CFD Modeling of the Feed Distribution System of a Gas-Solid Reactor

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ABSTRACT: *Granular flow simulation using CFD has received a lot of attention in recent years. In such cases, CFD is either, coupled with Discrete Element Method (DEM) techniques for appropriate incorporation of inter-particle collisions, or the Eulerian CFD approach is used in which granular particles are treated as they were fluid. In the present study, a CFD analysis was performed for granular flow in an industrial screw feeder to study the choking phenomena. Eulerian multiphase flow model, also known as two-fluid model in the case of two phases, was used along with the solids closures based on Kinetic Theory of Granular Flow (KTGF). The rotating effect of the half pitch screw was incorporated by using the immersed boundary method (IMB). Variation of mass flow through change in revolution per minute (RPM) and moisture content was studied in this work. A jump condition in the axial profiles of both the solid phase volume fraction and pressure was observed near the inlet. It was found that the jump condition in solid phase volume fraction and pressure profiles reduces by increase in the RPM of the screw.*

EYWORDS: *Computational Fluid Dynamics (CFD); Kinetic Theory of Granular Flow (KTGF); Immersed Boundary Method (IBM); Screw feeder.*

INTRODUCTION

From sand hour glass to catalytic reactor, granular materials can be found in almost all walks of life. Usage of granular materials for carrying out chemical reactions either as a reactant or as a catalyst can be found in several industries such as coal combustion, petroleum cracking reactors, metal ores, etc. There are also many naturally occurring phenomena like avalanches, debris flow, etc. which require the understanding of flow characteristics of the bulk granular materials [1]. In chemical process industry, granular materials play a significant role. It is, therefore, essential to know the exact hydrodynamic details of the equipment using these granular materials.

Studies have been performed to understand the dynamics of such materials. *Ghadiri* [2] investigated the effect of attrition and shear on the porous spherical catalyst carrier beads. The physics involved, in the moving granular materials, covers a wide variety of complex phenomena and applications ranging from mundane to celestial [3]. *Nedderman* [4] studied the stress distribution of granular materials in the storage bins. The major concern of the study was to analyze the stress acting on the walls of bins in which material is stored. In recent years, several efforts have been made to theoretically model flows involving the flow of solids

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in process equipment. For example, *Massoudi* [5] derived the governing flow equations for granular materials using a continuum approach. He also discussed and solved problem involving granular materials flowing down an inclined plane with radiation heat transfer [6]. *Wu et al.* [7] considered a three-dimensional flow of granular materials with viscous fluid flow in a channel using mixture theory. Transportation and conveyance of granular materials have been a tricky challenge.

Different methods have been used to transport and convey these materials from one location to another. For example, pneumatic transport of granular materials has been common in the food and pharmaceutical industry [8, 9]. Some industries use vibratory conveyors with a trough which is vibrated sinusoidally in time [10, 11]. Screw feeders are also used to transfer granular materials from one place to another depending upon their flow rate and torque [12, 13]. These types of feeders are mainly used in metallurgy, mining, food processing and pharmaceutical industries where screw feeders are used to transfer bulk materials over a short distance from storage bin. Screw feeders provide a precise throughput control. Normally, screw feeders consist of a storage bin with a screw conveyor. Rotation of screw draw bulk material from hopper and moves it forward with the screw [14, 15]. The flow of granular material is almost always accompanied by dissipation of energy they get from the conveying system, mainly due to collisions with neighbouring grains. Therefore, a continuous supply of energy is required to facilitate the flow and agitation of granular particles. The friction arising due to wall surface results in shearing of the bulk flow. Therefore, wall conditions have a significant effect on the flow profile of bulk granular material. It is, therefore, cumbersome to perform experiments for complete description of flow field.

