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Countercurrent Flow Simulation of Gas-Solid System in a Purge Column Using Computational Fluid Dynamics Techniques

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***Abstract*—**Purge columns or degasser vessels are widely used in the polyolefin process for removing trapped hydrocarbons and in-excess catalyst residues from the polymer particles. A uniform distribution of purged gases coupled with a plug-flow characteristic inside the column system is desirable to obtain optimum desorption characteristics of trapped hydrocarbon and catalyst residues. Computational Fluid Dynamics (CFD) approach is a promising tool for design optimization of these vessels. The success of this approach is profoundly dependent on the solution strategy and the choice of geometrical layout at the vessel outlet. Filling the column with solids and initially solving for the solids flow minimized numerical diffusion substantially. Adopting a cylindrical configuration at the vessel outlet resulted in less numerical instability and resembled the hydrodynamics flow of solids in the hopper segment reasonably well.

***Keywords*—**CFD, gas-solids flow, gas purging, species transport, purge column, degasser vessel.

I. Introduction

Several polyolefin processes that produce polyethylene and polypropylene polymers utilize a gas-phase fluidized-bed reactor coupled with a purge column to polymerize the hydrocarbon olefin and subsequently desorb the polymer resin from undissolved hydrocarbons [1]-[3]. Downstream of the column, polymer is then transferred to storage bins or silos for further processing. To administer the transition process, a rotary valve is placed at the bottom of the vessel. The valve is automatically triggered to allow specific amount of product to exit the vessel in contingent with product weight and flow conditions. Any irregularities in the process condition could render an undesirable product characteristics and financial losses. Thus, it is imperative to design the column properly to maintain financial gains and to adhere to product specification.

In this paper, we present a computational strategy for simulating a dense-phase gas-solids system using CFD approach. The aim is to provide CFD community of practitioners with an effective methodology to model the column operation and functionality. A countercurrent flow of descending solid pellets and ascending gases is modeled with the Eulerian granular approach. The k-ε turbulence model with a dispersed turbulent multiphase model approach was adopted. Medium-to-fine size mesh was applied in the overall computational domain except in the hopper zone where dense mesh was imposed to capture the solids and gas movement accurately. CFD predictions showed that outlet configuration of the column has a profound impact on the flow field in the hopper zone. For a fixed hopper height, adopting a cylindrical configuration at the vessel outlet resulted in more stable solution and resembled the hydrodynamics flow of solids in the hopper segment reasonably well in comparison to a conical configuration. Nevertheless, modeling the purge column with the Eulerian granular approach is still very challenging and deficient.

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II. Model Description

A. CAD Model Development

The model depicts a *similar design* to the discussed schematic in [1] (also displayed in Fig. 1 for illustrative purposes). The model contains two segments; a top silo (Cylindrical structure) and a bottom hopper (Conical structure) (Fig. 2). Two outlet configurations were studied to mimic the functionality of a rotary valve. Configuration 1 depicts a cylindrical outlet attached to the bottom of the hopper segment as per plant setup, whereas configuration 2 depicts a conical extension to the existing hopper outlet. In a plant setting, the length of the extended section is carefully selected to balance the solids weight or load needed to trigger the rotary valve to open and close as per polymer specification. An early or delayed discharge of polymer product from the column could have an adverse impact on the column flow characteristics and could lead to an off-specified product quality.

Six nozzles (N1 – N6) delivered nitrogen to the column (Fig. 2). Nozzles in the hopper segment delivered nitrogen at temperatures ranging from 30-40 ^{o}C while steam was introduced at much higher temperatures. Steam was fed to the vessel through a pipe extended inward into the center of an inverted cone structure embedded inside the hopper zone. The role of the steam is to deactivate the catalyst residues off the polymer surface before exiting the column. Finally, solid particles from the reactor bed were fed into the column through a top opening at temperatures close to the steam inlet temperature, descended downward towards the hopper zone by means of gravity-assisted flow then exited the system from the bottom of the hopper.

