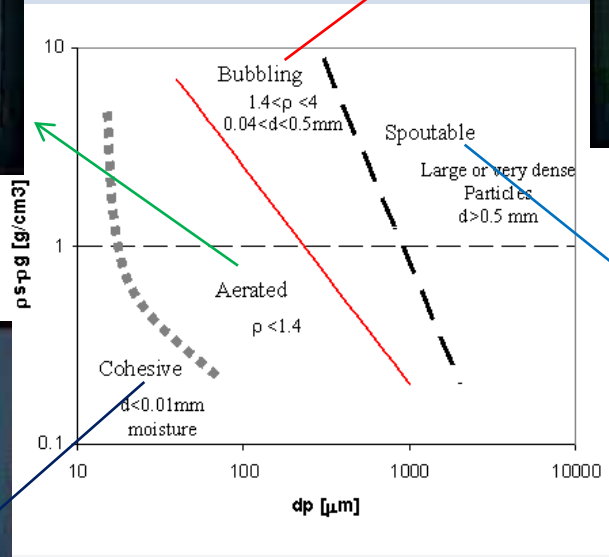
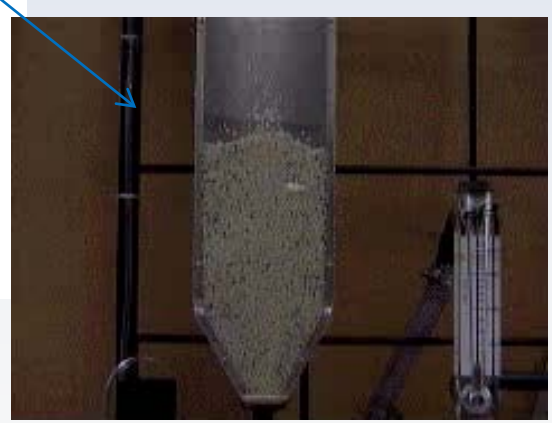
Gas-solid flows

Group A: small size and density like FCC powder

Group B: Most common Material Like Sand



Group C: Cohesive powder



Group D: Large and/or very dense particles

Courstesy: Prof. Martin Rhodes, Monash University, Australia.

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Classification of granular flows

- **Kinetic regime (diluted flow)**
  - grains randomly fluctuate and translate, these forms of viscous dissipation and stress is named kinetic effect.
- **Collisional regime (higher concentration)**
  - in addition to dissipation, grains can collide shortly, enhancing dissipation and stress, named collisional effect
- **Frictional regime (typically ε >50%)**
  - grains starts to endure long, sliding and rubbing contacts, which gives rise to a totally different from kinetic and collisional, named frictional effect.

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Dilute vs. Dense Flows

- **Average time between particle collisions:**

$$\tau_C = \frac{1}{f_C} = \frac{1}{n\pi d_P^2 v_r}$$

- Particle response time:

$$\tau_P = \frac{\rho_P d_P^2}{18\mu_C}$$

- Inter-particle spacing:

$$\frac{L}{d_P} = \sqrt[3]{\frac{\pi}{6\alpha_P}}$$

- **Dilute flow:**

$$\tau_P / \tau_C < 1$$

- Dense flow:

$$\tau_P / \tau_C > 1$$

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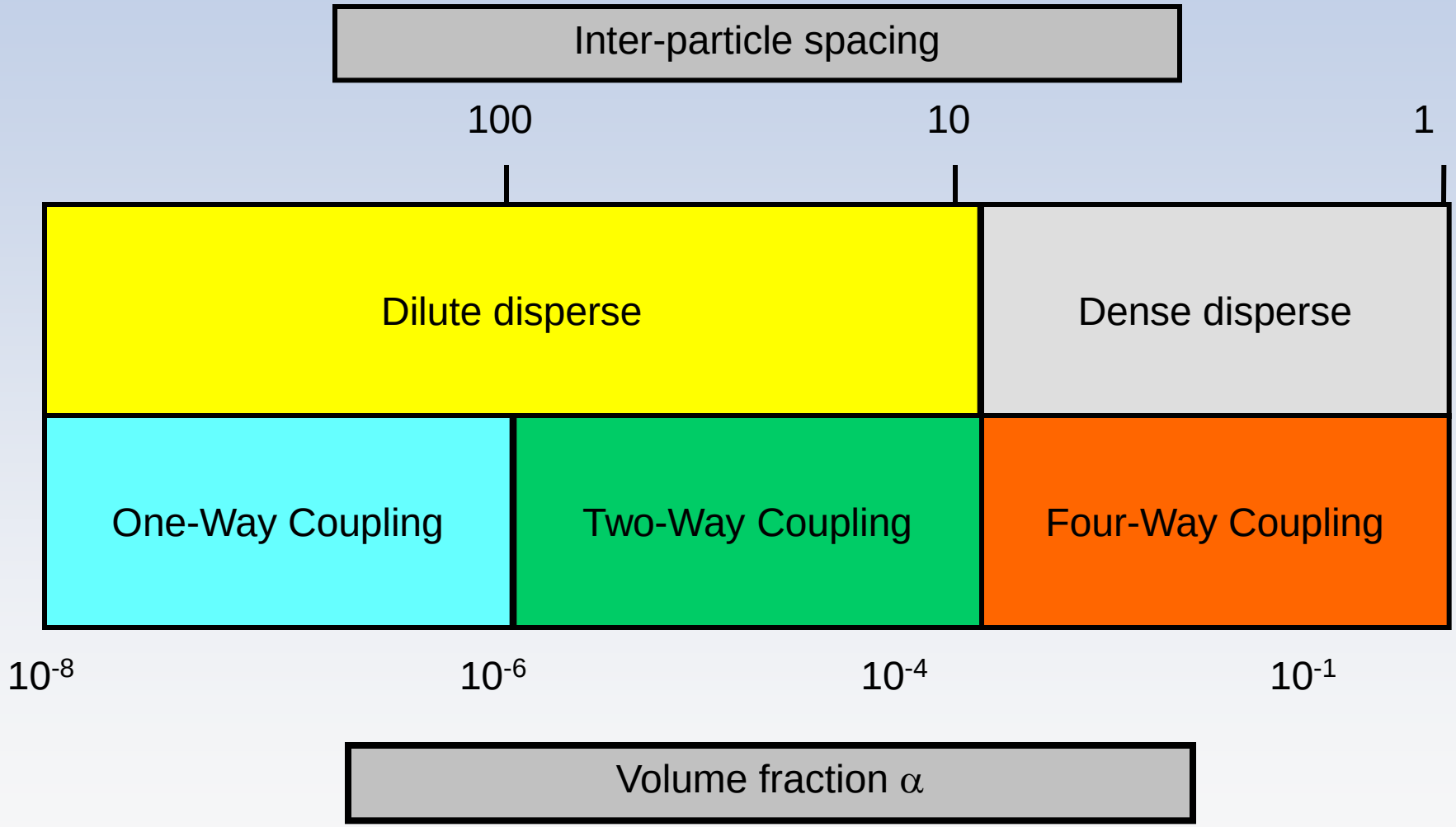
Dilute vs. Dense Flows



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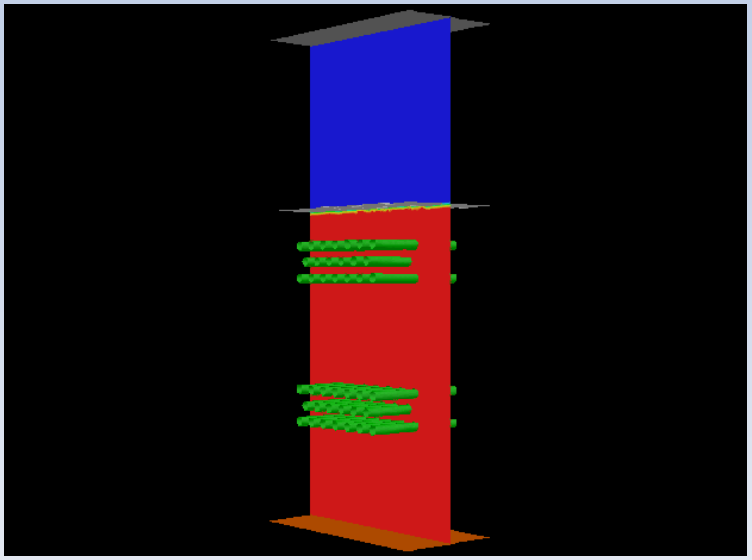
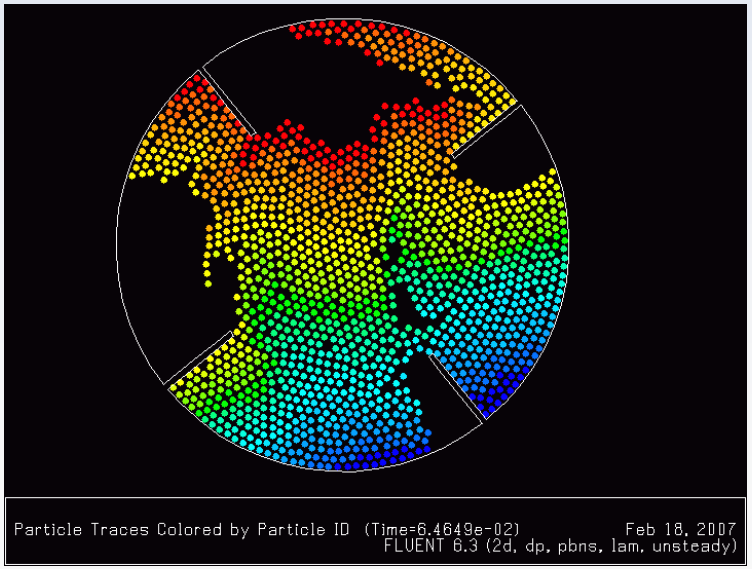
Common Multiphase Models

- **Modeling particulate flows has been of long-standing interest and commonly used models include:**
  - Lagrangian Models
    - DPM for dilute phase (steady and time dependent)
    - Macroscopic Particle Model (MPM) for large particles.
  - Eulerian Models
    - Euler-Granular with constitutive relations for particle stresses
  - Hybrid Methods
    - Dense Phase DPM for dense flows with large size distributions.
      - Stress modeled on GKT
      - Explicit contact