To this end, a promising alternative has emerged in recent years due to significant development of computational resources. This alternative allows for modeling and simulation of equipment dealing with granular flows. Several different computational techniques are available to simulate granular solids. Among the many methods available, Euler-Lagrangian method is one of the accurate techniques that can be used to simulate the granular flow field [16, 17]. This method has the limitation that it requires accurate closures for particle-particle interactions, which are generally not available. Moreover, this method can be used for equipment with relatively small number of particles as this method resolves complete balance equations for all particles [18]. An alternative to this approach is the Eulerian-Eulerian method where both the solid particles and fluid phases are considered as interpenetrating continuum fluids [19]. However, this method also requires closures for the solid phase parameters such as pressure, viscosity, stresses, etc. Gidaspow's work on development of kinetic theory of dense gas for application to granular flow has been seminal in this regard [20].

In the light of the above discussion, in the present work, we apply the Eulerian two-fluid model with closures from Kinetic Theory of Granular Flow (KTGF) to simulate the flow of granular particles being conveyed by a screw feeder. Next section presents the system details for simulations. Then simulation settings including boundary conditions are presented followed by the results of grid independence study. Finally, we identified the inhomogeneous flow distribution within the screw conveyor by plotting axial solid fraction and pressure profiles. The manuscript concludes with recommendations to avoid this inhomogeneous distribution.

SIMULATION METHODOLOGY

Accuracy of CFD results is highly dependent upon the meshing methodology as well as the discretization schemes used for spatial as well as temporal variables. Although the detailed study of effects of these parameters is not the subject of this paper; care has, however, been taken to use widely adopted scheme of things which would result in acceptable results. A CAD model of screw feeder was created using ANSYS® Design Modeler. Figs. 1 and 2 present the complete CAD model. This model consists of three main parts i.e., hopper, screw and the screw casing. Feed is introduced in the screw feeder from the hopper, which flows with the motion of the screw. The fluid domain is contained between the screw and its casing.

This CAD model was then exported to mesh generating software. The system was meshed using ANSYS® ICEM software. The structured hexahedral mesh was generated using multizone technique. Meshing parameters like aspect ratio, skewness, and element quality were specified within permissible limits to ensure

Table 1: Dimensions used for screw feeder.

Specifications	Dimensions (mm)
Length of screw casing	458
Length of screw	458
The diameter of the screw casing	52
Diameter of shaft	28
Depth of screw flight	10
Pitch of screw flight	25
The thickness of screw flight	10
Number of turns	15
Hopper (center) distance from the outlet	305
Hopper bucket bottom (length x width)	100 x 52
Hopper bucket top (length x width)	100 x 100
Height of bucket	50

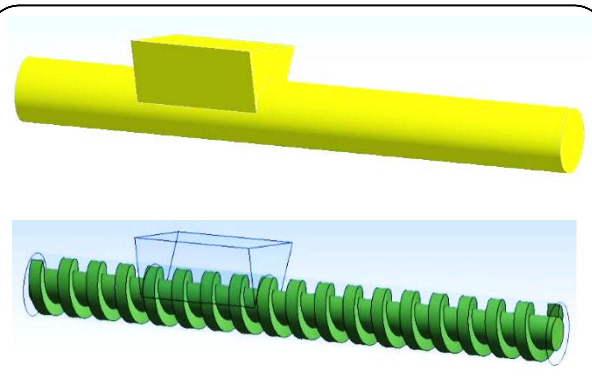

Fig. 1: Fluid domain with a bucket.

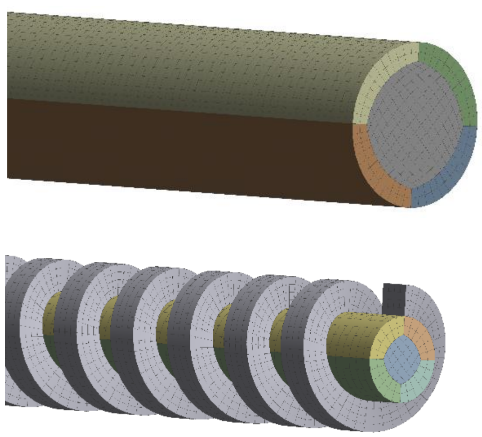

Fig. 2: Mesh of fluid domain and screw.

meshing quality. Table 1 shows the dimensions of the geometry used in the present work.

