A Numerical Study on Regenerator in the Fluid Catalytic Cracking Process

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Motivation

- Fluid catalytic cracking (FCC) is a primary step in petroleum refineries.
- FCC provides greater levels of high-octane gasoline and by-product gases than the out-dated thermal cracking process.
- In the FCC process, the cracking reactions in the riser-reactor result in deactivating the catalyst from coke formation.
- The regenerator plays a crucial role of combusting the accumulated coke and thus, re-activating the catalyst for a continuous process operation.

Multi-scale Problem

- Multiphase gas-solids fluidized bed reactors are of multiphase structure.
  - Single particles, particle clusters/bubbles, fluid dynamics, heat and mass transfer, and reaction kinetics are components of this multiphase structure.
- The problem is simplified, and we are considering a regenerator section of a fluid catalytic cracking (FCC) reactor.
  - Single particles, particle transfer and clustering within the main stream are considered.

Governing Equations (Eulerian-Eulerian Two-Phase Model)

- Each phase is treated as interpenetrating continua, identified by their phase fraction and exchange properties like momentum.
- Each of these continua is described by means of a continuity and a momentum equation.
- The gas and particulate phases are coupled through the interphase drag force term in their momentum equation.

Governing Equations (Eulerian-Eulerian Two Phase Model)

- Gas phase equations
  - Continuity $$\frac{\partial \alpha_g \rho_g}{\partial t} + \nabla \cdot \left(\alpha_g \rho_g \mathbf{U}_g\right) = 0$$
  - Momentum

$$\frac{\partial}{\partial t}\left(\alpha_g \rho_g \mathbf{U}_g\right) + \nabla \cdot \left(\alpha_g \rho_g \mathbf{U}_g \mathbf{U}_g\right) = \nabla \cdot \tau_g - \alpha_g \nabla p + \alpha_g \rho_g \mathbf{g} - K_{drag}\left(\mathbf{U}_g - \mathbf{U}_s\right)$$

$$\tau_g = \mu_g\left[\nabla \mathbf{U}_g + \nabla^T \mathbf{U}_g\right] - \frac{2}{3}\mu_g\left(\nabla \cdot \mathbf{U}_g\right)\mathbf{I}$$

- Particulate phase equations
  - Continuity $$\frac{\partial \alpha_s \rho_s}{\partial t} + \nabla \cdot \left(\alpha_s \rho_s \mathbf{U}_s\right) = 0$$
  - Momentum

$$\frac{\partial}{\partial t}\left(\alpha_s \rho_s \mathbf{U}_s\right) + \nabla \cdot \left(\alpha_s \rho_s \mathbf{U}_s \mathbf{U}_s\right) = \nabla \cdot \tau_s - \alpha_s \nabla p - \nabla p_s + \alpha_s \rho_s \mathbf{g} + K_{drag}\left(\mathbf{U}_g - \mathbf{U}_s\right)$$

$$\tau_s = \mu_s\left[\nabla \mathbf{U}_s + \nabla^T \mathbf{U}_s\right] + \left(\lambda_s - \frac{2}{3}\mu_s\right)\left(\nabla \cdot \mathbf{U}_s\right)\mathbf{I}$$

Governing Equations (Eulerian-Eulerian Two Phase Model)

- Interphase momentum transfer
  - GidasPow drag coefficient relation

$$K_{drag} = \frac{3}{4}\frac{C_d \alpha_g \alpha_s \rho_g \left|\mathbf{U}_g - \mathbf{U}_s\right|}{d_p} \alpha_g^{-2.65} \ \text{if } \alpha_s < 0.2$$

$$K_{drag} = 150\frac{\mu_g \alpha_s^2}{\alpha_g^2 d_p^2} + 1.75\frac{\alpha_s \rho_g}{\alpha_g d_p}\left|\mathbf{U}_g - \mathbf{U}_s\right| \ \text{if } \alpha_s > 0.2$$

$$C_d = \frac{24}{Re_p}\left(1 + 0.15 Re_p^{0.687}\right) \ \text{if } Re_p < 1000$$

