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# CFD-DEM modelling of powder flows and dust generation mechanisms - A review

Luke Stone

*University of Wollongong, les019@uowmail.edu.au*

Peter W. Wypych

*University of Wollongong, wypych@uow.edu.au*

David B. Hastie

*University of Wollongong, dhastie@uow.edu.au*

Stefan Zigan

*University of Greenwich*

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# CFD-DEM modelling of powder flows and dust generation mechanisms - A review

## **Abstract**

Dust generation forms a large part of the challenges that bulk materials handling engineers face throughout the life of their career. Dust generation can lead to health problems, explosion risks, material segregation and environment pollution [1-5]. These conditions are typical of run of mine dump hoppers, grain silos, coal train dump stations and alumina storage silos. Computational Fluid Dynamic (CFD) models have been used successfully for predicting fluid flows with a high level of accuracy with the benefit of being less computationally expensive than in the past. Although CFD programs such as ANSYS can be used to successfully model fluids, these models are not suitable for modelling non-homogenous substances, such as dust. Alternatively, the Discrete Element Method (DEM) has been primarily used for granular materials and has been unsuitable for modelling the effects that the surrounding environment has on the particles trajectories. By coupling these two methods, it may be possible to develop a more robust and accurate dust generation model. This paper investigates and reviews previous research on modelling powder flows and dust generation mechanisms using both analytical methods and CFD coupled with DEM. Additionally, the programs that are available are investigated and their suitability for use in CFD-DEM coupling is examined.

## **Disciplines**

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# CFD-DEM Modelling of Powder Flows and Dust Generation Mechanisms – A Review

**Luke E. Stone<sup>1</sup>, Peter W. Wypych<sup>1</sup>, David B. Hastie<sup>1</sup> and Stefan Zigan<sup>2</sup>**

1. Faculty of Engineering and Information Sciences, University of Wollongong, Northfields Avenue, Wollongong, N.S.W, 2522, Australia
2. School of Engineering, University of Greenwich, Central Avenue, Chatham Maritime, Kent, ME4 4TB, United Kingdom

**ABSTRACT** Dust generation forms a large part of the challenges that bulk materials handling engineers face throughout the life of their career. Dust generation can lead to health problems, explosion risks, material segregation and environment pollution [1-5]. These conditions are typical of run of mine dump hoppers, grain silos, coal train dump stations and alumina storage silos. Computational Fluid Dynamic (CFD) models have been used successfully for predicting fluid flows with a high level of accuracy with the benefit of being less computationally expensive than in the past. Although CFD programs such as ANSYS can be used to successfully model fluids, these models are not suitable for modelling non-homogenous substances, such as dust. Alternatively, the Discrete Element Method (DEM) has been primarily used for granular materials and has been unsuitable for modelling the effects that the surrounding environment has on the particles trajectories. By coupling these two methods, it may be possible to develop a more robust and accurate dust generation model. This paper investigates and reviews previous research on modelling powder flows and dust generation mechanisms using both analytical methods and CFD coupled with DEM. Additionally, the programs that are available are investigated and their suitability for use in CFD-DEM coupling is examined.

## 1. INTRODUCTION

Computer use has been increasing exponentially in the engineering field over the past few decades and this has led to more efficient use of engineers' resources and hence increased productivity. Although this increased use of computers has aided engineers in many areas such as structural analysis using Finite Element Analysis (FEA), fluid analysis using Computational Fluid Dynamics (CFD) and granular modelling using the Discrete Element Method (DEM) there are still limitations to the degree to which natural phenomena can be modelled with an accuracy that is acceptable. In today's society it is of paramount importance to have a reliable model for dust transportation mechanisms. Dust emissions do not only pose a health risk to workers through respiration and cause a damaging effect on the local environment [1-5], it also has the possibility to ignite under the correct conditions creating an explosion hazard [6-10]. This risk of dust explosion is ever present in many areas of materials handling, from coal mine dump stations to the filling of grain silos. Therefore, this review must be undertaken to lay the ground work for further research to ensure that the lacking information is identified and existing work is validated correctly.