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Hybrid Models

- **A general framework in which the continuous phase is solved on an Eulerian grid and the particulate phase in a Lagrangian frame.**
- **Accounts for the volume fraction of the particulate phase and particle size distribution.**
- **Provides cell-averaged information from Lagrangian to Eulerian frame.**
- **Accounts for particle-particle and particle-wall interactions (GKT or explicitly).**

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Transport equations for Eulerian granular flow

Continuity

$$\frac{\partial}{\partial t}(\alpha_s \rho_s) + \nabla \cdot (\alpha_s \rho_s \vec{u}_s) = \dot{m}_{fs}$$

Mass transfer

Momentum

Shared pressure

Inter-phase terms

$$\frac{\partial}{\partial t}(\alpha_s \rho_s \vec{u}_s) + \nabla \cdot (\alpha_s \rho_s \vec{u}_s \vec{u}_s) = -\alpha_s \nabla p_f + \nabla \cdot \bar{\tau}_s + \sum_{s=1}^{n} (\vec{R}_{fs} + \dot{m}_{fs} \vec{u}_{fs}) + \vec{F}_s$$

Solids Stress

Note

Transport equations for fluid-fluid system and fluid-solid system differ only in the treatment of stress tensor and inter-phase terms

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Solids stress tensor

- **Constitutive equations needed to account for interphase and intraphase interaction:**
  - Solids stress $\nabla \cdot \bar{\tau}_s$
  - Accounts for interaction within solid phase. Derived from granular kinetic theory

$$\bar{\tau}_s = -P_s \bar{\mathbf{I}} + 2\alpha_s \mu_s \bar{\mathbf{S}} + \alpha_s (\lambda_s - \tfrac{2}{3}\mu_s) \nabla \cdot \vec{u}_s \bar{\mathbf{I}}$$

where,

$\bar{\mathbf{S}} = \frac{1}{2}\left(\nabla \vec{u}_s + (\nabla \vec{u}_s)^T\right)$ Strain rate

P_s Solids Pressure

g_o Radial distribution function

λ_s, μ_s Solids bulk and shear viscosity

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Algorithm of the Dense Discrete Phase Model

Particle equation of motion, Collision force“

$$\frac{d\vec{u}_s}{dt} = F_D\left(\vec{u}_f - \vec{u}_s\right) - \frac{1}{\rho_p}\nabla p + \vec{g}\left(\frac{\rho_p - \rho_f}{\rho_p}\right) + \vec{a}_{other} + \vec{a}_{col}$$

Cell based averaging

$$< \phi > = \frac{\sum_i n_i \ \phi_i}{\sum_i n_i}$$

$< \alpha_s \rho_s \vec{u}_s >$ mass flux

$< \alpha_s >$ vol. fraction

$$\vec{a}_{col} = -\frac{1}{\rho_p \alpha_p}\nabla P_s$$

Kinetic theory

$$\frac{3}{2}\left(\frac{\partial}{\partial t}\left(< \rho_s \alpha_s > \theta + \nabla \cdot \left(< \rho_s \alpha_s \vec{u}_s > \theta\right)\right)\right) =$$

$$= \bar{\tau}_s : \nabla < \vec{u}_s > + \nabla\left(k_\theta \nabla \theta\right) - \gamma_\theta + \phi_{ls}$$

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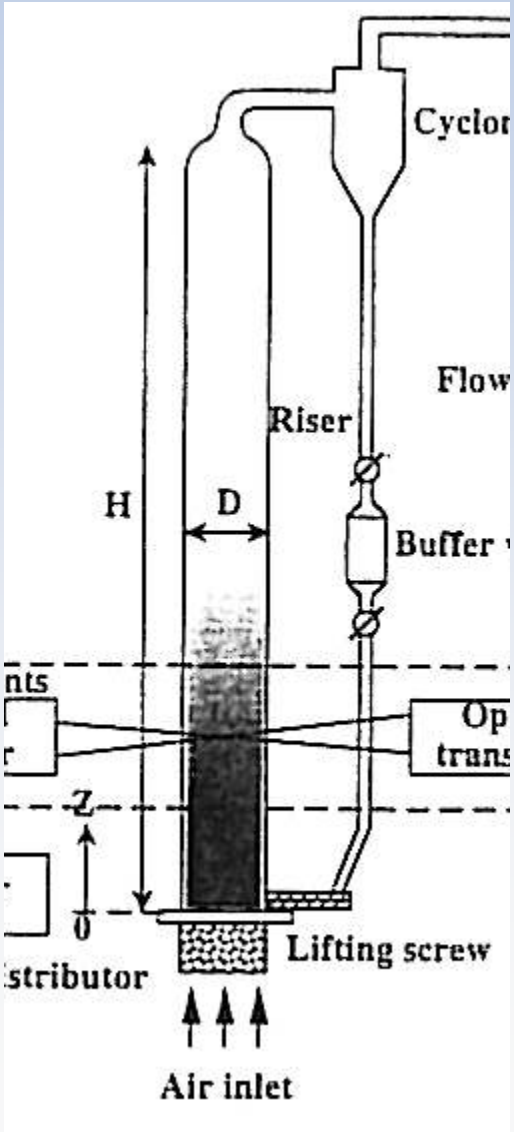
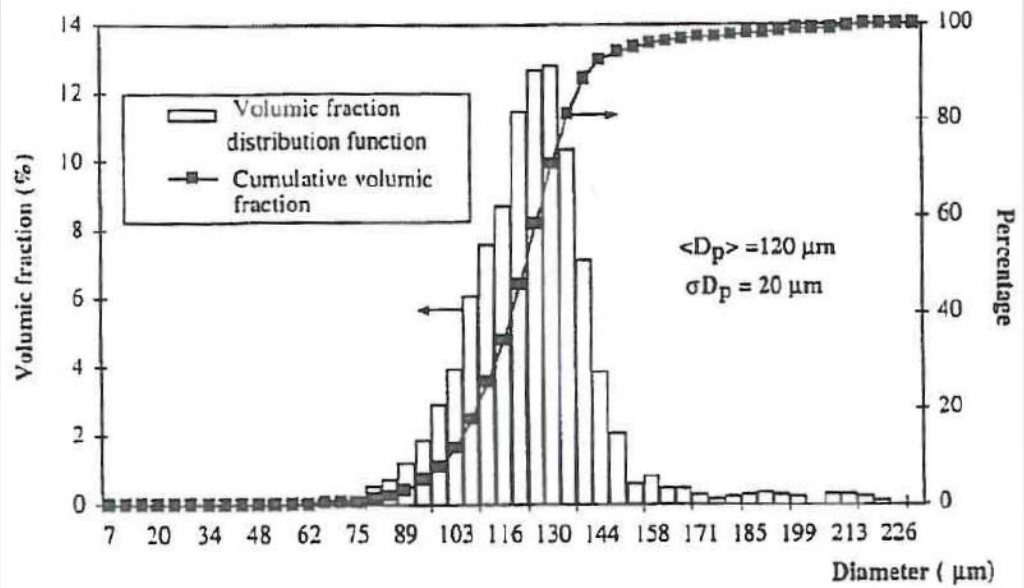
Circulating Fluidized Bed Investigation of Particle Segregation



Particles	$\rho_p = 2400\ \frac{kg}{m^3}$ $\alpha_p \leq \alpha_{max}$
Gas	$\rho_g = 1.225\ \frac{kg}{m^3}$ $u_g \approx 1,\ 1.1\ \frac{m}{s}$



T. Van den Moortel et. al. Chemical Engineering Science, Vol 53 (1998)

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Circulating Fluidized Bed Investigation of Particle Seggration

Settings

Model	Dense Discrete Phase, Multi Fluid
Drag	Morsi-Alexander
Grids	2d: 64k cells 3d: 20k, 114k, 264k cells
Number particles	2d: 523k in steady state 3d: 314k, 1.57 mio, 3.14 mio
Time	60s
Time step	0.001s
Computing time for 1000 time steps	160 min on 40 CPUs for fine mesh

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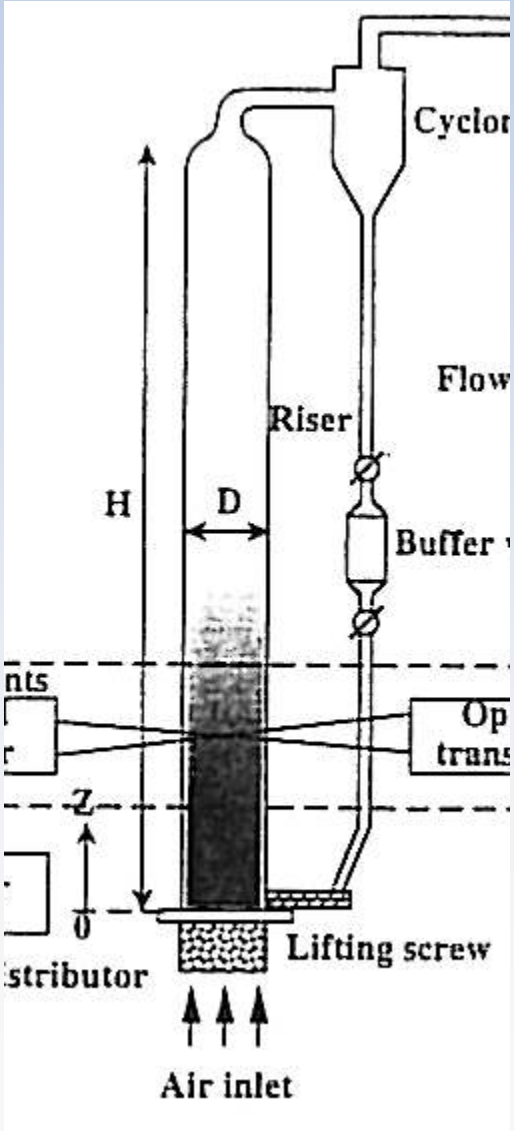
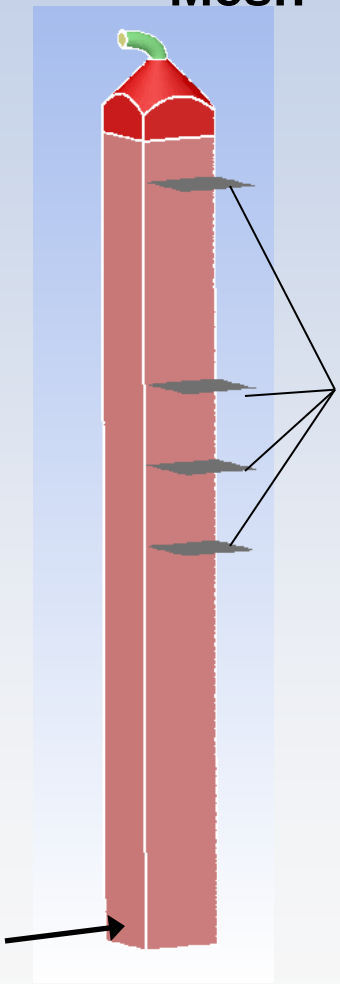
Circulating Fluidized Bed Setup