B. CFD Model Development

Both phases were simulated using Eulerian-Eulerian two-fluid model in ANSYS Fluent V19.2. This model incorporates the kinetic theory of granular flow (KTGF) to describe the gas-solids flow in the dense-bed system. ANSYS Design Modeler and ANSYS Workbench were utilized for geometry creation and meshing, respectively. Simulation was carried out using ANSYS Fluent multiphase flow solver. The meshed model is shown in Fig. 3.

It is a common practice to apply hexahedral type elements in the direction of the flow as this approach proved to be of superior quality over other type elements. Hence, it was applied in this study in the silo segment to capture the flow properties more accurately. In the gas-purging segment however where gas-purging nozzles are placed, tetrahedral and mixed type elements were implemented. In addition, finer mesh was implemented in this region and in the hopper segment to capture the flow pattern in both regions effectively (Fig. 3).

The governing equations were solved for an incompressible gaseous flow for nitrogen and steam, whereas a granular flow approach was applied to capture the solids movement in the column. A pressure-based, phase coupled SIMPLE algorithm with double-precision solver was adopted to solve a transient solution with time step of 0.001 s. The solution converged in nearly 4 days of wall-clock time with the speed of a 16-Core 32-node Intel processor. Residual mean values for convergence were set below 10^{-4} for flow and turbulent equations; whereas, for energy and species transport equations, it was set at 10^{-6}.

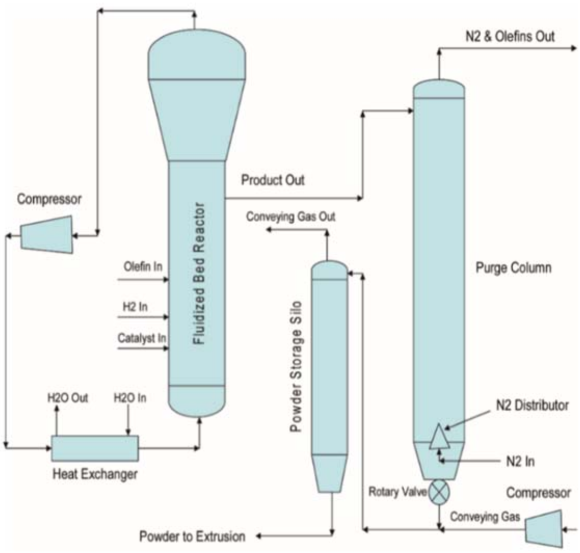

Fig. 1 Schematic of reactor & purge column (taken from [1])

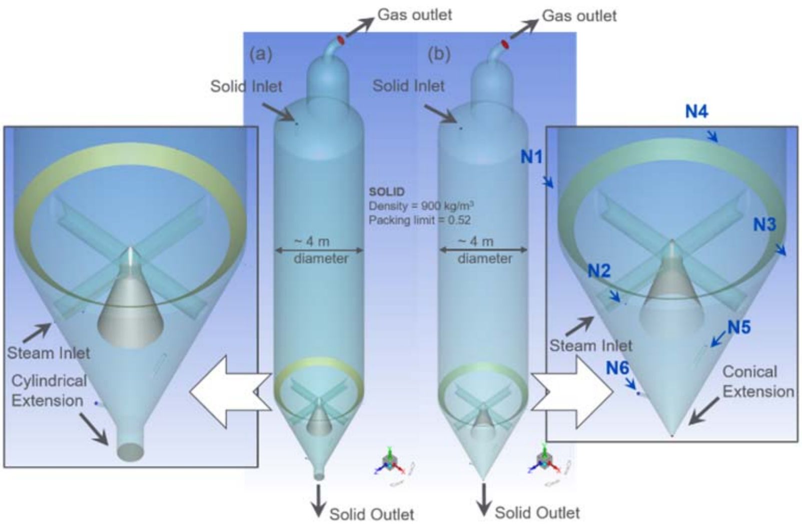

Fig. 2 3-D CAD model (a) Outlet configuration 1 and (b) Outlet configuration 2

At the inlets of the computational domain, steam and nitrogen were injected at mass flow rates ranging from 120 to 800 kg/h, respectively. Solids were introduced to the column at rates ranging from 63,000 to 66,000 kg/h. At the domain outlet, a pressure outlet condition was specified such that at the top, a gauge pressure of zero was assigned, whereas at the bottom, a static pressure of roughly 70 KPa was assigned to support a bed height of 20 m. In addition, a back-flow volume fraction of 0.4 was assigned at the bottom outlet to balance the loss of solids from the column during operation.