This paper will focus exclusively on the software available, both commercial and open source codes, used to model the complex interaction of gas and solid mixtures. In addition to the review of software available, previous modelling of dust and small particle interactions will be reviewed to determine where there is lack of knowledge, as well as verification and validation which has, in recent years, become a growing concern as outlined by Grace and Taghipour [11]. To ensure that this is a well-defined (and verifiable) investigation, the software has been limited to the software codes most used in industry and by researchers. Firstly, on the commercial side, the two main software products used are ANSYS' Fluent [12] and CFX packages [13], which have multiple methods to calculate multiphase flows, and EDEM software developed by DEM Solutions [14] primarily used for granular modelling. On the other hand, two open source products have been investigated, OpenFoam [15] which is not a software package, rather a C++ Library that contains a number of utilities and applications, and LIGGGHTS DEM package [16] for granular modelling. These packages in the last few years have released coupling capabilities and present an intriguing avenue for researchers looking for more control over simulations – the actual solvers are investigated and explained in the following section.

## 2. COMPUTATIONAL PROGRAMS

As outlined in the introduction to this paper the four main programs and developers considered in this review include: ANSYS' Fluent and CFX; OpenCFD's OpenFoam; DCS Computing's LIGGGHTS; and DEM Solutions' EDEM. This chapter will serve as a brief overview of the abilities and limitations of these packages and the potential for use in dust generation modelling. A more in depth paper by van Wachem and Almstedt [17] investigates the formulation of the models employed in these software packages and is worth reading for a more thorough investigation on modelling multiphase flows from a fundamental level. In addition, the paper by Balachandar and Eaton [18] on turbulent dispersed multiphase flow also is worth reviewing for a greater understanding of the complications faced when modelling multiphase phenomena.

### 2.1. Commercial Software

#### 2.1.1. Computational Fluid Dynamics (CFD)

ANSYS Inc. has been at the forefront of commercial software for a number of years and has become one of the most heavily used computational packages available. In particular, the variety of problems that can be solved in ANSYS is what creates its appeal. The relevant solvers in this instance are "Fluent" and "CFX" – the key difference between these two solvers is the method that they use to discretise a problem. CFX uses finite elements, similar to a mechanical analysis, whereas Fluent uses finite volumes. Although these solvers are both capable of modelling multiphase flow problems, it appears that Fluent has been the most popular among researchers.

Multiphase flows can be modelled using four models that exist in ANSYS, these are: Discrete Phase Model; Volume of Fluid (VOF); Mixture; and Eulerian. These models have been developed to successfully model the interaction and behaviour of multiphase flows of varying concentrations and loading scenarios.

The Discrete Phase Model is the only true Lagrangian model available in ANSYS – in this model individual particles are able to be tracked by the user. However, due to the high computation power required it is limited to small concentrations of less than 10% solid to fluid loading. Although this solver is limited to low concentrations of solids it has the added feature of two-way coupling, which leads to an Eulerian-Lagrangian model being used where the fluid is modelled as a continuum.

Alternatively, the loading cases where the secondary phase concentration exceeds 10% may be modelled using an Eulerian-Eulerian approach. The other methods within Fluent (Volume of Fluid, Mixture and Eulerian) can be used to model larger concentrations of multiphase flow leading to the two phases both being modelled as continuums.

Additionally, the standard viscous models can be used such as: laminar; k-epsilon; k-omega; and Large-Eddy Simulation. It appears that k-epsilon is the most realisable and popular model due to its good agreeance for single phase fluid flows.

#### 2.1.2. Discrete Element Method (DEM)

EDEM is an application developed by DEM solutions for modelling granular material such as coal, mined ores, soil, tablets and powders. The program uses a DEM solver to model each particle individually solving equations within a defined domain for a range of interactions: bonded particle; cohesion; Hertz-Mindlin; linear spring; and moving surfaces. Although this solver is suitable for larger particles it is unsuitable for modelling smaller dust particles due to being a one way solver and relying on simple drag laws for particle trajectories. Hence, DEM Solutions have recently released '*EDEM-CFD Co-Simulation*' [19] allowing ANSYS to be coupled to this software package and hence allowing Fluent multiphase models to be used.