Mesh



PDA measurement planes

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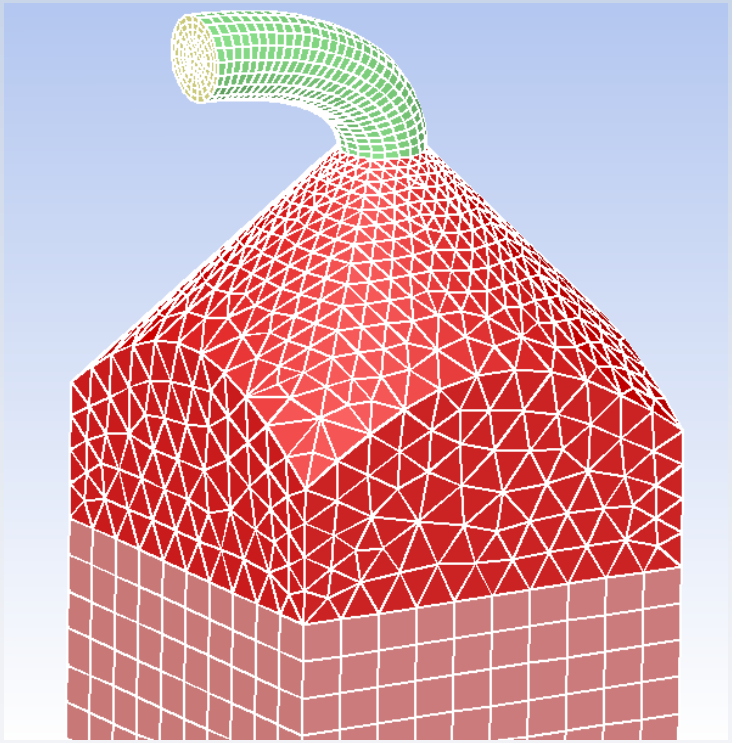
Circulating Fluidized Bed Mesh

hexahedral mesh
at exit



tet mesh
for transition

hexahedral mesh
in riser

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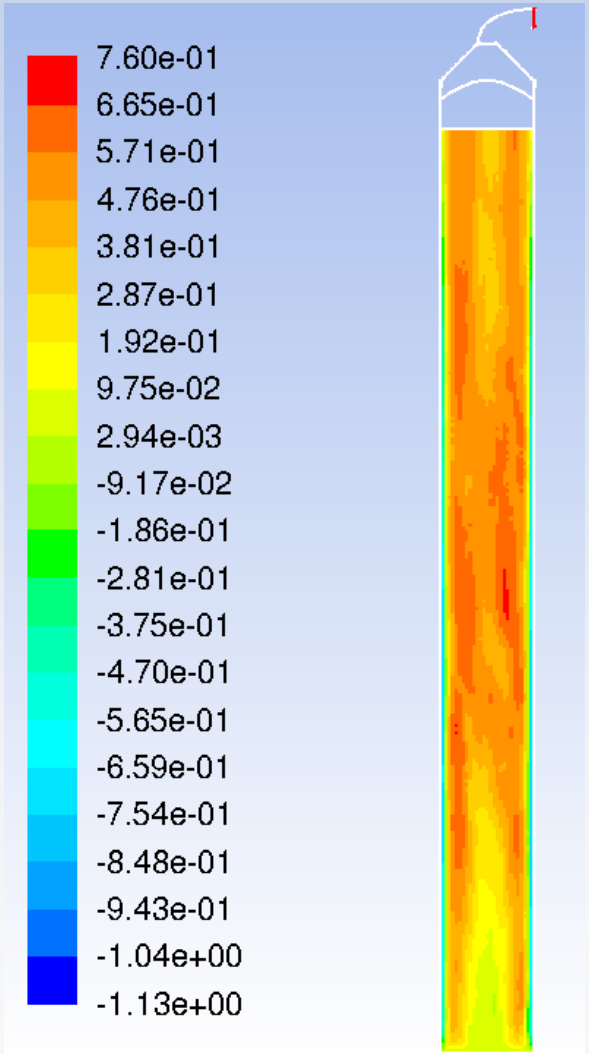
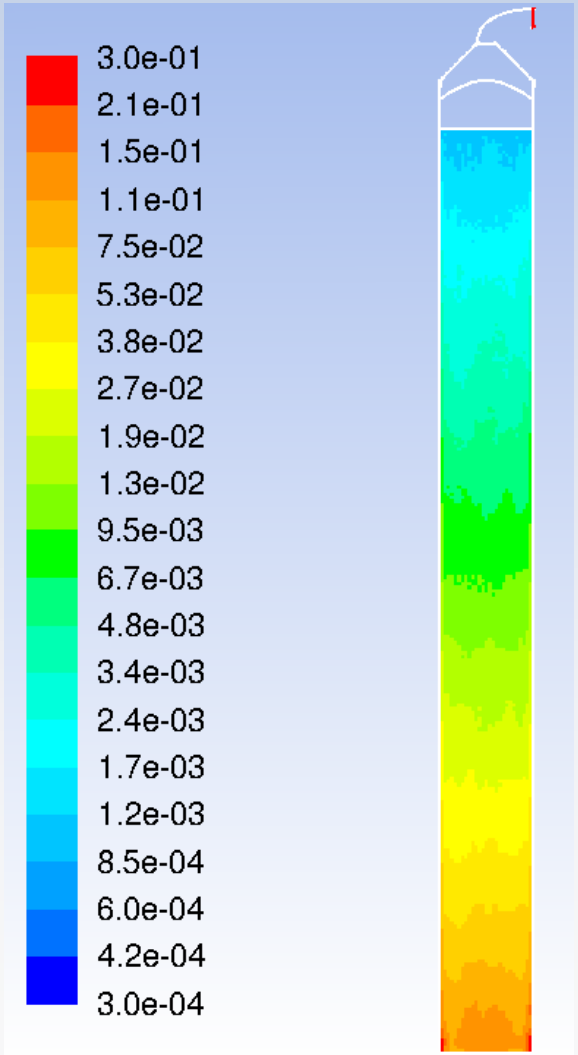
Circulating Fluidized Bed
Results Averaged for 30 Seconds

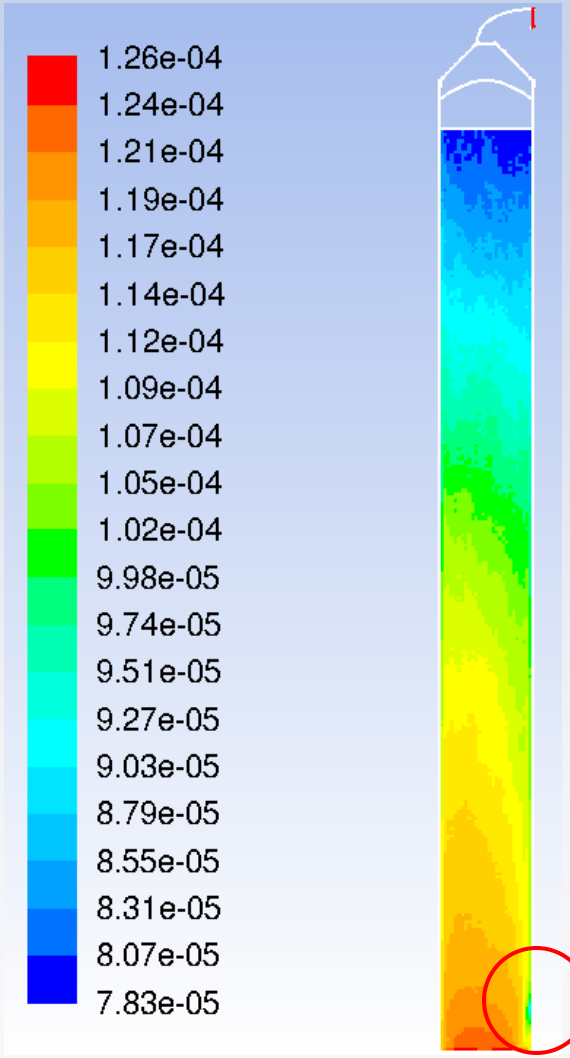
axial particle velocity



particle volume fraction



d10 diameter



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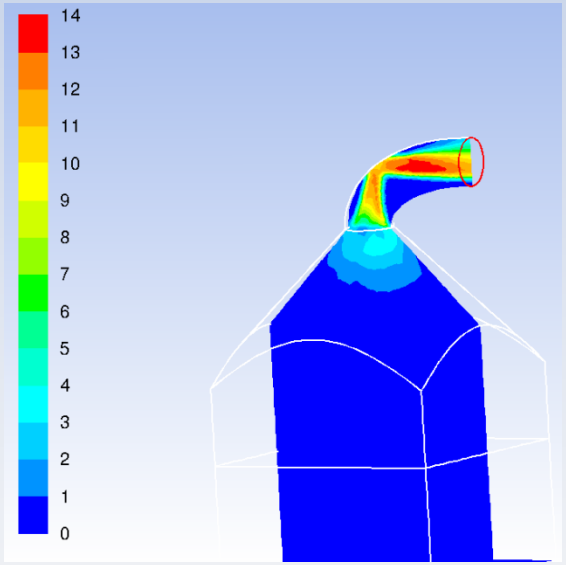
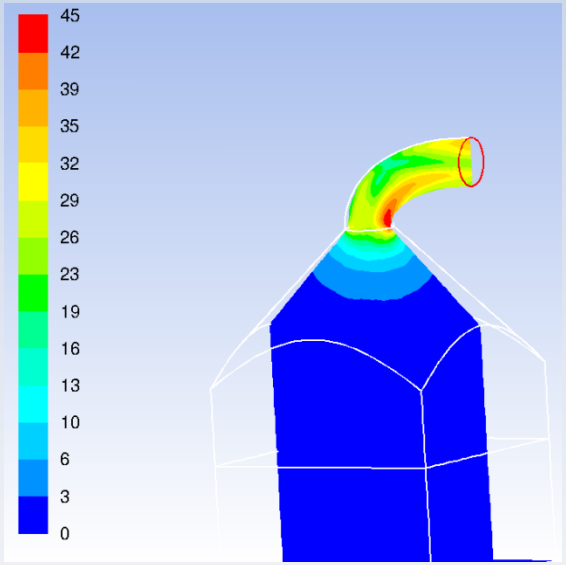
Circulating Fluidized Bed Flow at Exit