Kinetic theory for granular flow

Euler-Euler approach is preferred for the systems where a number of particles is huge and DEM simulations are computationally expensive, if not impossible. However, Eulerian approach also requires closures for solid phase e.g. stresses, viscosity etc. To achieve this, KTGF is used in conjunction with Eulerian methodology. Granular particles are taken as smooth spherical particles which dissipate energy on collisions with neighboring particles. In the Eulerian approach, individual particle trajectories are not simulated while an attempt is made to represent the physics of these trajectories and particle-particle collisions. In present work, Gidaspow radial distribution function was used for granular particles. The solid shear viscosity, the solid pressure model and the solid bulk viscosity were computed as a function of granular temperature. Granular temperature is proportional to the kinetic energy of random motion of particles. Algebraic equilibrium approach was used to calculate the granular temperature. As this model predicts very large granular temperature in regions where the solid phase volume fraction is low so the upper bound for granular temperature was applied to circumvent this limitation of the algebraic equilibrium model [1, 21].

Governing equations

ANSYS® CFX 14.5 was used for solving the discretized hydrodynamics equations [22]. Inhomogeneous hydrodynamics equations solved in this work are as follows.

Continuity Equation

$$\frac{\partial}{\partial t}(r_\alpha \rho_\alpha) + \nabla \cdot (r_\alpha \rho_\alpha U_\alpha) = S_{MS\alpha} + \sum_{\beta=1}^{N_p} \Gamma_{\alpha\beta} \tag{1}$$

Momentum Equation

$$\frac{\partial}{\partial t}(r_\alpha \rho_\alpha U_\alpha) + \nabla \cdot (r_\alpha (\rho_\alpha U_\alpha \otimes U_\alpha)) = \tag{2}$$

$$-r_\alpha \nabla p_\alpha + \nabla \cdot \left(r_\alpha \mu_\alpha \left(\nabla U_\alpha + (\nabla U_\alpha)^T \right) \right) +$$

$$\sum_{\beta=1}^{N_p} \left(\Gamma_{\alpha\beta}^{+} U_\beta - \Gamma_{\alpha\beta}^{+} U_\alpha \right) + S_{M\alpha} + M_\alpha$$

Volume Conservation Equation

$$\sum_{\alpha=1}^{N_p} r_\alpha = 1 \tag{3}$$

The solid powder considered in this work was composed of spherical particles having diameter of 10 microns with a density of 2500 kg/m^3. In this simulation, the moisture was not included as a separate entity in the simulation setup. The fluid phase was considered as a mixture of air and moisture with effective properties.

Interphase momentum transfer

Interfacial area density is calculated by using the particle model. This model assumes that one phase is continuous and other one is dispersed and dispersed phase is present in the form of spherical particles with mean diameter d_β.

$$A_{\alpha\beta} = \frac{6r_\beta}{d_\beta} \tag{4}$$

Drag force acting on a single particle can be expressed as

$$D = \frac{1}{2} C_D \rho_f A_p \left| U_f - U_p \right| \left(U_f - U_p \right) \tag{5}$$

Where C_D is the non-dimensional drag co-efficient and is calculated by using the Wen Yu drag model when the volume fraction of continuous phase is greater than 0.8 and for volume fractions less than 0.8 Gidaspow model is used [22, 23].

$$c_{\alpha\beta}^{(d)} = 150 \frac{(1-r_c)^2 \mu_c}{r_c d_p^2} + \frac{7}{4} \frac{(1-r_c)\left|U_c - U_d\right|}{d_p} \tag{6}$$

Fluid Prandtl number and Particle Reynolds number can be used to correct the dimensionless coefficient of the interphase transfer. They can be expressed as.

$$Re_{\alpha\beta} = \frac{\rho_\alpha \left| U_\beta - U_\alpha \right| d_\beta}{\mu_\alpha} \tag{7}$$

$$Pr_{\alpha\beta} = \frac{\mu_\alpha C_{P\alpha}}{\lambda_\alpha} \tag{8}$$

Table 2 shows the pre-input simulation settings for present work.