$$C_d = 0.44 \ \text{if } Re_p \geq 1000$$

$$Re_p = \frac{\rho_g d_p \left|\mathbf{U}_g - \mathbf{U}_s\right|}{\mu_g}$$

Kinetic Theory of the Granular Flow

- Fluid dynamic properties of the particulate flow are calculated coupling the kinetic theory of the granular flow with frictional stress models .
- Granular Energy Equation:

$$\frac{3}{2}\left[\frac{\partial}{\partial t}(\alpha_s \rho_s \Theta_s) + \nabla \cdot (\alpha_s \rho_s \mathbf{U}_s \Theta_s)\right] = (-p_s \mathbf{I} + \tau_s) : \nabla \mathbf{U}_s + \nabla \cdot (\kappa_s \nabla \Theta_s) - \gamma_s + J_{slip} + J_{vis}$$

- Particle Phase Shear Viscosity:

$$\mu_s = \mu_{s,col} + \mu_{s,kin}$$

$$\mu_{s,col} = \frac{4}{5}\alpha_s^2 \rho_s d_p g_0 (1 + e_s)\left(\frac{\Theta_s}{\pi}\right)^{1/2} \qquad \mu_{s,kin} = \frac{10 \rho_s d_p \sqrt{\Theta_s \pi}}{96 g_0 (1 + e_s)}\left[1 + \frac{4}{5}(1 + e_s)\alpha_s g_0\right]^2$$

Kinetic Theory of the Granular Flow

- Particle Phase Bulk Viscosity:

$$\lambda_s = \frac{4}{3}\alpha_s^2\rho_s d_p g_0(1+e_s)\left(\frac{\Theta_s}{\pi}\right)^{1/2}$$

- Particle Pressure:

$$p_s = \rho_s\alpha_s\Theta_s + 2\rho_s\alpha_s^2 g_0\Theta_s(1+e_s)$$

$$g_0 = \frac{1}{1-\left(\frac{\alpha_s}{\alpha_{s,max}}\right)^{1/3}}$$

- Conductivity of granular energy:

$$\kappa_s = \frac{150\rho_s d_p\sqrt{\Theta_s\pi}}{384 g_0(1+e_s)}\left[1+\frac{6}{5}(1+e_s)\alpha_s g_0\right]^2 + 2\alpha_s^2\rho_s d_p g_0(1+e_s)\left(\frac{\Theta_s}{\pi}\right)^{1/2}$$

Kinetic Theory of the Granular Flow

- Restitution Coefficient: $e_s = 0.8$
- Dissipation Term due to Inelastic Collisions:

$$\gamma_s = 3(1 - e_s^2)\alpha_s^2 \rho_s g_0 \Theta_s \left[\frac{4}{d_p} \sqrt{\frac{\Theta_s}{\pi}} - \nabla \cdot \mathbf{U}_s \right]$$

- Dissipation of Granular Energy due to Viscous Damping: $J_{vis} = -3K_{drag}\Theta_s$
- Production of granular energy due to slip between gas and particles:

$$J_{slip} = \frac{81\alpha_s \mu_g^2}{g_0 d_p^3 \rho_s \sqrt{\pi \Theta_s}} \left| \mathbf{U}_g - \mathbf{U}_s \right|^2$$

Frictional Stress Models

- When particles are closely packed, the behavior of the granular flow is influenced by continuous contact among the particles.
- Johnson & Jackson proposed a frictional-kinetic closure for the particle shear stress:

$$\tau_s = \tau_{s,kt} + \tau_{s,f}$$

$$\tau_{s,f} = p_{s,f}\mathbf{I} - \mu_{s,f}[\nabla\mathbf{U}_s + (\nabla\mathbf{U}_s)^T]$$

$$p_{s,f} = \begin{cases} 0 & \text{if} \quad \alpha_s < \alpha_{s,f,min} \\ F\dfrac{(\alpha_s - \alpha_{s,f,min})^r}{(\alpha_{s,max} - \alpha_s)^s} & \text{if} \quad \alpha_s \geq \alpha_{s,f,min} \end{cases}$$

Numerical Platform

- The OpenFOAM toolkit is employed as an open-source finite-volume C++ code.
- The multiphaseEulerFoam solver within OpenFOAM is employed to solve the governing equations.
- Pressure-momentum coupling is addressed through the PIMPLE algorithm.
- Simulations are performed on BP America HPC machines.