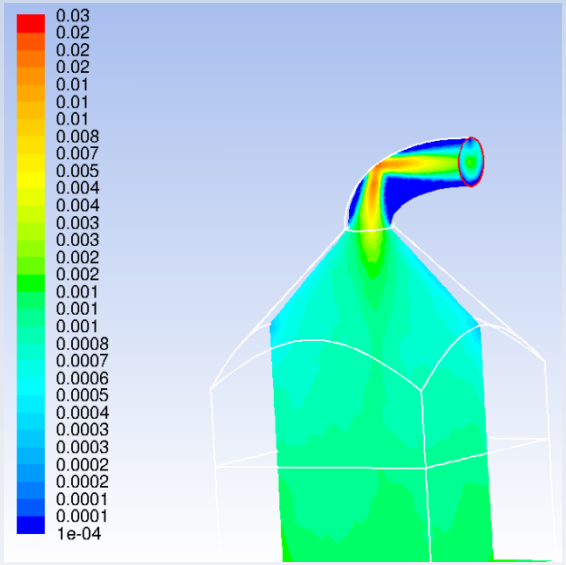
particle velocity



gas velocity



particle volume fraction



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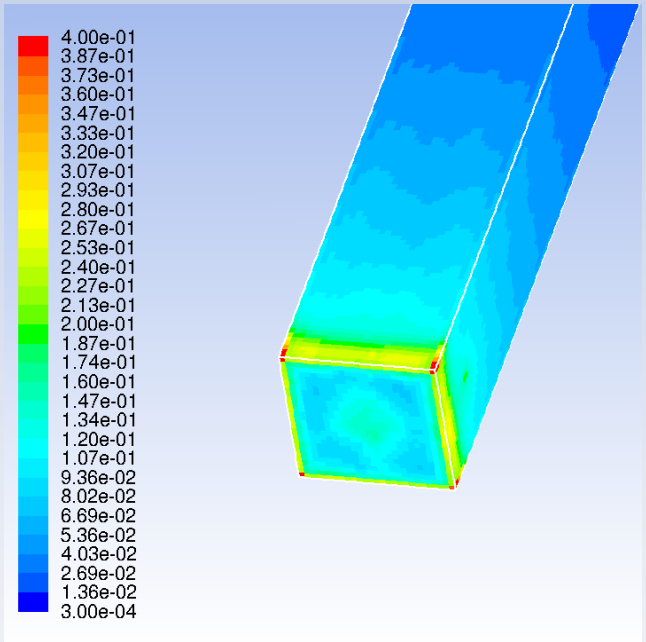
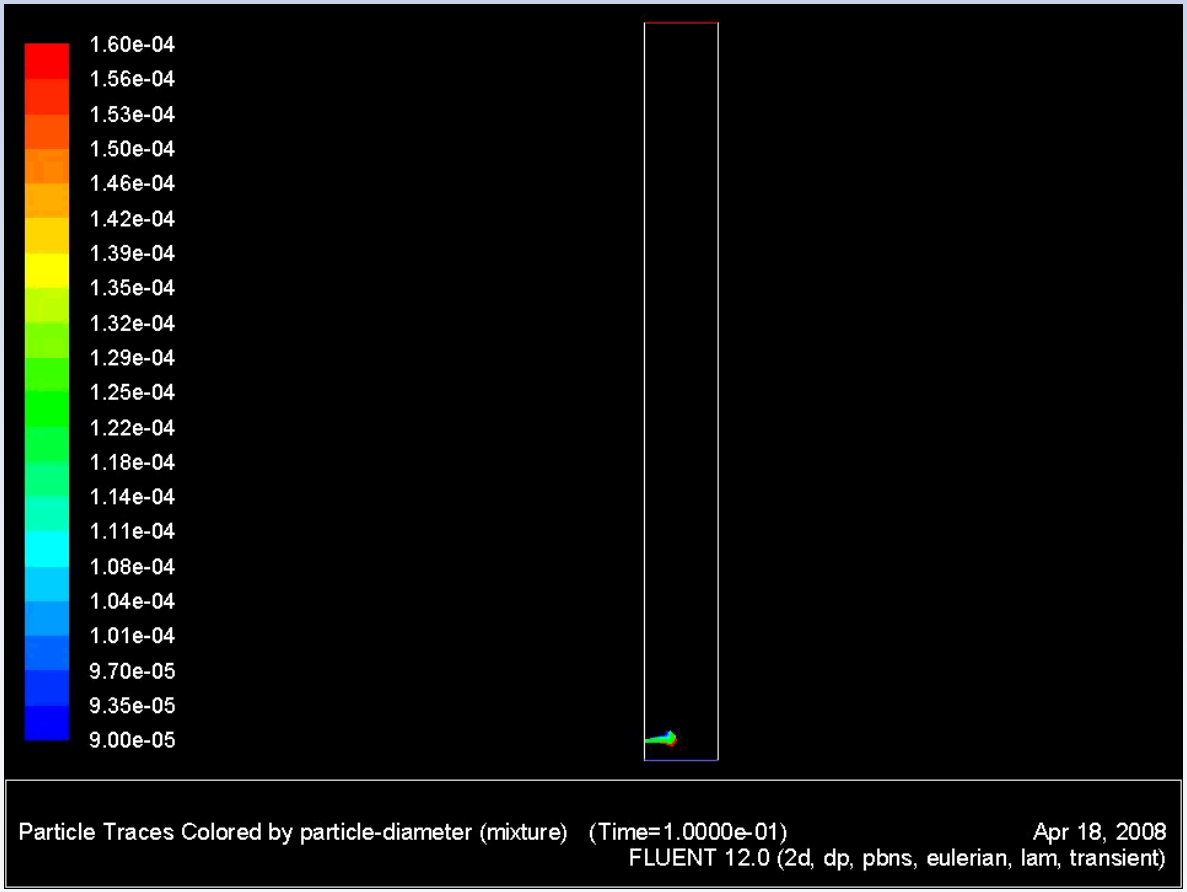
Circulating Fluidized Bed
Particle Accumulation at Bottom



particle volume fraction



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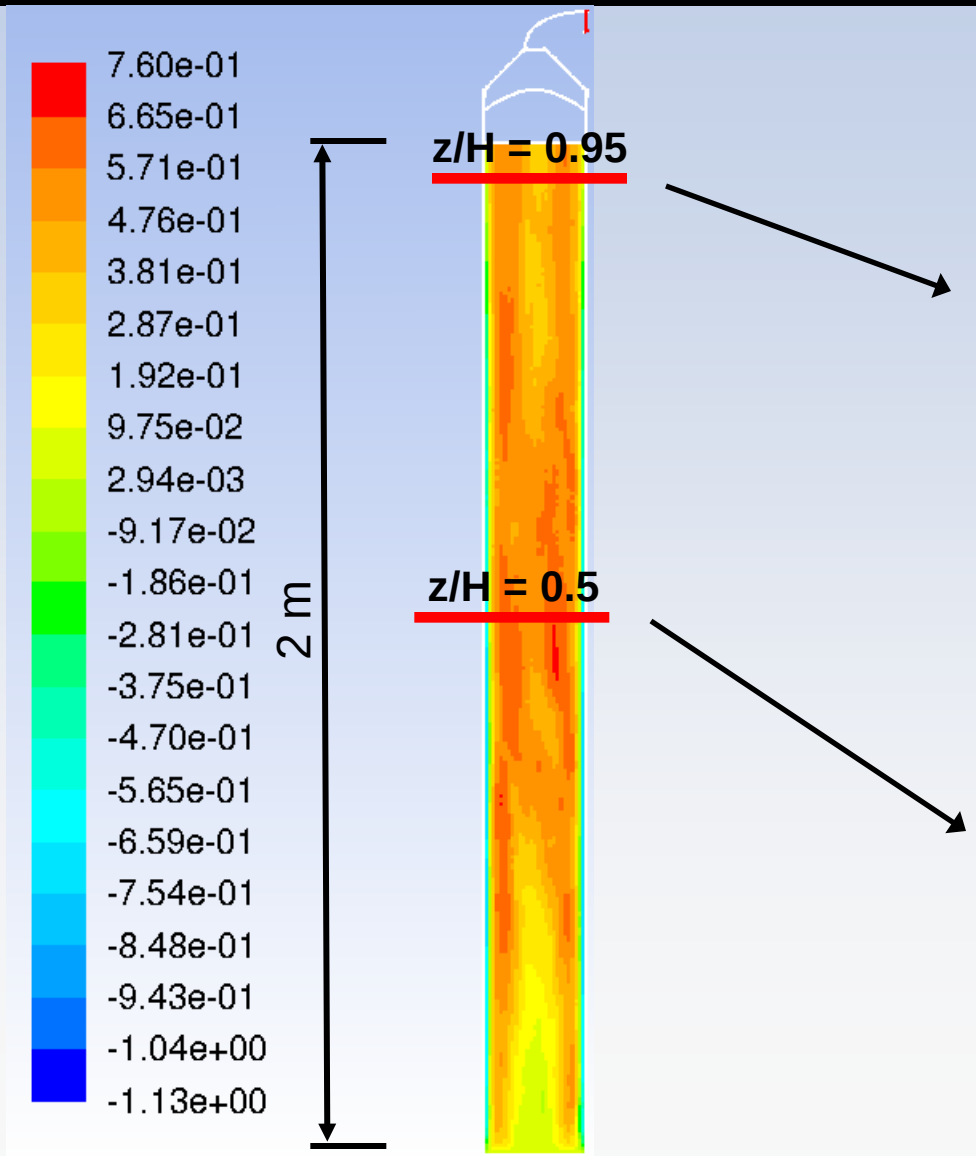
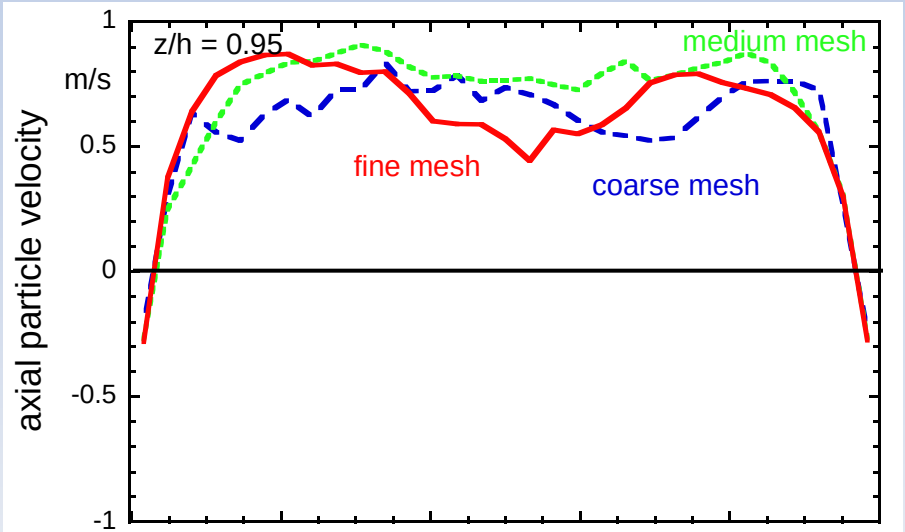
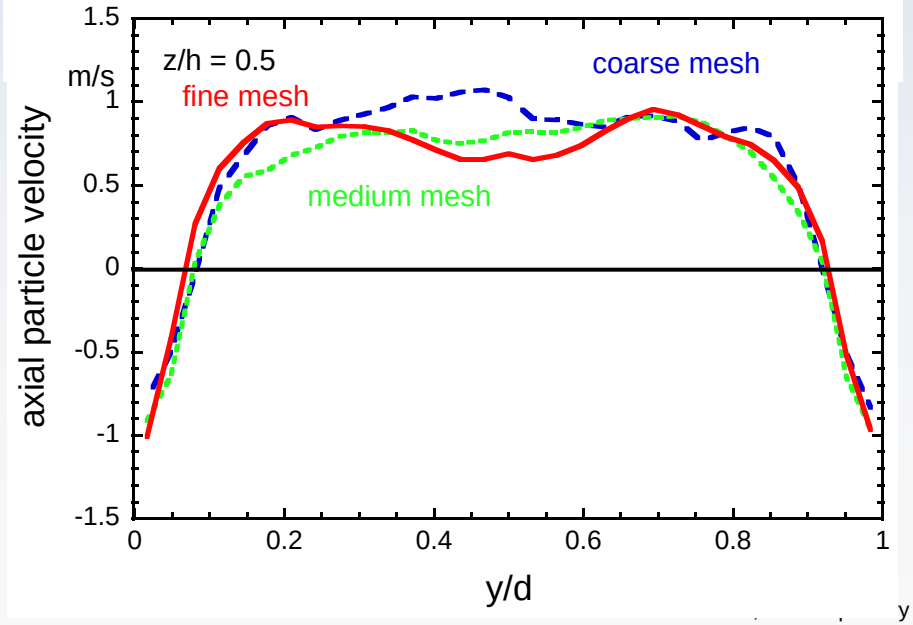
Circulating Fluidized Bed
Influence of the Mesh Resolution