### 2.2. Open Source Software

#### 2.2.1. Computational Fluid Dynamics (CFD)

Open source software has been growing in use over the past few years and has led to some powerful tools being released to the research community free of charge with restrictions on commercial use. One such example is OpenFoam, a Linux based C++ library. Various precompiled applications, or solvers, are also released with this

package. Further there is the potential for the user to create their own application utilising other models available within the package. A number of applications exist for solving multiphase fluid based flows, such as:

- *Compressible Multiphase InterFoam*, a solver for compressible, non-isothermal immiscible fluids using a VOF (volume of fluid) phase-fraction.
- *Multiphase EulerFoam*, a solver for a system of compressible fluid phases including heat-transfer.
- *Reacting Multiphase EulerFoam*, a solver for a system of compressible fluid phases with a common pressure, but otherwise separate properties.

However, there is no discrete model available to model dispersed particles using the Lagrangian approach or to incorporate solid–fluid interactions. This has led to the coupling of OpenFoam with LIGGGHTS, which is discussed later in this chapter.

### 2.2.2. Discrete Element Method (DEM)

*LIGGGHTS* (LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) Improved for General Granular and Granular Heat Transfer Simulations) open source software package has been released to the general community as a part of the CFDEM® project hosted by DCS Computing. Simply, LIGGGHTS is a DEM solver offering basic functionalities for DEM simulations. Similar to EDEM, there is support for cohesion, rolling friction and Hertz-Mindlin, as well as Hooke’s Law. However, it does not have capabilities for fluid flows and therefore requires OpenFoam coupling to allow for multiphase fluid–solid flows to be modelled.

## 2.3. Limitations

As discussed earlier, limitations exist with the previously mentioned software packages. These limitations have been but one of the many challenges faced when attempting to model dust and dust emissions accurately. Each of the programs have their own set of limitations: ANSYS places restrictions on the number of cells for the academic license, as well as recommendations for each solver’s use; OpenFoam can only be used for fluid modelling; EDEM and LIGGGHTS are both discrete solvers with no interaction with the fluid phase.

For the ANSYS fluent solver using the discrete method to model solid particles, it is recommended that the user not use this model for cases where the loading of solids to fluids is greater than 10 %. If the user is using this model outside the guidelines placed by ANSYS then there cannot be a guarantee on the accuracy and hence, would require a great deal of validation before it could be confirmed that this method is suitable for other loading concentrations. Additionally, as there are many small particle interactions, as the injection rate increases and hence, the concentration of particles to fluid, the simulation times also increase – this needs to be addressed also and provides another limitation. This means that modelling a full scale silo may take anywhere from days to months on a standard desktop computer. Further limitations exist within ANSYS when using the academic version in regards to mesh sizes. When creating a mesh, the user is limited to 512000 cells limiting the capabilities to model dust accurately on a large scale as the cell sizes must increase to maintain a level of 512000 or below. This can be avoided by using a non-academic licence; however when undertaking research funding is limited and the likelihood of this occurring is small.

On the other hand, there is OpenFoam which is an open source package available to the research community. Although this software is highly customisable and allows for greater control over simulations, it is currently limited to two phase simulations involving fluids. This means that for an Euler–Lagrangian simulation to be undertaken it must be coupled with a discrete solver to model the particle interactions. As discussed earlier through the CFDEM® project, it is possible to use the DEM solver LIGGGHTS and OpenFoam together.

EDEM and LIGGGHTS are both DEM packages for use with granular materials, although they have the potential to model down to 1 micron, they are limited in use where the surrounding air has an appreciable effect on the particle stream. Hence, to overcome this limitation they must be coupled with a fluid solver, such as Fluent or OpenFoam.

Finally, a common limitation amongst some of the programs is that the particles are modelled as spheres and hence, faceted particles with complex shapes aren’t modelled realistically as a shape factor must be applied. The determination of this shape factor is what will determine if a simulation is valid or not and hence, relies on experimental data to set a baseline for the simulations. An exception to this is EDEM which can be used to create particles of more complex shapes, such as tri particles. Although there is a limitation on modelling complex particles, calibration technology can be used to verify and scale bulk material properties and behaviour

such as the work conducted by Grima *et al.* [20, 21]. However, this calibration work has been limited to bulk material flow streams rather than dispersed dust and may require further validation.

### 3. PREVIOUS RESEARCH

After undertaking a thorough literature review it has become clear that the majority of work conducted has been focused on a variety of areas surrounding the use of both CFD and DEM. However, although there is some progress in the area of dust modelling there is also a lack of validation and verification presented. Authors have claimed to have ‘good agreeance’ without providing an explanation of how the data was collected and collated.