Immersed boundary method

Two general approaches are in common use these days for the simulations involving a moving boundary within a fluid domain. First, moving or sliding mesh method and second is the use of the Immersed Boundary Method (IBM). In the moving mesh method, continuous deformation and regeneration of the grid is necessary which is very tedious and computationally expensive work as the solver must generate a new mesh after each time step [23]. This regeneration of mesh on each time step also compromises the quality of the mesh. Therefore, a good quality mesh on each time step is required to carry out the simulations. While second method does not require regeneration of the mesh on each time step. Furthermore, the discretized governing equations in moving mesh method are much more complex than those for fixed Cartesian grids, which increase the computational cost and decrease the numerical stability considerably. While immersed boundary method does not require regeneration of mesh on each time step. In this technique, the moving body is considered as a momentum forcing function in the Navier-Stokes equation rather than a real moving rigid body. Therefore, flow involving complex geometries can be easily simulated by using this technique [24-27].

RESULTS AND DISCUSSIONS

Grid independence study

Refining of mesh is necessary to avoid numerical errors in the result. Grid size plays a significant role in the results. For present work, four different meshes, with 0.15 million, 0.307 million, 0.367 million and 0.615 million cells were tested. The simulation time taken for the coarse mesh with 0.15 million elements took approximately 35 hours of wall clock time to simulate 20 seconds. The time is taken by the finest mesh of 0.615 million elements took around four days for 20 seconds of simulations. Multiple variables were checked at each mesh for grid independence. Fig. 4 shows the variation of mean mass flow and pressure difference across inlet and outlet with mesh size. Based on these results, the mesh with 0.367 million cells was selected for further simulations. The focus of this study is to find that either flow is being chocked in the screw conveyor or in the hopper above.

The location where flow chocked is the point where the maximum accumulation of the solid particles occurs. To find the point of maximum accumulation multiple simulations were performed by varying different parameters.

Effect of moisture content

The maximum amount of moisture allowed in the granular material to be conveyed is only 0.5%. This choice of the moisture content was based on the literature

Table 2: ANSYS CFX pre-input settings for transient simulations.

Model	Parameters	Values and Comments
	Simulation type	Transient Simulation
Fluid:	Fluid list	Air at 25^0C and Solid particles
	Reference pressure	1-atm
	Buoyancy option	Buoyant
	Domain motion	Stationary
	Fluid models	Eulerian-Eulerian
	Turbulence model	k-ε model
	Fluid details	Air at 25°C as continuous fluid, Solid particles as dispersed phase
	Particles diameter	10 μm
	Restitution coefficient	0.9
	Kinetic theory	Granular temperature model: Algebraic equation model
	Radial distribution function	Kinetic theory
	Solid pressure model	Kinetic theory
	Solid bulk viscosity	Kinetic theory
	Solid shear viscosity	Kinetic theory
	Interphase transfer	Particle model
	Drag force used	Gidaspow
Wall boundary details:	Wall contact model	Volume fraction used
	Wall roughness	Smooth wall
	Air at 25°C	No Slip
	Solid particles	No Slip
Fluid inlet (opening):	Fluid region	Subsonic: Normal speed 0.3 mm/s
	Air volume fraction	0.4
	Solids volume fraction	0.6
	Turbulence Intensity:	Medium: 5%
Fluid Outlet (opening):	Fluid region	Subsonic:
	Mass and momentum	Average Static Pressure: 0.0Pa
	Turbulence	Zero gradient
Solver control:	Discretization (Advective) scheme	High Resolution
	Transient scheme	Second order Backward Euler
	Convergence Criteria	RMS
	Residual target	1.0E-04
	Equation class setting	Continuity
	Time step	1.0E-03s
	Total Time	20 s