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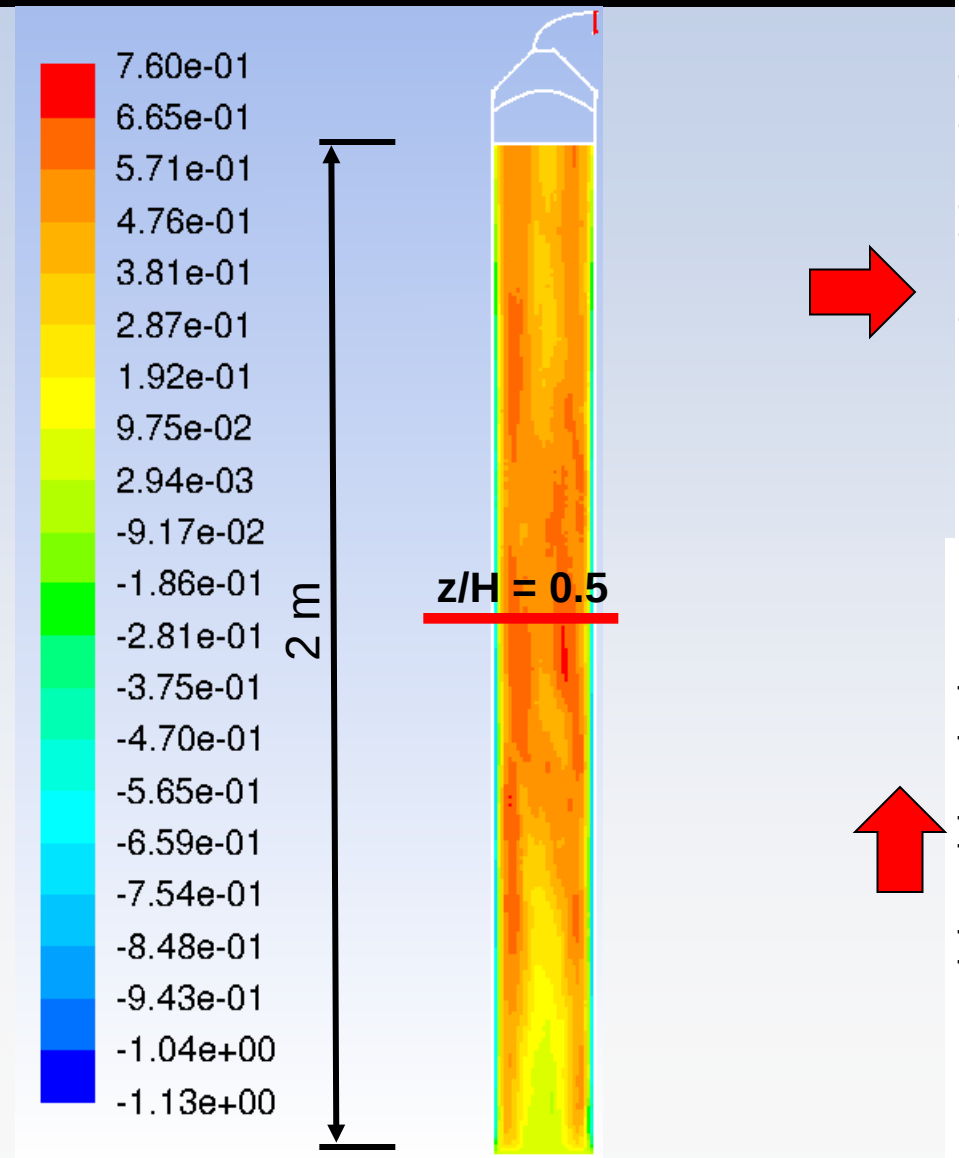
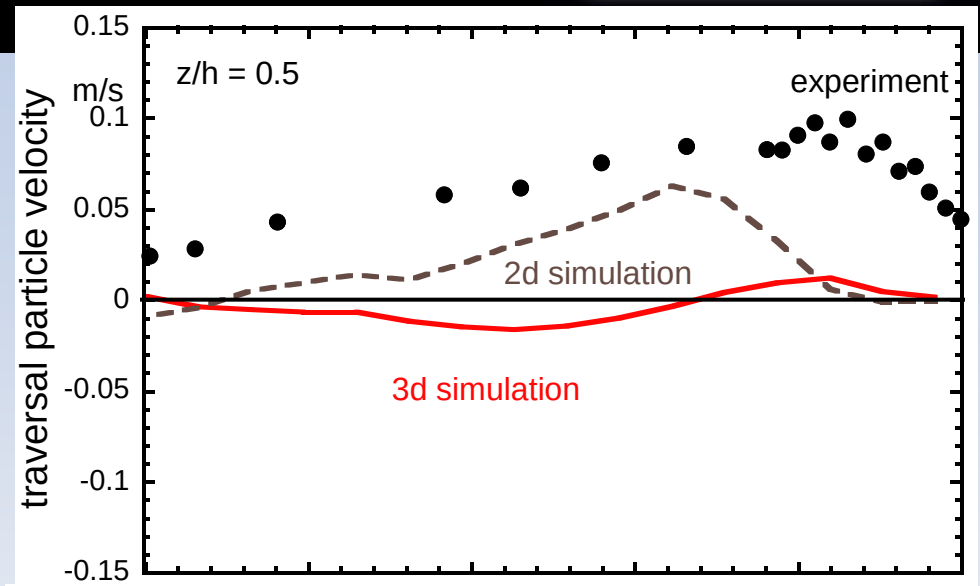
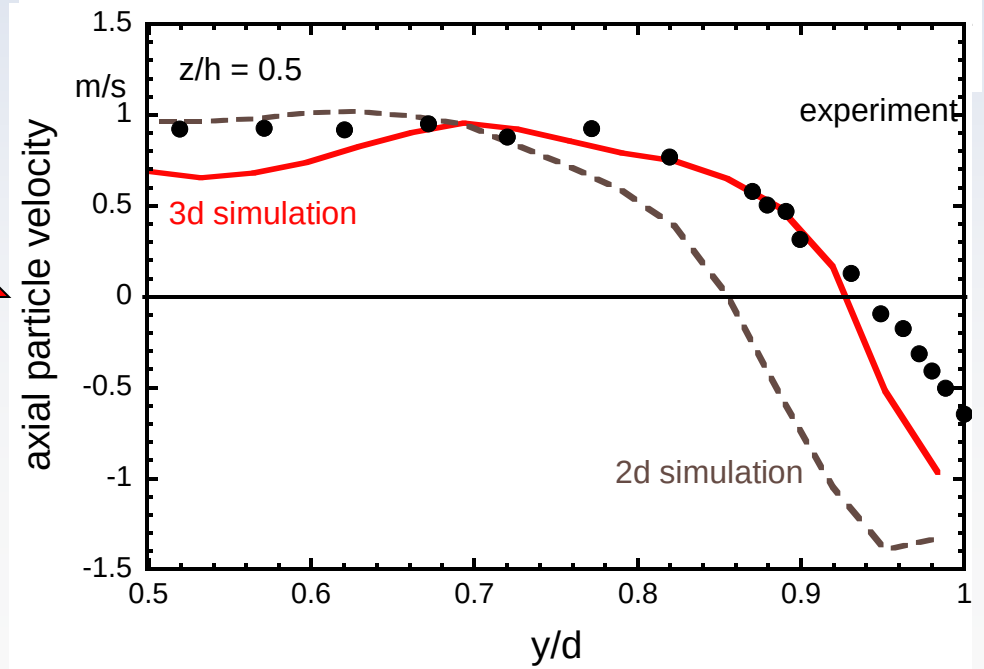
Circulating Fluidized Bed
Axial/Transverse Velocity z/H = 0.5