Numerical Schemes

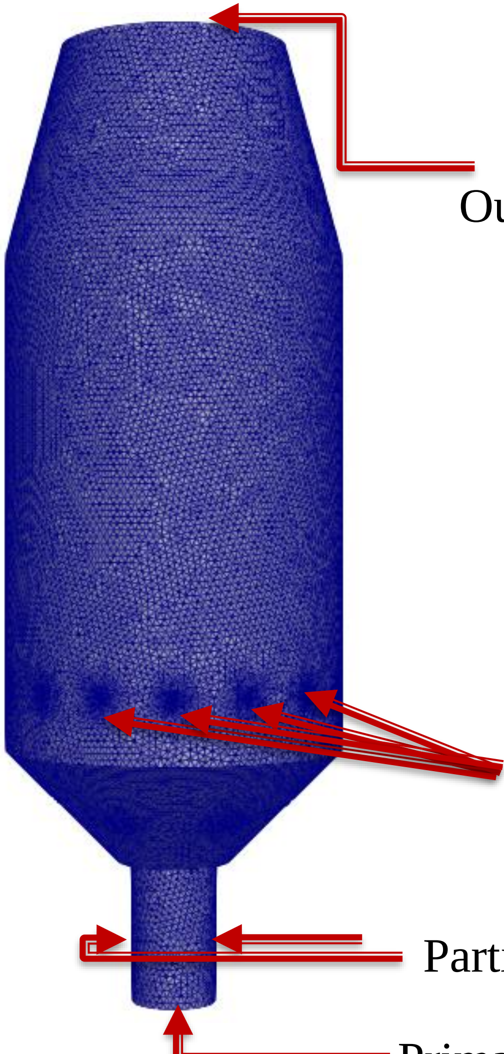
- Volume-fraction divergence term: vanLeer or upwind schemes are utilized.
- Laplacian term: second-order central differencing
  - To account for non-orthogonality and maintain second-order accuracy, an explicitly corrected surface normal gradient scheme is employed.
- Gradient terms: Gauss or second-order least squares
  - The multidimensional cell-limited scheme is employed to limit the gradient such that extrapolated centroid values at faces satisfy the maximum principle.

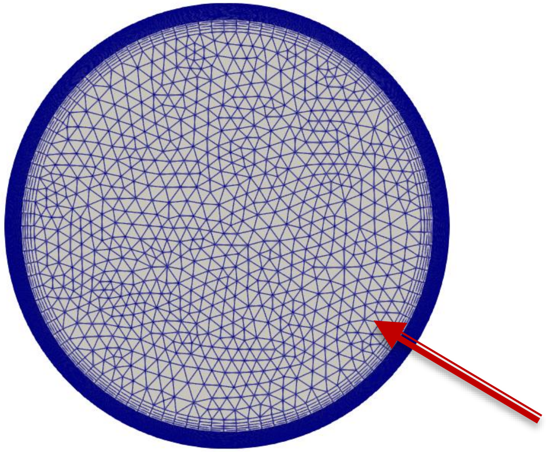
Numerical Settings

- The convergence criterion for pimple algorithm is set for pressure residual and equal to 10^{-5}.
- For further stabilization, under-relaxation value of 0.3 is used for pressure field and value of 0.7 is used for momentum equation.
- Iterations
  - Outer correctors: 20
  - Inner correctors: 1
  - Non-orthogonality correctors: 1

Computational Domain and Boundary Conditions

- 2,647,382 unstructured grid cells
- Particulate inlets $\alpha_s = 0.6, \alpha_g = 0.4$
- Airflow inlets $\alpha_s = 0, \alpha_g = 1$





Defined Cases and Objective

- Case A
  - Gauss linear gradient and upwind volume-fraction related divergence schemes
- Case B
  - Least squares gradient and vanLeer volume-fraction related divergence schemes
- All other schemes are identical between two cases
- Particle clustering in lower parts of the regenerator and volume fractions in upper parts of the regenerator and outlet are investigated.