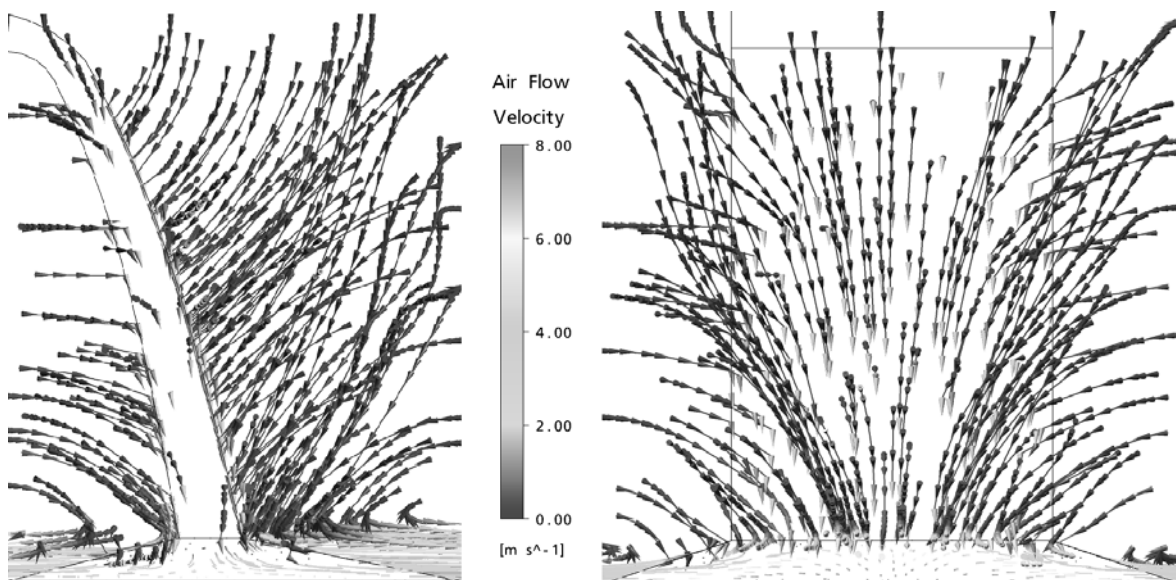
Some authors have taken the approach of pure numerical methods [22-34] others have focused on using CFD to model cyclone separators [28, 35-39] while others have focused more on CFD and DEM in attempting to model flows in channels, free fall and fluidised beds [40-45] . Of the research conducted the following paragraphs discuss the work conducted around dust modelling which show promise for the development of a reliable modelling method.

Currently there are two methods to model powder flows and dust generation.

- CFD Eulerian – Eulerian approach used by [46-51]
- CFD Eulerian – Lagrangian approach used by [52-59]

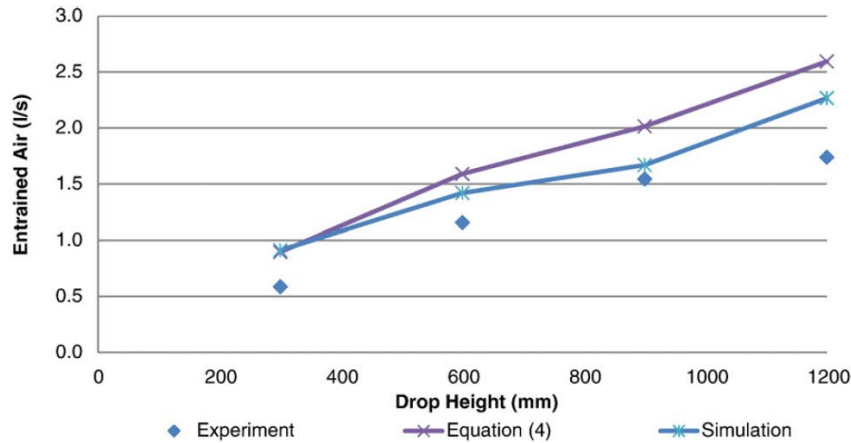
Notable papers investigated by the author are discussed in the preceding section to determine the most suitable method for modelling dust in a free falling stream, the selection of papers have fallen under the headings of Eulerian-Eulerian and Eulerian-Lagrangian methods for multiphase modelling.