In dense systems such as in the hopper segment of the column, collisional dissipation of energy due to particle-particle and particle-wall collision plays a crucial role in dictating the flow upstream of the hopper outlet. For highly elastic particle collision, a restitution coefficient of 0.999 is often assigned. As particle collision becomes less and less elastic as in this study, a restitution coefficient of 0.8 to 0.9 (partially to slightly elastic) is more representative of this collision. In this study, a value of 0.8 will be simulated. Furthermore, as particles descend near the column wall, they follow the partially slip condition with a specularity coefficient in the range of 0.4 to 0.6. In this study, 0.6 was used. Finally, to evaluate the heat transfer between the gas and solids phases, Gunn correlation [4] for Nusselt number was adopted. This correlation is widely used and accepted in fluidized bed and fixed bed systems. It corrects for the gas holdup within the moving solids as shown in (1).

$$Nu = (7 - 10\boldsymbol{\varepsilon} + 5\boldsymbol{\varepsilon}^2)(1 + 0.7Re^{0.2}Pr^{1/3}) + (1.33 - 2.4\boldsymbol{\varepsilon} + 1.2\boldsymbol{\varepsilon}^2)(Re^{0.7}Pr^{1/3}) \quad (1)$$

In (1), *Nu* stands for Nusselt number, ε is the gas holdup, *Re* is Reynold's number, and *Pr* is Prandtl number.

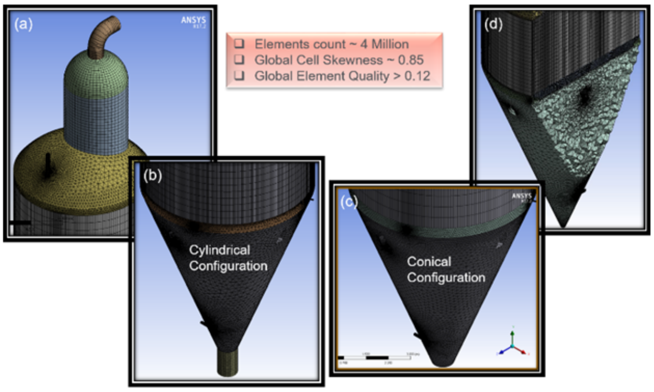

Fig. 3 Meshed model (a) Enlarged top section, (b) Enlarged outlet segment for cylindrical configuration, (c) Enlarged outlet segment for conical configuration (d) Cut-section view of meshed model

Parameters pertaining to granular properties were calculated based on correlations given in Table I. These correlations are widely used for fluidized-bed systems. They have shown to be indicative of the solid-solid and gas-solids interaction in these systems with minor deviation from experimental observations.

In a plant setting, polymer solids are of porous structure. This adds another degree of complexity to the posed problem. However, since it is the hydrodynamic characteristics we are after in this study, diffusional mass transfer in the solids pores will not be considered. Consequently, polymer was considered as mono-sized solid particles spherical in shape.