Particle Characteristics

- Particle diameter is considered to be 75 μm.
- Particle velocity is specified at the oulets.
  - 1.1645 m/s with 45 degrees upward angle
- Based on the height of the regenerator (12.5 m), one flow-through time for the particles takes about 10 seconds.

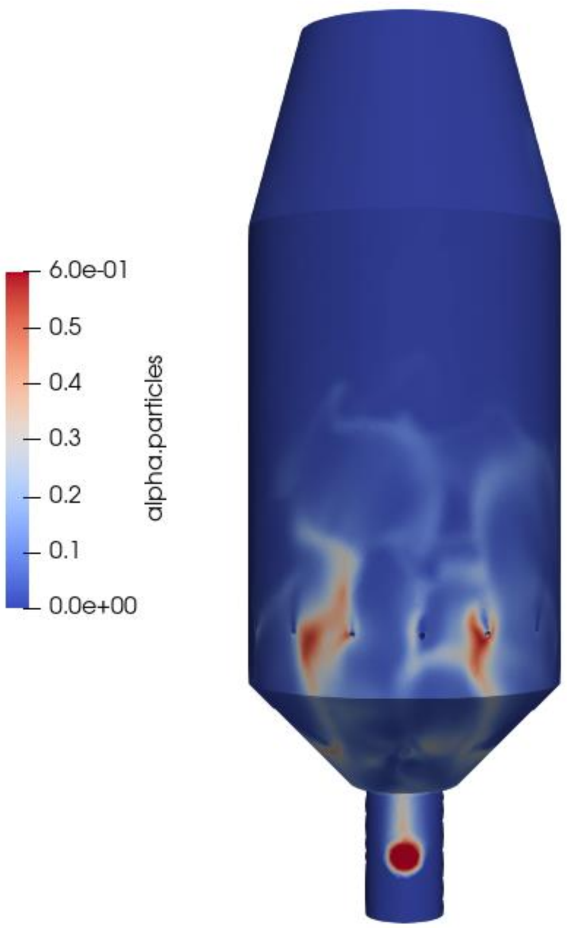
Results and Discussion

- The following results are still in preliminary stages and under development.
- Contours of particle volume fraction and their distribution range are discussed in addition to the particle velocity contours.

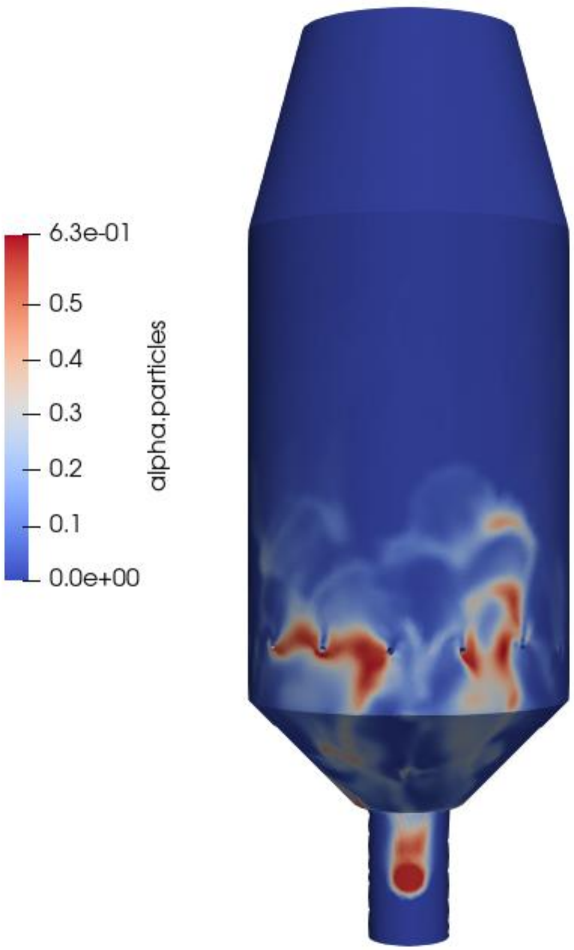
Three-dimensional Contours of Particle Volume Fraction