An alternative approach for investigating dust generation in bulk solids handling was presented by Donohue *et al.* [47] where CFD and DEM were used uncoupled. In this paper a conveyor transfer was investigated using DEM and CFD utilising a stepped approach. Firstly, the material stream is modelled in DEM software to obtain a porosity associated with the free-falling stream. After the porosity is determined, the transfer is modelled in CFD software as a chute with a porous medium which the air travels through. The focus of this work was not on the dust generation but rather on the induced air through the action of free falling particles and the influence on dust. Although, this method shows the quantity of air induced, it does not represent the dust very accurately as particles larger than 10 microns will typically not follow the air flow completely. This method may provide a novel way to check more complex coupled CFD–DEM simulations, such as Derakhshani *et al.* [53].



**Figure 1** Velocity Streamline Of Air Surrounding The Falling Material (Adapted From [47])

Donohue *et al.* [47] continued this work as a co-author in two papers presented by Esmaili *et al.* [48, 49], which were focused on the study of air velocity for free falling coarse material. This work was compared with experimental results obtained using the Particle Image Velocimetry (PIV) method. Although the results showed good agreeance, PIV has its own limitations based on the camera resolution and potential for particle overlaps to induce errors in the velocity calculations. *Figure 2* shows a comparison of the results obtained in this study.



**Figure 2** Air Entrainment Results From The CFD Simulations For 3mm Glass Beads (Adapted Form [49])

One key result from this work is the observation that the free-falling particle stream will have a lower particle concentration with larger particles when compared to the same material comprised of smaller particles. This leads to a lower surrounding air velocity for larger particles when compared to the smaller particles of the same material and free fall conditions. Additionally, it was seen that the k-epsilon model tended to overestimate predicted air and solid velocities while on the other hand the shear stress transport model results were closer to the experimental outcomes.

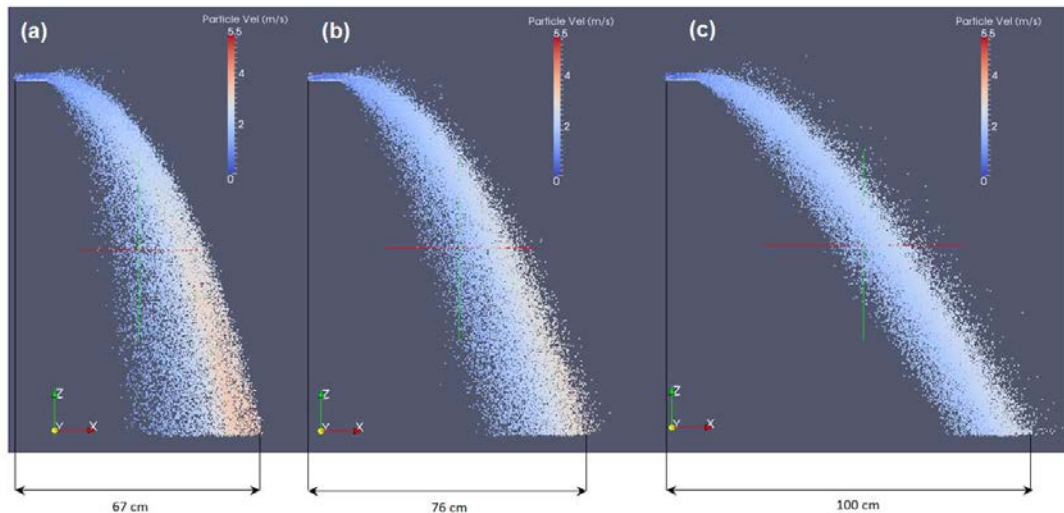
Unlike the previous papers Chen *et al.* [50] model a conveyor transfer using Fluent and a two-phase Euler-Euler approach with six transfer chute configurations. Sheets of plastic were placed on the floor within an enclosure to capture dust that had settled after running an experiment. The author then compared this dust settlement to recorded experiment velocities and CFD simulated velocities. Although not presented with the data, the author commented on the overall trend where the magnitude of the velocities of Chutes D, E and F agreed with the corresponding experimental results within 30%. However, the chutes labelled A, B and C had velocities that were considerably lower. Further to this, the results showed that the Euler-Euler approach is suitable for quantifying likely dust emission rather than actual dust emissions.