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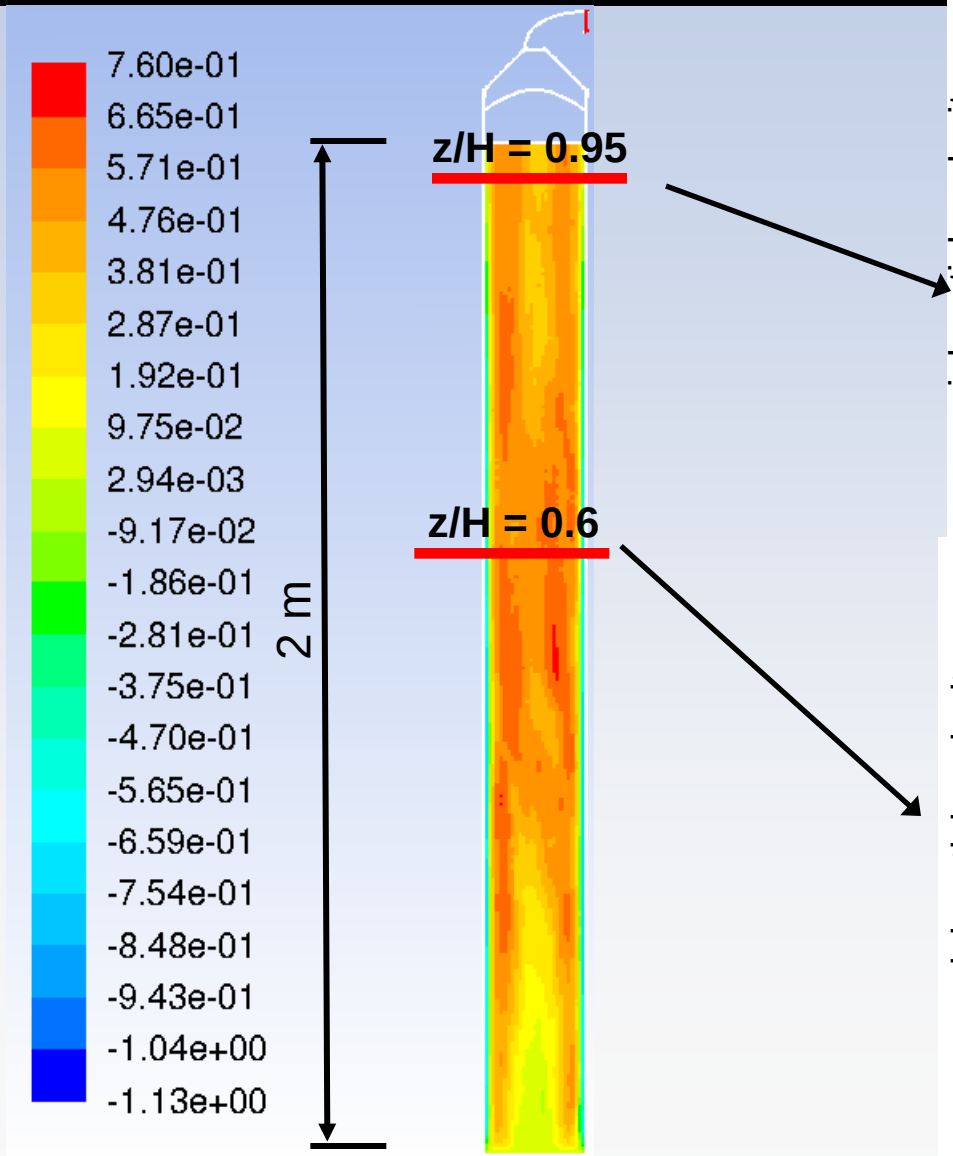
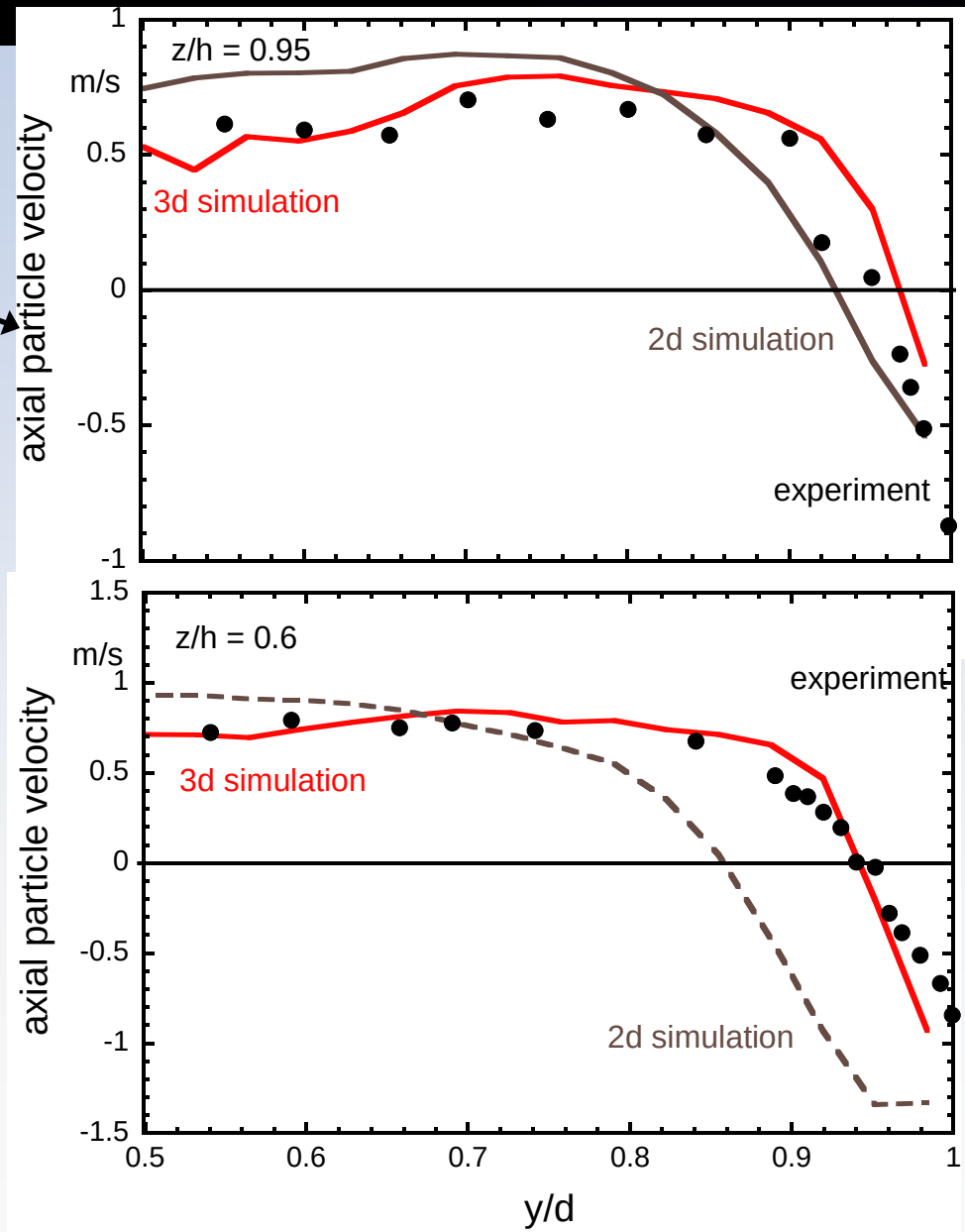
Circulating Fluidized Bed
Axial Velocity at z/H = 0.6/0.95





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Summary of results

- **Riser simulation:**
  - Validation of particle seggregation effects in circulating fluidized bed.
  - DDPM predicts proper distribution of velocity profiles.
  - Results clearly show 3-dimensional effects.
- **Further studies needed to investigate**
  - drag models,
  - turbulence models,
  - averaging procedures
- **DDPM highly efficient for particle size distributions at all volume fractions.**

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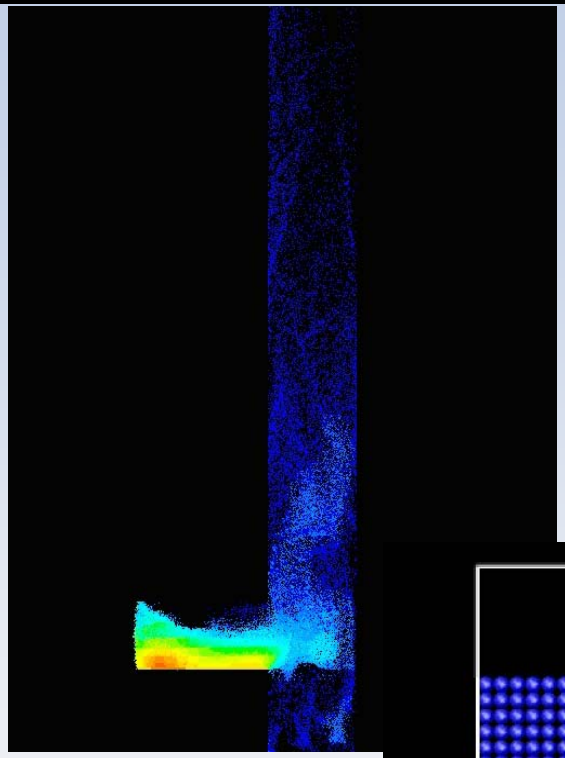
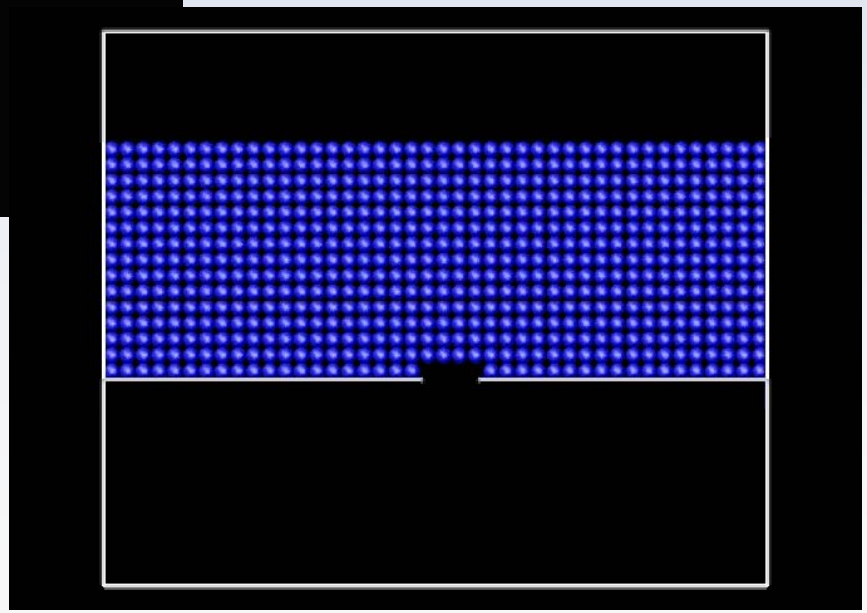
Modeling contacts explicitly