$t_{sim} = 3.4$ sec

Case A



Case B

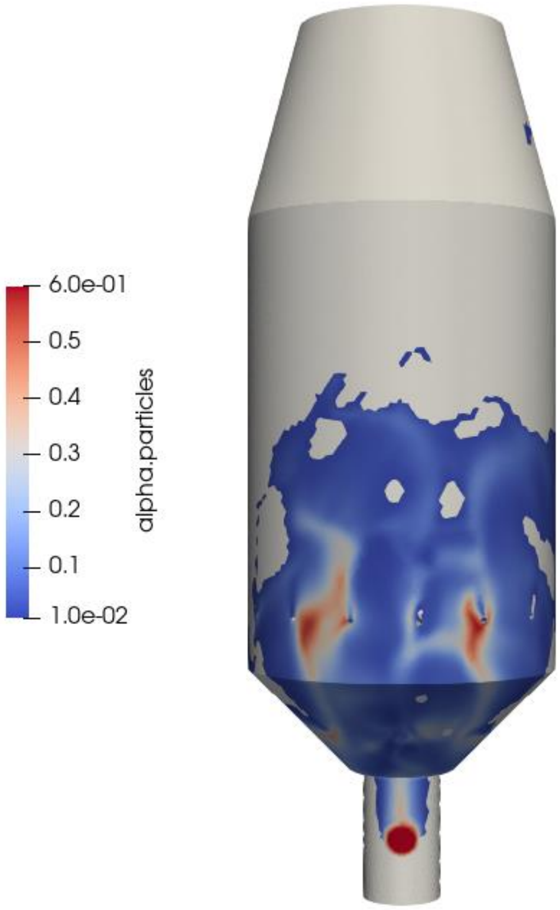


Three-dimensional Contours of Particle Volume Fraction

$t_{sim} = 3.4$ sec

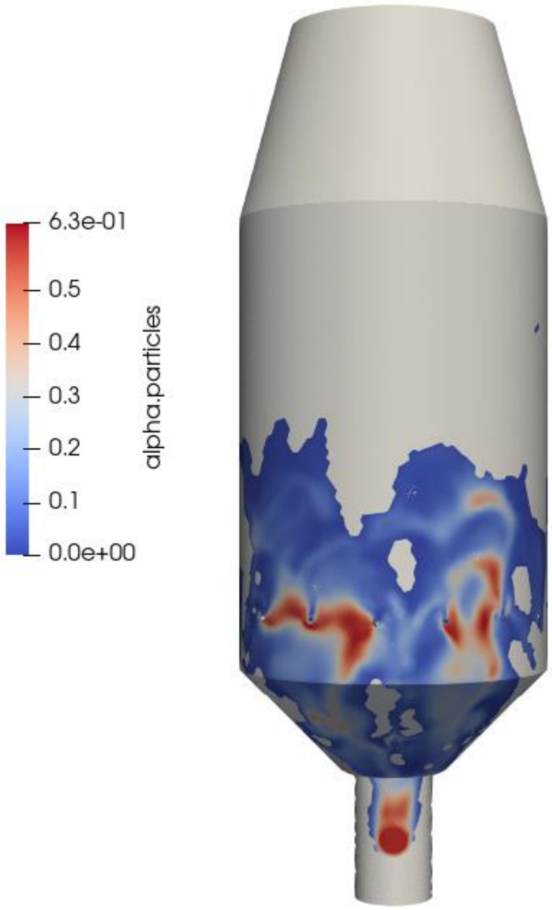
Case A