As discussed earlier the limitations that exist currently in OpenFoam may be avoided by coupling the software with LIGGGHTS DEM package, similarly, the other limitation on modelling dust in free falling materials is the large computation times required to derive a solution. Hager *et al.* [52] and Derakhshani *et al.* [53] show this coupling in practice and provide further advances in the methods used to couple OpenFoam with LIGGGHTS allowing for fully coupled simulations with smaller simulation times.

Firstly, Hager *et al.* [52] presents an improved algorithm for parallel resolved coupling between OpenFoam and LIGGGHTS, as stated by the author, these programs are already parallelized but by improving this coupling the simulation times can be reduced. Although the particles used in this paper are much larger than what would be expected for dust modelling, and in lower concentrations, the principles for reducing the simulation time can be applied to future simulations to investigate if the algorithm can still work.

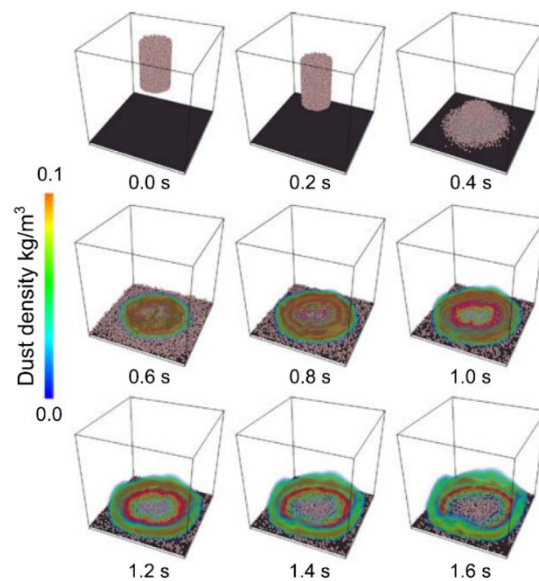
Secondly, Derakhshani *et al.* [53], under-took an investigation of dust liberation at a belt conveyor transfer point. Conveyor transfer points are a key area for generation of fugitive dust and therefore are of great importance when investigating dust generation methods. This paper focused on a purely computational based approach and provides no experimental results to compare to the models used. However, despite lacking verification and validation by experimental means, the ability to couple OpenFoam and LIGGGHTS in this way is clearly demonstrated. The effect that CFD has on the DEM code can be seen when comparing the results side by side (see *Figure 3*) and shows the potential for use in modelling smaller particles using this method.





**Figure 3** Effect Of Wind Velocity On The Trajectory Of Particles For Wind Velocity Of: (A) 0.0 m/s; (B) 0.5 m/s; And (C) 1.0 m/s (Adapted From [53])

Hilton and Cleary [54] presented a paper on dust modelling focusing on dispersal of airborne dust from stock piles. As part of this work the authors conducted a simulation of dust production during a vertical drop in which a cylinder of material was dropped onto a stationary plate. This simulation work shows the potential for CFD-DEM coupling and modelling dust generation of falling particle streams and requires further research to validate the results obtained.



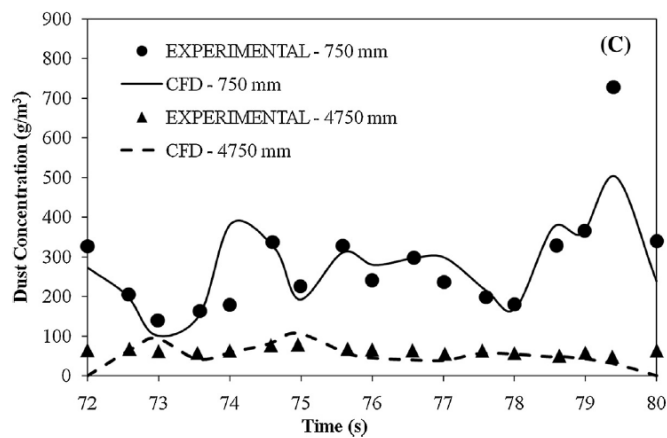
**Figure 4** Dust Generated By Falling Column Of Particle Of 2cm Diameter Dropped 0.5m Onto Flat Plate (Adapted From [54])