- **An extension of the DDPM takes into account the explicit contacting of particles through collision detection.**
- **Soft sphere based models**
  - Soil mechanics: Cundall and Strack (1979)
  - Fluidized beds: Tsuji, Hoomans (1998*)
  - Pneumatic conveying: Tsuji, Herrmann (1999*)
  - Parcel based approach: Joseph (2001)





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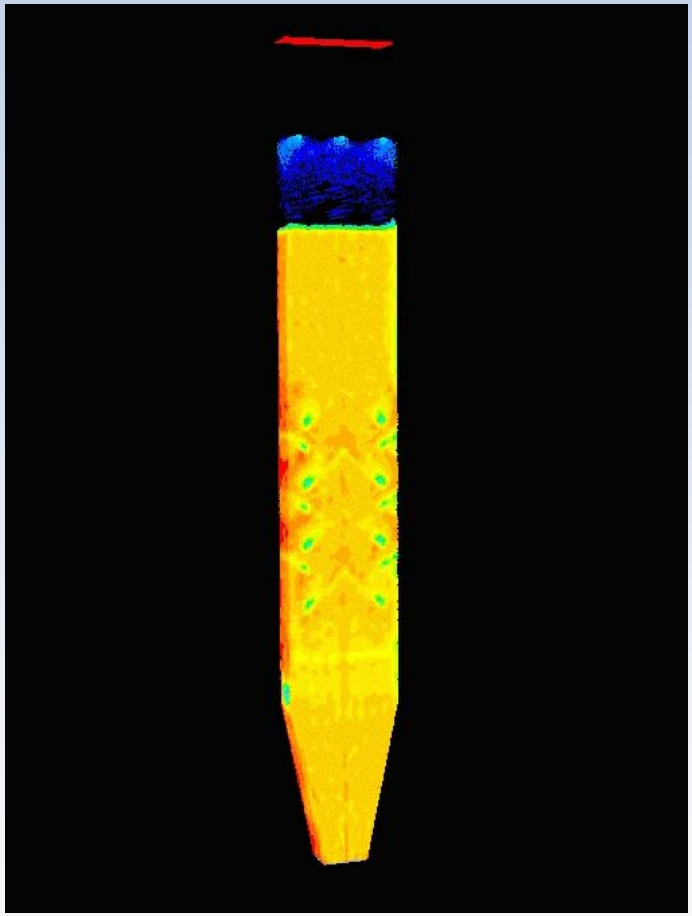
Current implementation

- **Accounts for explicit contact of parcels**
  - The forces at contact are determined by using a soft-particle spring dashpot model
  - The contact law is customizable
  - Ability to include more complicated physics
- **The framework is extendable to include heat transfer, reactions and is parallelizable**



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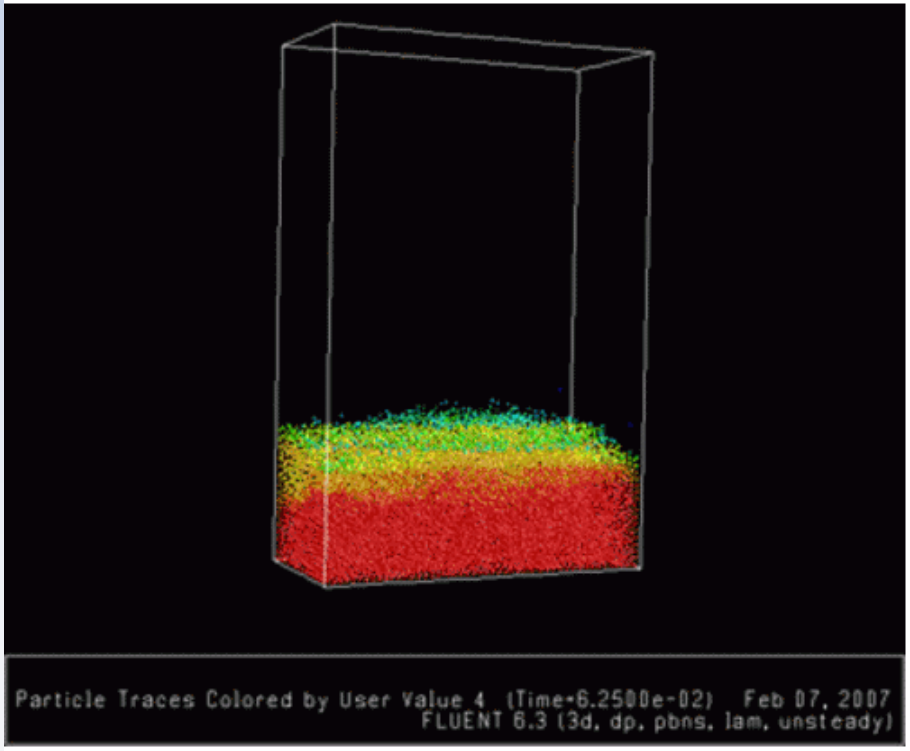
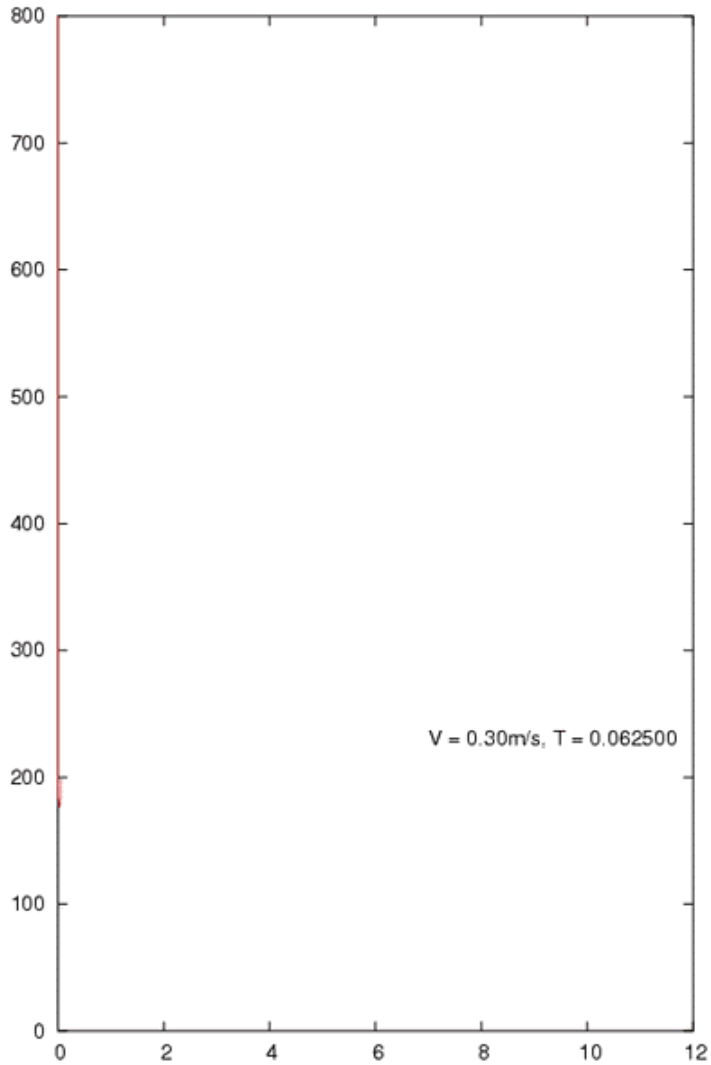
Structure of the bed for various gas velocities





Pressure at the inlet

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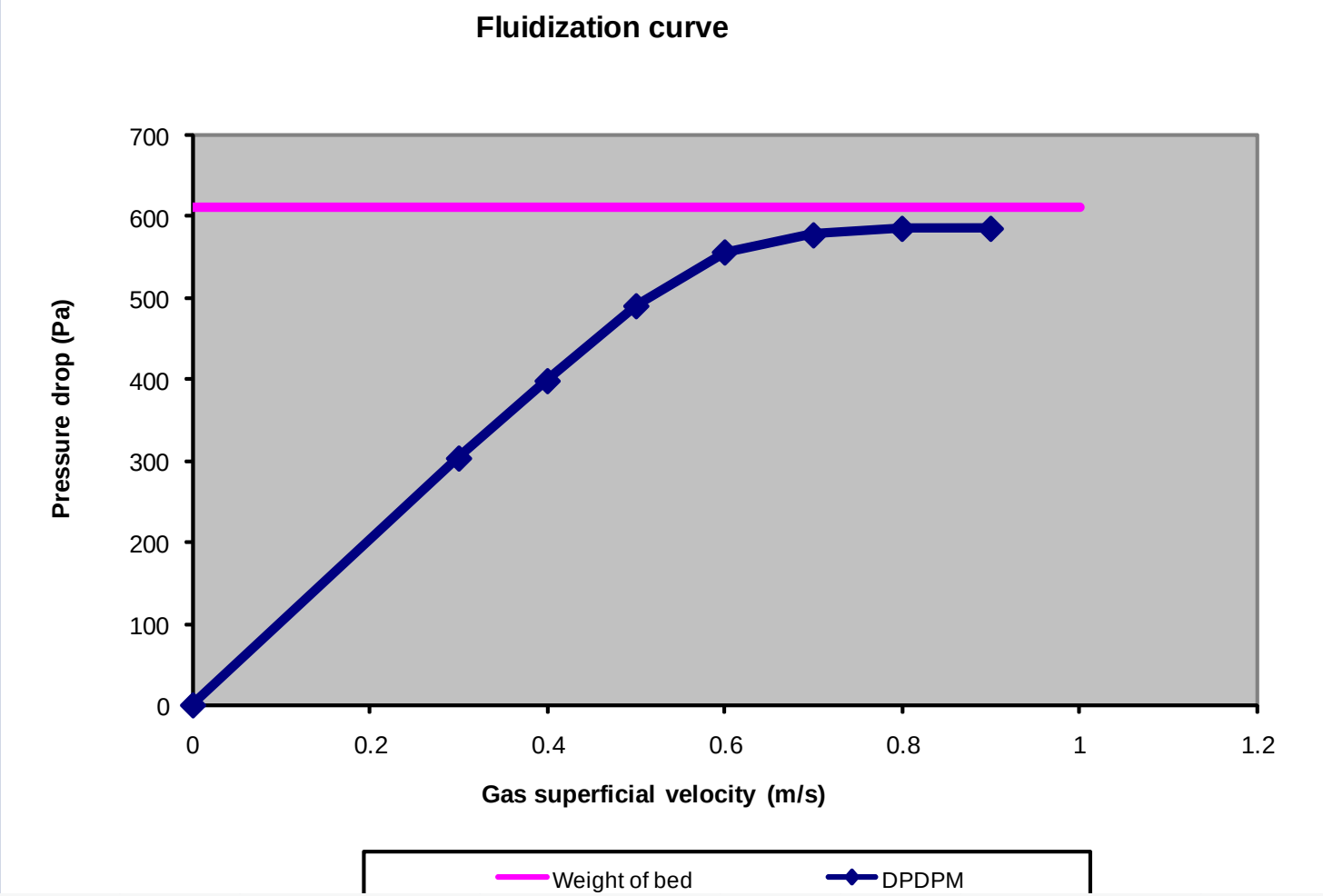
The fluidization curve