$0.01 < \alpha_s < 0.63$



Case B

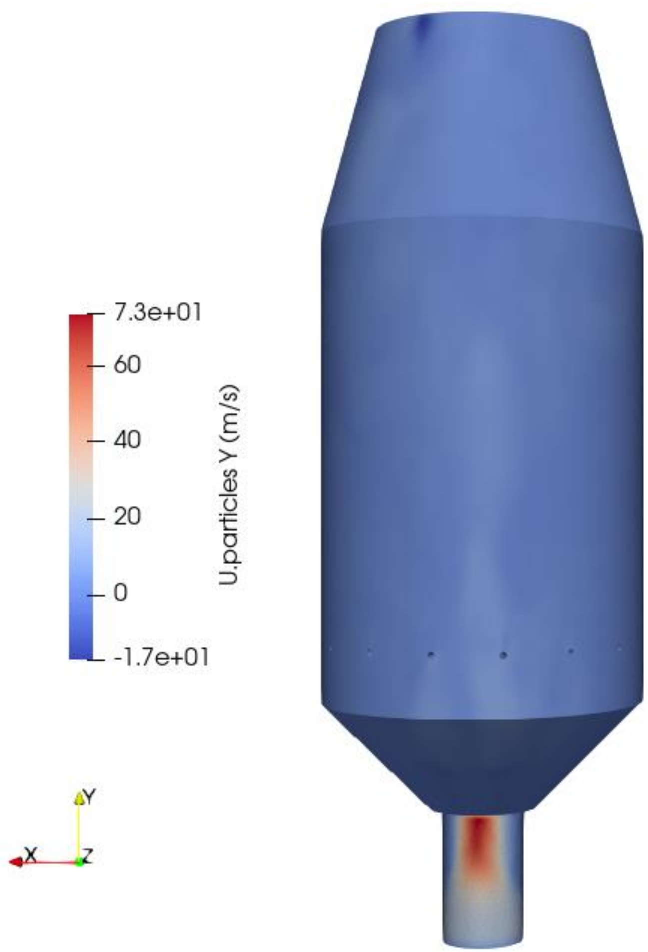
$0.01 < \alpha_s < 0.63$



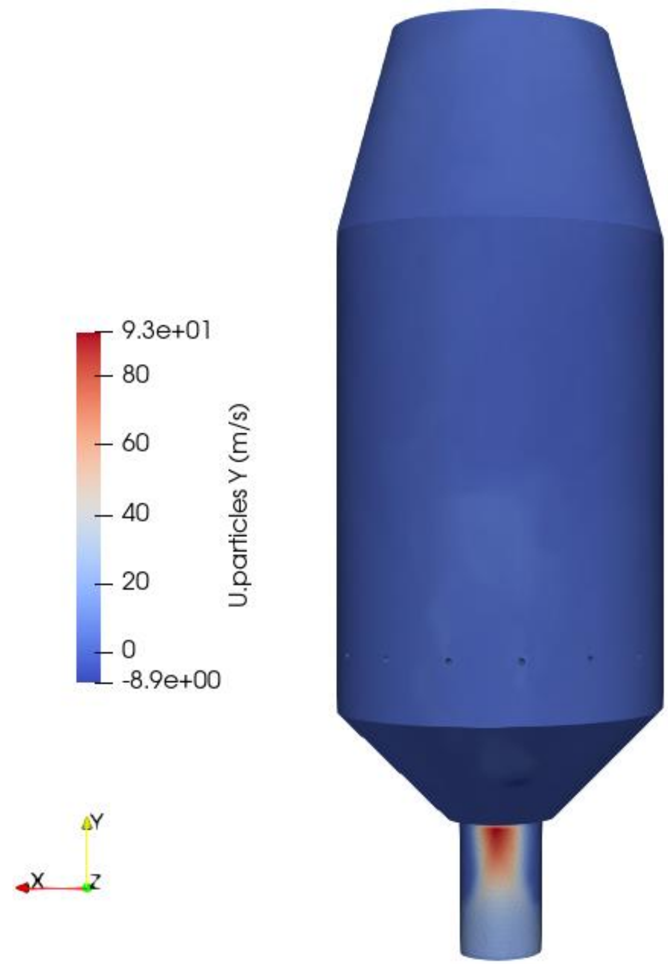
Three-dimensional Contours of Particle Vertical Velocity