Other work conducted around free falling particle streams has been in the area of filling silos. Klippel *et al.* [55] and Rani *et al.* [56] have presented papers in which dust concentrations were modelled using CFD. Firstly, Klippel *et al.* took the approach of modelling two different injection methods and compared these to experimental data that they had collected. It was found that the tests depended heavily on the material properties, humidity and temperature and in some cases the experiments varied from one another by over 30%. Despite this the author claims good agreement between measured and simulated dust concentrations with the exception of an over prediction for settling velocity for the pneumatic filling case. Although, due to the large

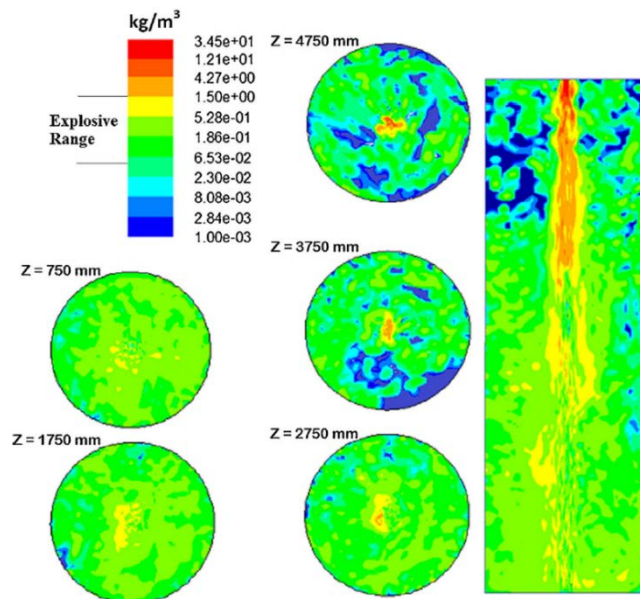
variance in experimental results these results are questionable and the validation of this method needs further work.

Similarly, Rani *et al.* [56] focused on the modelling of dust concentrations for a particular silo investigated previously by Hauert and Vogl (see [56] for reference). Rani *et al.* [56] used the Reynolds average Navier Stokes (RANS) and Re-Normalisation group (RNG) k-epsilon turbulence model and applied a Lagrangian approach for the corn starch particles. A rosin-rammler distribution was used with a minimum particle diameter of 4.5 microns and maximum of 100 microns. The simulation used a time step size of 5 milliseconds and 35 iterations per time step which resulted in a very lengthy simulation taking around a month to complete.

After the simulation was completed it was found that the simulated dust concentration had a fair agreement with the experimental data obtained by Hauert and Vogl (see *Figure 5*). This paper shows potential for tracking particles in large scale simulations and the ability to model dust when considering free falling streams (see *Figure 6*), however, the simulation needs further experimental verification before it can be deemed suitable for other applications and additionally the simulation time needs to be reduced for this method to be viable for commercial applications.



**Figure 5** Comparison Of Dust Concentration Data Points Between Rani *Et Al.* [56] And Hauert And Vogl (Adapted From [56])



**Figure 6** Dust Concentration At Different Silo Heights Key Corresponds To Corn Starch Concentration (Adapted From [56])

#### 4. CONCLUSIONS

Although software limitations have affected the ability to model dust in the past and many researchers have tried to model the phenomenon, currently there is a lack of research focused on powder flows and dust generation mechanisms for free-falling streams of material. The ability of present-day software coupled with the increase in cheap computational power shows promise of the complex particle interactions to be modelled successfully with an Eulerian–Lagrangian approach. Additionally, as open source software improves it appears that there is new scope for modelling dust emissions through two-way coupling of software packages with a high level of customisability of the solvers.

From literature, the k-epsilon viscous turbulence model has been most favoured and shown good agreement in most cases, however some researchers have found that the shear stress transport (SST) model is more agreeable in their comparison to experimental data. It is recommended that when modelling turbulence a comparison be undertaken to ensure the experimental data compares accurately to the results obtained and thus to choose the best model for the particular case study being undertaken.

The ability to use multiple models for specific areas is of a great benefit when investigating material falling streams in the future, such as modelling air as an Eulerian continuum, the falling particle stream as a secondary Eulerian continuum and finally a Lagrangian discrete phase for the dust particles influenced by the two Eulerian continuums. Further, two way coupling of a package dedicated primarily to CFD and a second package dedicated primarily to DEM should be investigated as this will potentially create a more reliable and accurate modelling approach where the user has greater control.

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