TABLE I
GRANULAR PARAMETERS USED IN THE STUDY

Parameter	Model/Correlation
Granular diameter [micrometer]	760
Granular viscosity [kg/m-s]	Syamlal - Obrien [5]
Granular bulk viscosity [kg/m-s]	Lun et al. [6]
Granular temperature	Algebraic
Solids pressure [Pa]	Lun et al. [6]
Radial distribution function [-]	Syamlal - Obrien [5]
Drag coefficient [-]	Gidaspow [7]

III. DISCUSSION OF RESULTS

The pressure profile along the height of the column is displayed in Fig. 4 for both outlet configurations. Similar pressure distribution is predicted with similar hydrostatic pressure values. This indicates matching solids loading for both columns. Similarly, velocity profiles for the solids phase were similar for both columns above the bed surface as depicted in Fig. 5. Nevertheless, that was not the case when comparing solids velocities in the hopper segment as shown in Fig. 6. It can be clearly seen in the figure that distinct flow pattern existed in the hopper region for both configurations; nevertheless, none of the predicted profiles achieved a plug flow. This flow is desirable in the silo and hopper segments for this type of industrial application to maintain an optimum vessel performance. Any abnormalities in the process could lead to undesirable product specification and inefficient vessel performance.

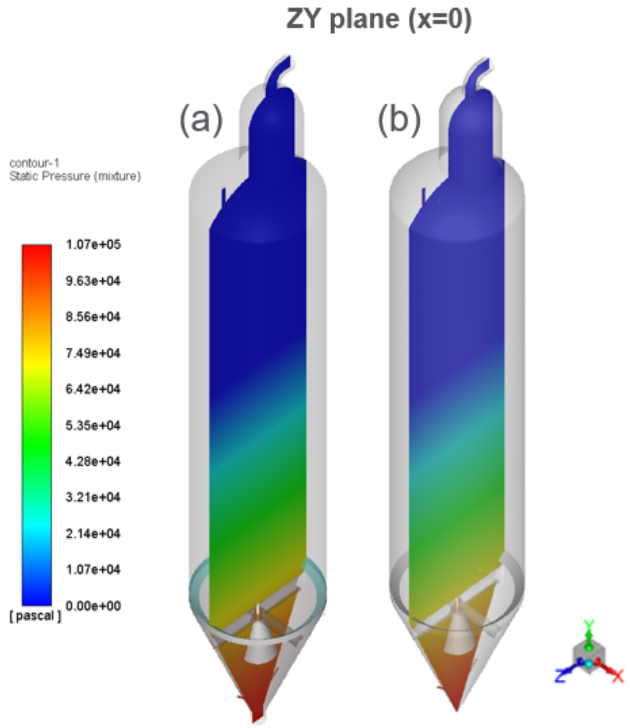

Fig. 4 Pressure profile in the column for both outlet configurations (a) Cylindrical and (b) Conical

Fig. 6 also showed an accelerating solids movement towards the outlet of the vessel, an anticipated flow pattern to satisfy the conservation of mass principle. However, this pattern should have extended further upstream of the vessel outlet to maintain a plug flow performance. In addition, pockets of higher solids velocity were predicted around the inverted cone structure in both configurations, needless to mention that asymmetrical flow pattern was obvious for the case of conical configuration. It can be postulated that the reason behind this flow abnormality is the tangling of upward moving steam with the descending solids. This hypothesis seems impractical due to the enormous weight of solids in the vessel. These systems can handle up to 300 tons of solids and therefore, fluidizing the whole bed requires more sophisticated distribution system and not simply gas purging with flow rates as low as those mentioned in this paper. Therefore, this study reveals a deficiency in the capability of Eulerian-Eulerian approach to address the hydrodynamic profile in these systems with sufficient accuracy. It can also be concluded that solids movement is more chaotic in the conical configuration versus its cylindrical counterpart.