$t_{sim} = 3.4$ sec

Case A



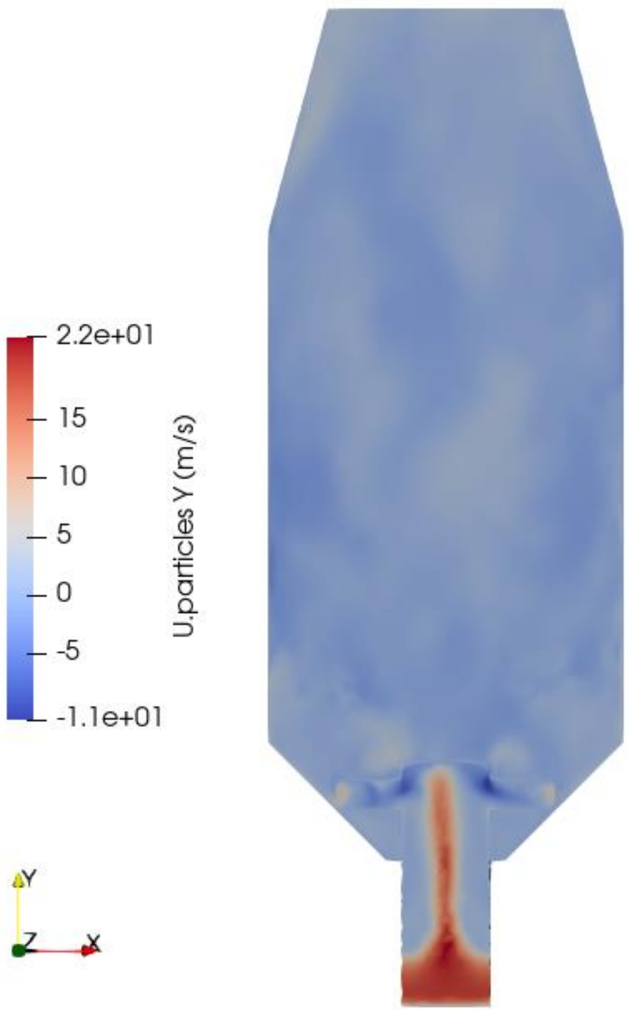
Case B



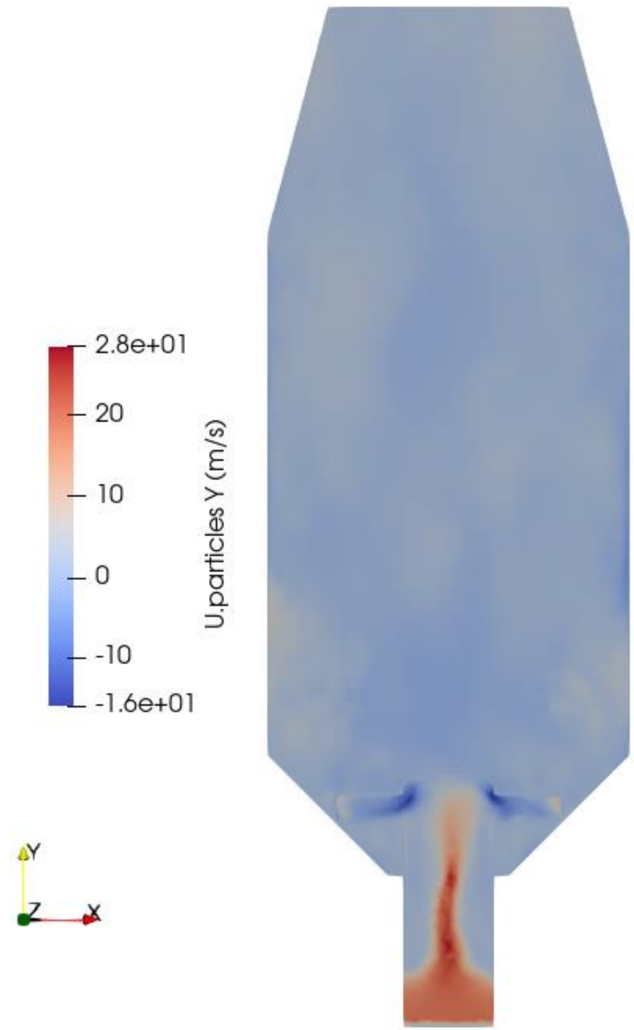
Two-dimensional Contours of Particle Vertical Velocity