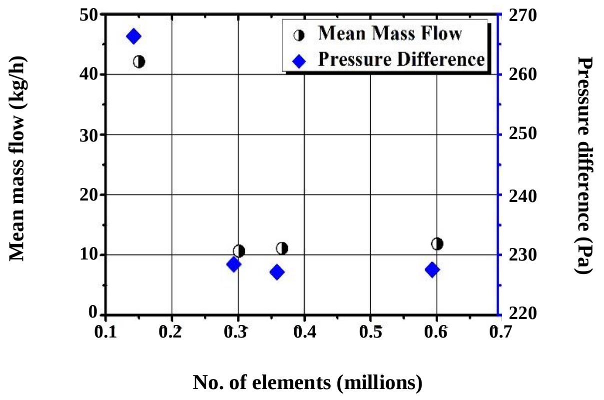

Fig. 3: Mesh independence study.

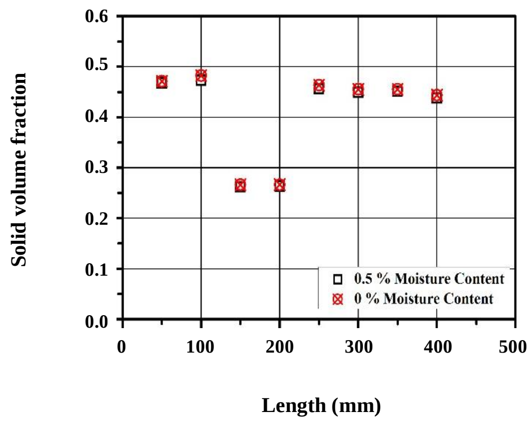

Fig. 4: Solid Volume Fraction along the length of the conveyor

values which varies from 0.2 to 0.5 % for the powders [28]. To study the effect of moisture on the flow field two simulations having moisture content 0% and 0.5% were performed using ANSYS® CFX 14.5. In general, when moisture is present in the powder, it will try to put particles together and hence increases the packing limit. Moisture is present in the free space between the particles and tends to bind the particles with each other. Further increase in the moisture content may cause problems such as formation of lump like structures or stick to the wall of screw. This will reduce the flow area resulting in the chocking of flow.

Area average values of solid phase volume fraction were calculated along the length after 20 seconds. When these values were plotted against the length of conveyor we found a jump condition at the position where hopper is attached to the conveyor. Fig. 4 shows the solid particles volume fraction plotted along the length of conveyor. It can also be seen that with moisture content present particles tend to settle down instead of forming a dusty cloud. As the moisture present is only 0.5% which is also uniformly distributed in the solid powder so the change observed is not of much significance. It is possible for the case of localized moisture content that a lumpy piece can be formed in the conveyor which tend to chock the flow.

The contours of the solid particles volume fraction are shown in Fig. 5, show the fact that solid particles tend to bind together in the presence of moisture.

By comparing the contours shown in Fig. 5, we can see an increase in the maximum packing limit of the particles (from 0.6892 to 0.7042) as moisture content increases from 0 to 0.5%, which also justify the fact that solid particles tend to bind together more tightly if moisture is present. However, the size of the lump has reduced in the presence of the moisture. The effect is not much significant as shown in Fig. 5 due to the small contents of moisture. The increased amount of moisture may enlarge this tightly packed lump and promote chocking. Hence, drying of the granular material may require in such situations. This should not be confused with the slurry, which has significantly higher percentage of the moisture contents.

Effect of revolutions per minute

Multiple simulations were performed at different rpm to see the effects of this variation on the flow field. Firstly, the solid particles tend to settle down in the lower part of the conveyor which is physically understandable. Secondly, with the increase in rpm, the maximum packing limit of the solid particles decreases. Demonstrating the fact that with greater force or torque, lumpy materials generated in the conveyor either by sticky nature of the conveying material or by moisture, are broken down to smaller manageable pieces. Variation in the rpm shows the fact that by increasing the rpm, the granular powder is evenly distributed within the feeder. Table 3 contains the maximum packing calculated by simulation at different rpms. It can be seen clearly that its value is decreasing with increasing the rpm.