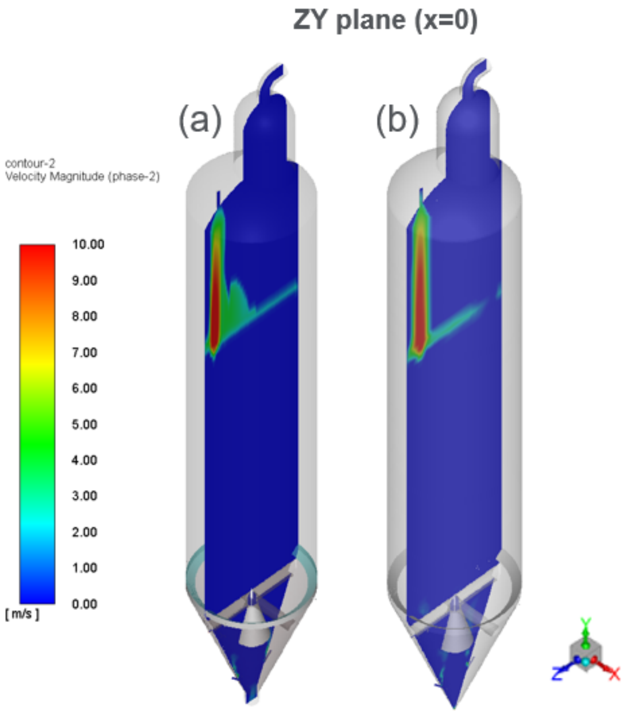

Fig. 5 Solids phase velocity in the plenum above bed surface for both outlet configurations (a) Cylindrical and (b) Conical

A plot of flow streamlines colored by gas phase velocity is displayed in Fig. 7. It shows the direction in which gas phase elements traveled within the computational domain or column. A close look at the plot reveals that gas phase distribution in the vessel is not channeled effectively throughout the vessel radial and axial directions. For a dense system such as the one considered in this study, it is expected to obtain wider distribution of gas phase among solids particles. In addition, the residence time of the gas in the hopper is short as can be estimated from the pseudo unidirectional flow rushing towards the silo segment. It is worth to mention that for an efficient deactivation and degassing processes, the gas phase should be in contact with more polymer particles and should be distributed more uniformly across each surface along the column height. This finding sheds more skepticism into the effectiveness and accuracy of the granular correlations used for this type of industrial system.

Finally, a contour plot of molar concentration of steam is illustrated in Fig. 8. Axial and radial profiles are shown for better visualization of the steam distribution in the column. The objective is to detect axial and radial dispersion of the introduced steam in the column segments. For similar industrial application, steam is introduced through the inverted cone structure into the hopper zone to deactivate the catalyst residues off the surface of polymer product. Residence time of steam in the hopper segment is very crucial to obtain a desired product specification and to adhere to environmental guidelines. It can be concluded from the figure that steam was not distributed efficiently in the hopper at rates that are one order of magnitude lesser than the introduced steam rate (Fig. 8 (b)); however a uniform distribution of steam was obtained at concentration rates that are two order of magnitudes less, Fig. 8 (c). These predictions are consistent with plant observation for similar industrial application.