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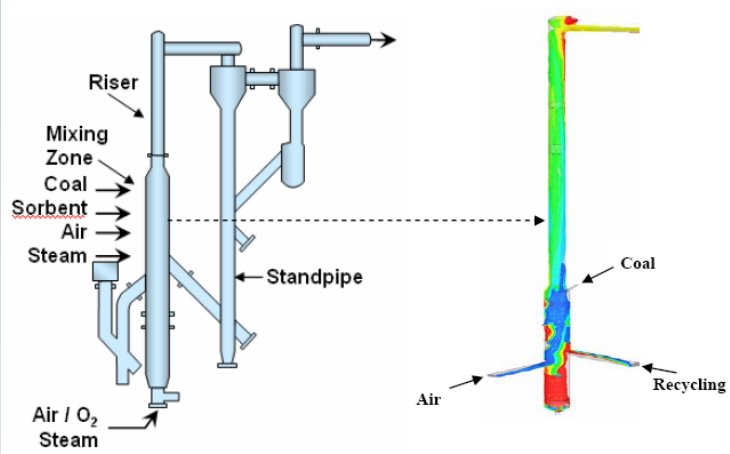
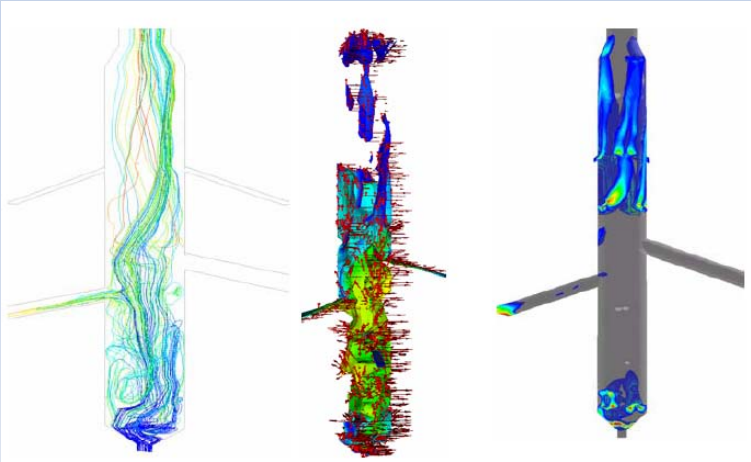
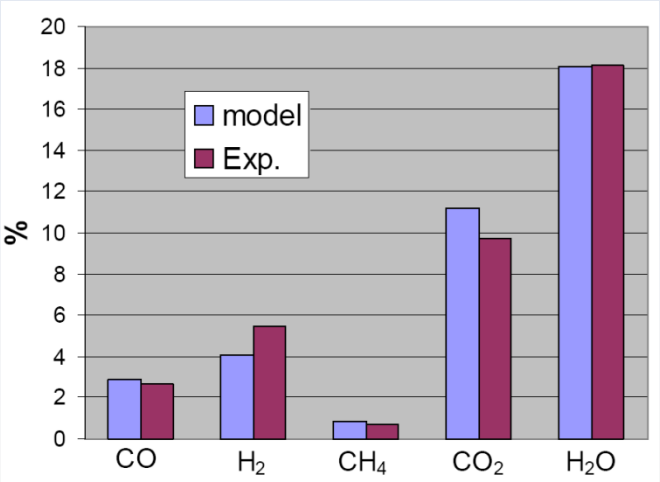
NETL partnership - Gasification







- **Gasification UDF for Euler-Granular model**
  - Developed under funding from NETL
  - Based on the work reported by Syamlal and Bissett (1992) and Wen *et. al.* (1982)
  - H_2 and CO combustion reactions also included
  - Used heterogeneous stiff chemistry solver of Fluent12 to take care of the stiffness of these reactions

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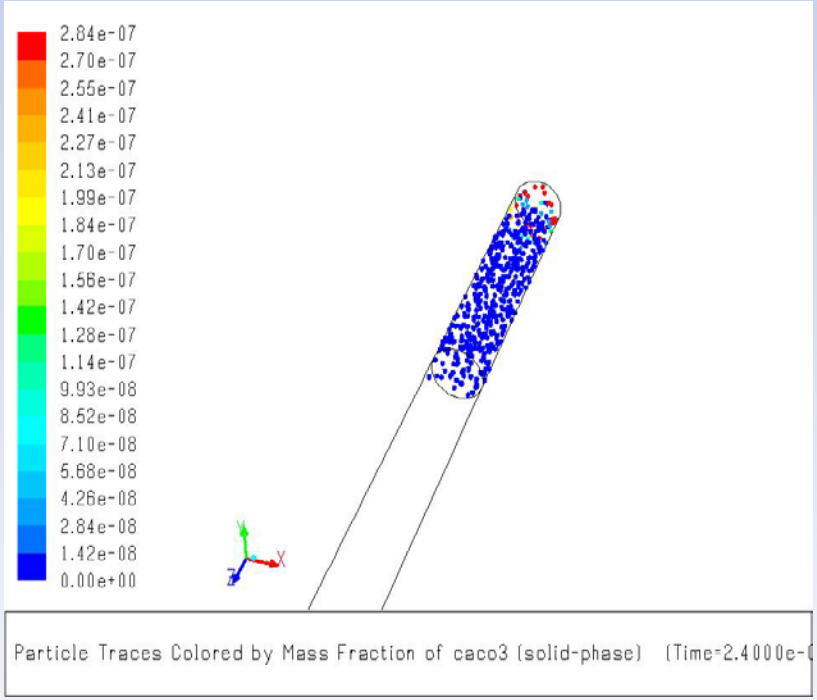
NETL partnership – Carbon capture

- 5 m tall cylindrical domain
  - Fluid bed height = 0.5 m
- Flue gas (12% CO_2, 10% H_2O, rest N_2) moves upward through the limestone bed (all size distributions under one secondary phase).
- **Particle Surface reaction takes place (gas temperatures 600-850 C)**
  - $CO_2(g) + CaO(s) = CaCO_3(s)$
- **Last picture shows start of limestone conversion to $CaCO_3$ at the bottom.**



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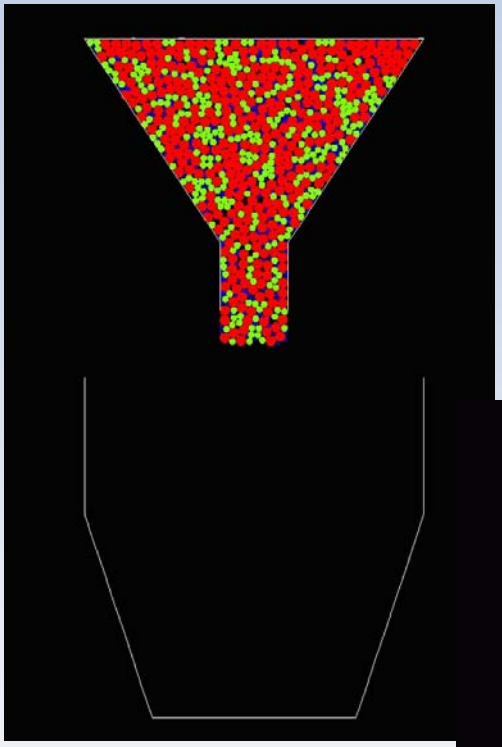
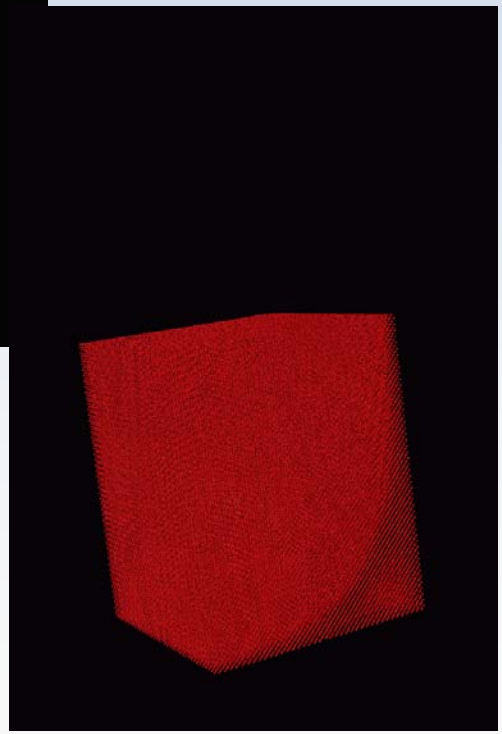
Conclusion

- **ANSYS is committed to providing “best in class” technology for modeling dilute to dense granular flows.**
- **Continue to improve speed and fidelity through experimental validation of results.**





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