Area average solid volume fraction is also calculated along the length at different points. And when these values were plotted against the length a similar jump condition was found as in the case of moisture content. Fig. 7 show the values of the average solid volume fraction along the length of conveyor.

Table 3: Maximum packing at different rpms.

rpm	Max Packing Achieved
30	0.6910
40	0.6547
50	0.6403
60	0.6401
70	0.6170

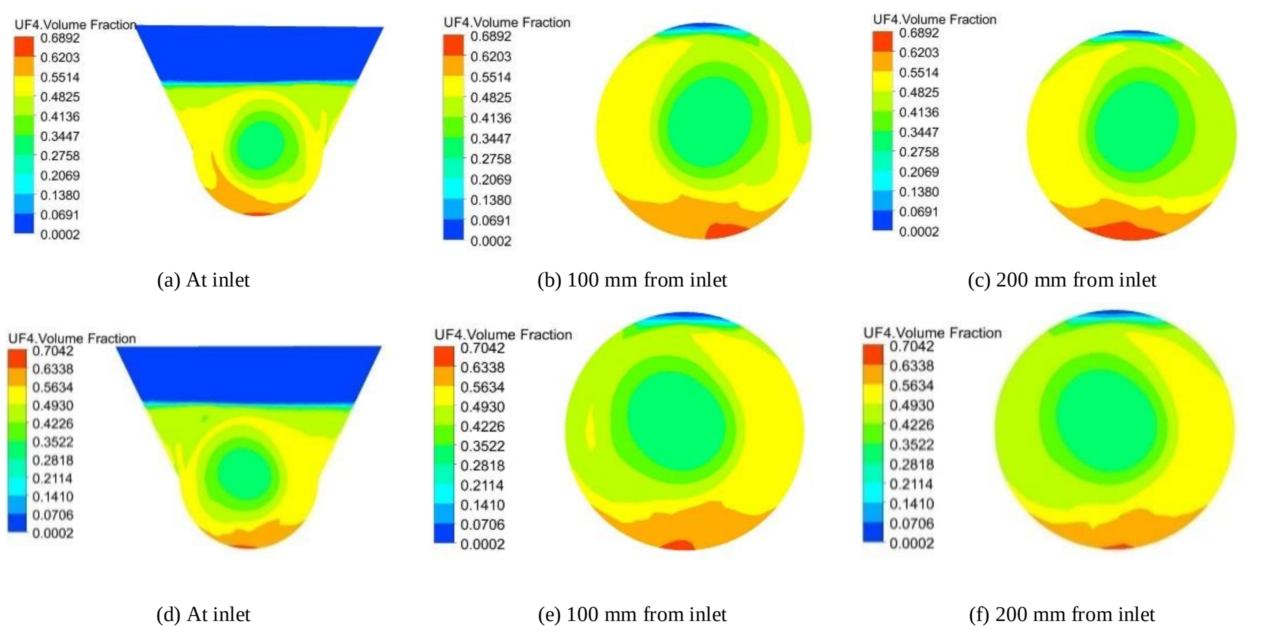

Fig. 5: Instantaneous (at 20 seconds) solid volume fraction contours (a,b,c) with 0% moisture (d,e,f) with 0.5% moisture.

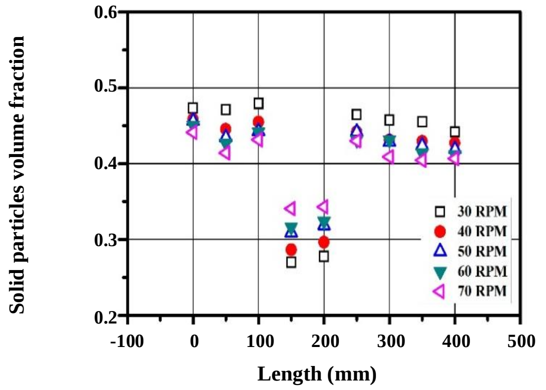

Fig. 6: Solid volume fraction along the length of the conveyor.