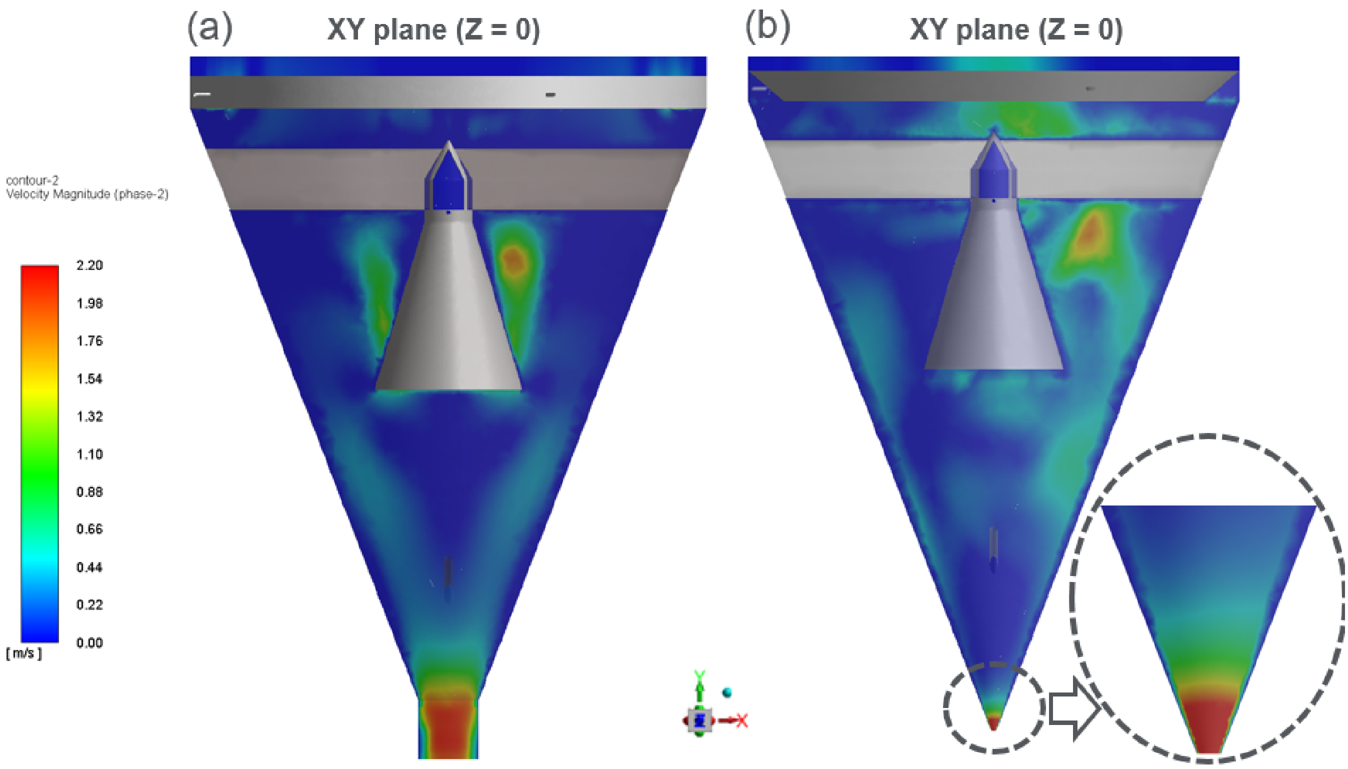

Fig. 6 Contour plot of solids phase velocity in the hopper segment for both outlet configurations (a) Cylindrical and (b) Conical