$t_{sim} = 3.4\ \mathrm{sec}$

Case A



Case B

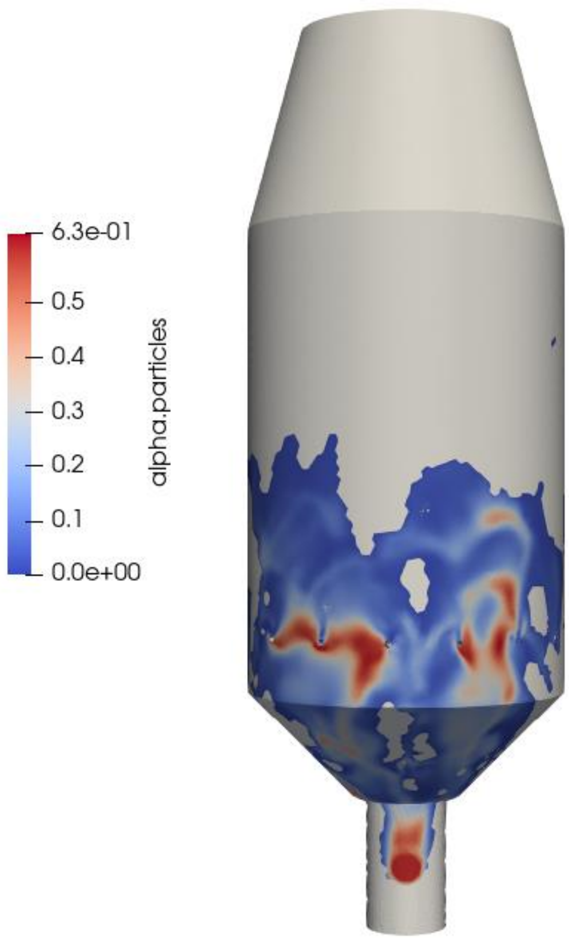


Particle Distribution Ranges in Regenerator

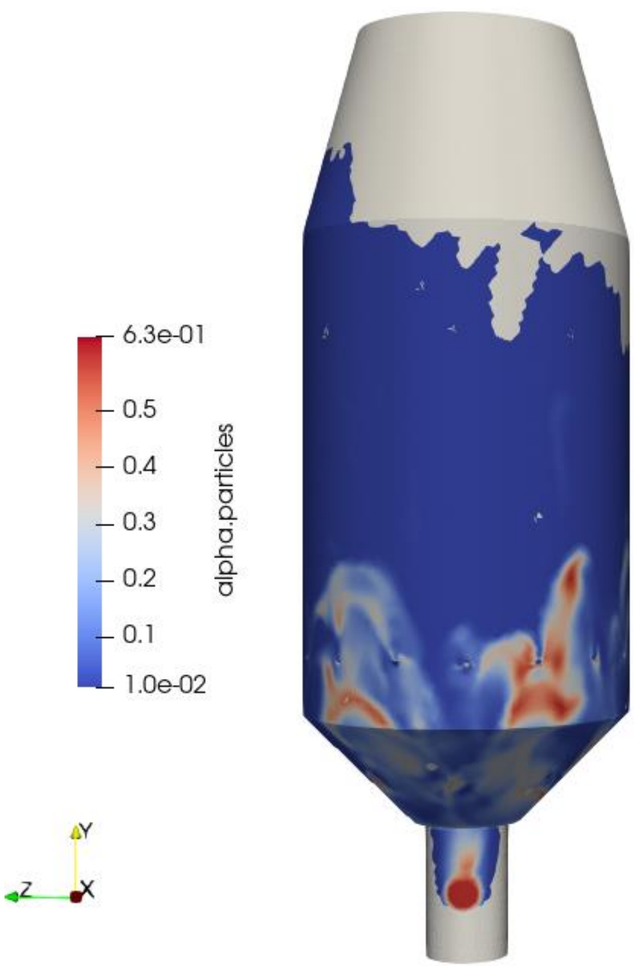
$t_{sim} = 4.3$ sec

Case B

$0.01 < \alpha_s < 0.63$



$0.001 < \alpha_s < 0.63$



Conclusions and Future Work

- An Euler-Euler numerical model is employed to simulate the solid-gas multiphase flow inside regenerators in fluid catalytic cracking refinery units.
- A comparison between first and second-order gradient and volume-fraction related divergence schemes is performed.
- The case with first order schemes provided peak values of velocity field and volume fraction lower than the second-order case.
- Future work:
  - Implementation of filtered models to reduce the computational cost.
  - Provide a more complex computational domain that considers other constituting parts of the FCC riser such as the outlet tubes and inlet pipes.