From Fig. 6, if we focus on the jump condition we can see that for 30 rpm the jump is largest and then gradually decreases with an increase in rpm and finally for 70 rpm this jump is smallest. This again shows the same fact that an increase in the rpm will lead to the even distribution of solid particles. Further increase in rpm may result in uniform distribution. The general range of rpm is 30-70 for the existing set-up. Increase in rpm would eliminate the jump condition. However, higher rpm is not allowed by the mechanical/structural design of existing plant. In order to operate the plant at higher rpm, the design of current setup has to be revisited. Fig. 7 show the contours along the length of conveyor at time t = 20 seconds. Absolute pressure is also plotted against the length of conveyor, and similar results were obtained. Again, a jump in value of absolute pressure has been observed at the entry point, as shown in Fig. 8 for solid volume fraction. It can be seen from Figs. 6 and 8 that

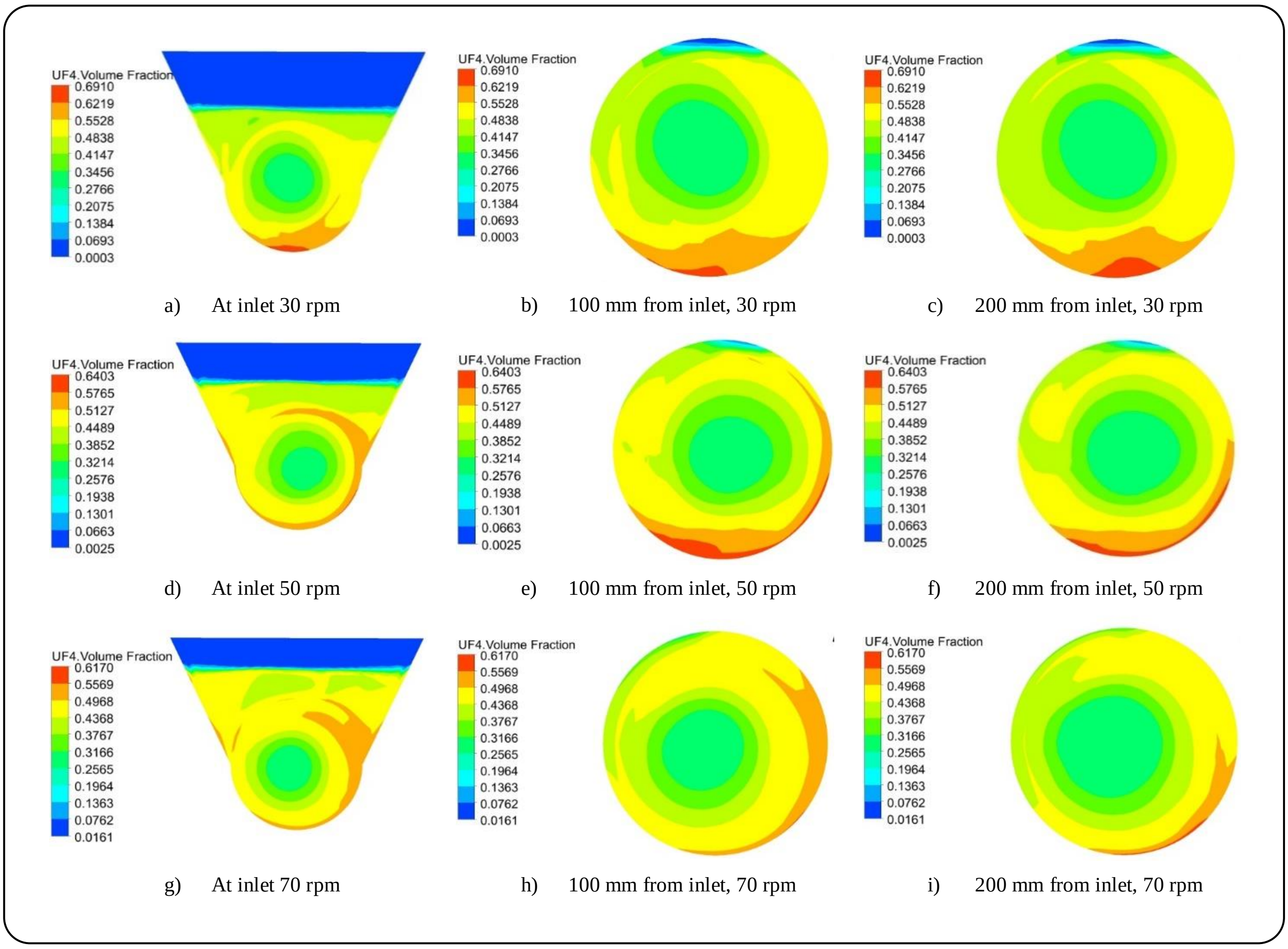

Fig. 1: Instantaneous (at 20 seconds) solid volume fraction contours (a,b,c) at 30 rpm (d,e,f) at 50 rpm (g,h,i) 70 rpm.

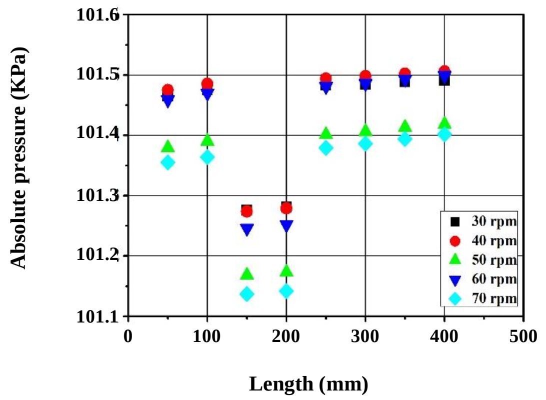

Fig. 8: Absolute pressure along the length of the conveyor.

with an increase in the rpm of the screw the difference in the solid particles Volume Fraction across the jump decreases. On the other hand, the lowest packing limit has been found to increase with increase in the rpm, as shown in Figs. 6 and 7. This increase in the lowest packing limit and decrease in the highest packing limit as mentioned above shows that the homogeneity of the distribution of material is increasing. This will result in a smooth flow of the material and no accumulation will take place. This effect will not only avoid the chocking of the material but also provide improved contact of the granular material with the gas if this material is to be taken as the feed of the gas-solid reactor.