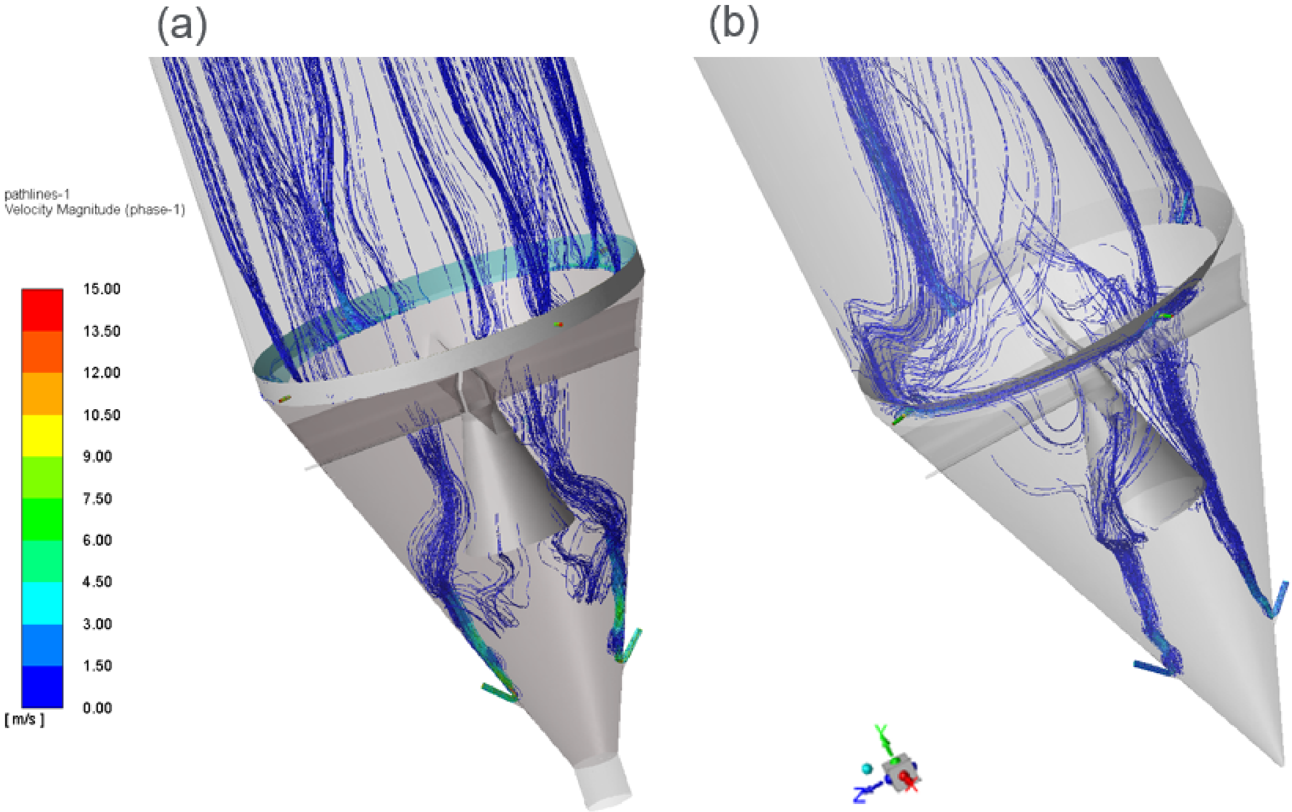

Fig. 7 Streamlines colored by gas phase velocity for both outlet configurations (a) Cylindrical and (b) Conical

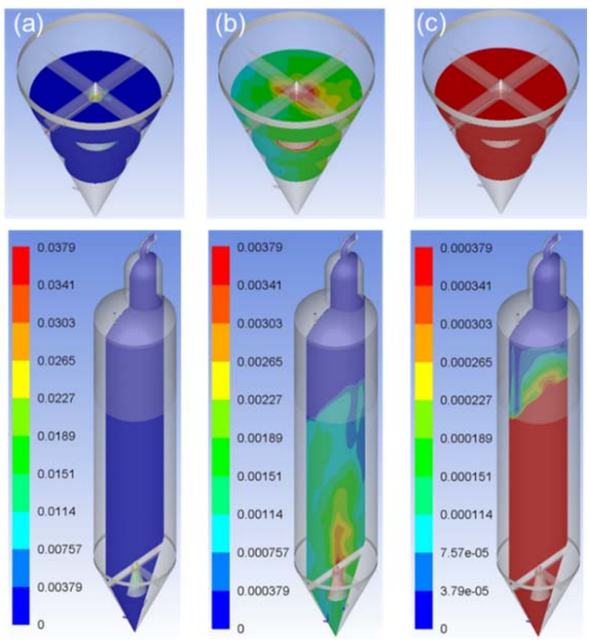

Fig. 8 Steam molar concentration in the column for chosen range (a) Maximum species concentration (b) One order of magnitude less and (c) Two order of magnitude less

IV. Conclusion

A CFD study was carried out to predict the multiphase flow of gas and solids in an industrial scale purge column. Predictions showed that the Eulerian-Eulerian approach coupled with the KTGF formulation addressed the hydrodynamic behavior of the column contents within an acceptable range. The interaction between the gas and solids phases however revealed a potential deficiency in the adopted model and the considered interphase correlations.

In order to minimize numerical instability and to obtain a converged solution, it is recommended to initially fill the column with solids and solve for the continuity and momentum equations while the product outlet is shut. This would also eliminate substantial drainage of solids from the column during the filling process.

Modeling the column with a cylindrical outlet configuration surpassed the conical counterpart. This option produced less numerical instability, less asymmetrical flow profile and more realistic solids acceleration in the hopper segment.

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