CONCLUSIONS

Eulerian CFD was successfully employed to predict the hydrodynamic behavior of a screw feeder. The powder containing 0.5% moisture content was found to attain a maximum packing limit of 0.7042, which is higher than the normal packing limit of dry powder. This shows that minute moisture content promotes cohesion between the powder particles which results in an increase of agglomeration of the material. At low rpm, the material residence time is greater than at high rpm which also results in an increase of maximum packing limit for 30 rpm and the smallest at 70 rpm. As the rpm is increased from 30 to 70, the value of maximum packing limit decrease from 0.691 to 0.617. On the other hand, the minimum packing limit is increased from 0.0003 to 0.0161. Hence more uniform distribution of the material fraction has been obtained at higher rpm. Axial profile of solids volume fraction shows a jump in the volume fraction at the inlet. The difference in volume fraction of solid phase across the jump is decreases as the rpm of screw conveyor is increased. Uniform distribution of the solid granular particles will also improve the gas-solid contact and hence the reactor performance.

In this work mass flow was controlled by fixing the inlet velocity, it can be improved via applying inlet boundary conditions where particles flow under gravity. This study was performed using IBM technique, however, moving mesh method can also be tried and compared with present work.

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NOMENCLATURE

ρ_α	Density of phase α
r_α	Volume Fraction of phase α
U_α	Velocity of phase α
$\Gamma^{+}_{\alpha\beta}$	Mass flow rate per unit volume from phase β to phase α
λ_α	Thermal conductivity
$S_{M\,S\alpha}$	Mass source specified by user
M_α	Interfacial force
μ_α	Viscosity of phase α
$C_{P\alpha}$	Heat capacity of phase α
$c^{(d)}_{\alpha\beta}$	Drag Coefficient

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