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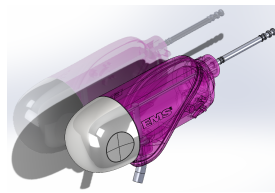
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# Multiphase Simulation for Powder Chamber

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## Abstract

During this intern, we used both open-sourced and commercial software to simulate the behaviors of the mixture of the powder/solid particles and the injected air. With the help of real experimental data and preliminary visualization of the simulation results in the animation, we can check whether the simulation models are approximating the real ones. The values we care about are inlet pressure  $P_{in}$ , outlet pressure  $P_{out}$ , inlet velocity of the mixture  $v_{in}$ , outlet velocity of the mixture  $v_{out}$ , mass flow rate of the outlet  $mfr_{out}$ , and the distribution of the volume fraction across the chamber  $VF_c$ .

The report begins with introduction on the background and goals of our project and difficulties of the gas-(solid)particle systems need to handle, and other extant available methods and software to study the dynamics of the powder inside the chamber in either simulation or physically experimental ways.

Then the open-sourced software MFiX Multiphase Flow Simulation is introduced for its strong versatility for computational applications of gas-liquid-solid systems and then we introduce the procedure on how MFiX should be connected with computing cluster SCITAS.

We first tried COMSOL Multiphysics software, in which the mixture model and the more generic Euler-Euler model are used to simulate the behaviors of our gas-solid(particles) systems. The mixture model method succeeded to converge with homogeneous drag force model and unrealistic small residence time of the powder mixture across the chamber while the Euler-Euler model method failed to converge with default solver configuration.

Then we used the more CFD-dedicated software Cradle from Hexagon company. The software provides full-Eulerian and mixture model methods as well and more stable solver compared to the COMSOL. But it does not provide the options for solid particle materials when using dispersed multiphase flow analysis type.

Finally, we studied several models with different configurations of parameters based on Cradle, output the evolution curves of  $mfr_{out}$  and visualized the distribution of  $VF_c$  and the mixture velocity magnitude distribution across the chamber.

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# 1 Introduction

The working process of the airflow chamber for air-powder mixture can be regarded as the fluidization process, in which the granular material is converted from a static solid-like state to a dynamic fluid-like state. This process occurs when a fluid is passed up through the granular material, in our case the high-speed air is injected into the chamber and mixed with the powder. The powder particles are forced by particle-particle mutual interaction, drag force induced by relative velocity with the air, and gravity.

## 1.1 Fluidization systems

In our case the particles are fluidized at a high enough gas flow rate, the velocity exceeds the terminal velocity of the particles. The upper surface of the powder bed disappears and, instead of bubbles, we can observe a turbulent motion of solid particle clusters and voids of gas of various sizes and shapes. The powder fluidization Beds under these conditions are called turbulent beds.

Not every particle can be fluidized. The behavior of solid particles in fluidized beds depends mostly on their size and density. A classic classifications of the powders by Geldart is shown as Fig. 13 in which the characteristics of the four different powder types are categorized as follows [1]:

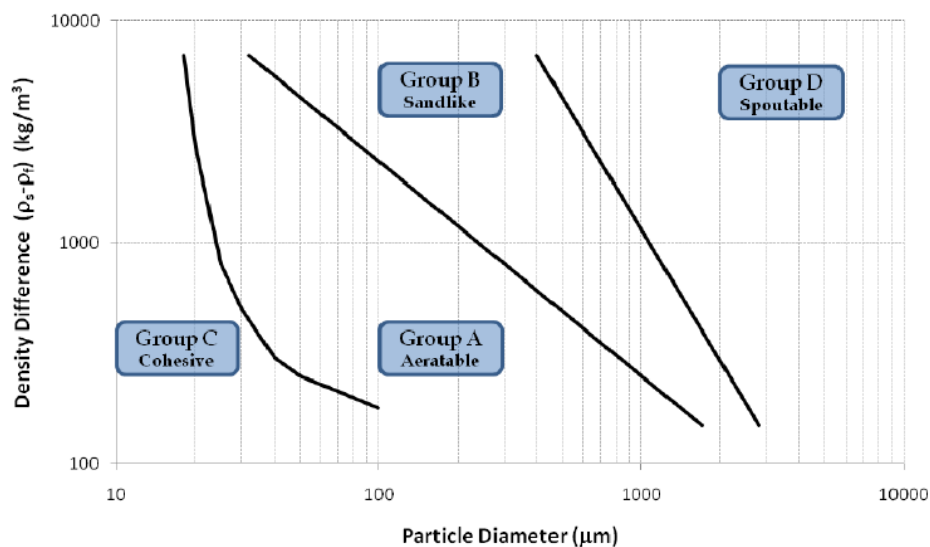


Figure 1: Classification of powders based on density and size

- Group A is designated as ‘aeratable’ particles. These materials have small mean particle size ( $d_p \leq 30\mu\text{m}$ ) and/or low particle density ( $\leq 1.4\text{ g/cm}^3$ ). These solids fluidize easily, with smooth fluidization at low gas velocities without the formation of bubbles.
- Group B is called ‘sandlike’ particles and some call it bubbly particles. Most particles of this group have size  $150\mu\text{m}$  to  $500\mu\text{m}$  and density from  $1.4$  to  $4\text{ g/cm}^3$ . For these particles, once the minimum fluidization velocity is exceeded, the excess gas appears in the form of bubbles. Bubbles in a bed of group B particles can grow to a large size. Typically used group B materials

are glass beads (ballotini) and coarse sand.

- Group C materials are ‘cohesive’, or very fine powders. Their sizes are usually less than  $30\mu m$ , and they are extremely difficult to fluidize because inter-particle forces are relatively large, compared to those resulting from the action of gas. Examples of group C materials are talc, flour and starch.
- Group D is called ‘spoutable’ and the materials are either very large or very dense. They are difficult to fluidize in deep beds. Unlike group B particles, as velocity increases, a jet can be formed in the material bed and the powder may then be blown out with the jet in a spouting motion.

It can be seen that our powder belongs to the group C at large.

## 1.2 Drag force impact

The drag force is the friction that a fluid imposes on an object, and the friction the object imposes on the fluid.

In a fluidized bed, it is the drag force that counteracts the force of gravity which results in the bed being fully suspended. At high superficial gas velocities, particles become entrained and leave the bed. For a single particle, the determination of the drag force is straightforward, and is typically described by the kinetic energy times the cross sectional area times a drag coefficient .

However, for particles in a fluidized bed, particles are affected by more than just a single drag force. Collisional stresses can change the direction and rotation of a particle. Particles, especially small particles, can cluster which results in a larger aerodynamic drag. A particle in front of another particle can reduce the drag on the following particle due to a fluid velocity reduction from the hydrodynamic shedding of the advancing particles.

Thus, using a single particle drag force relationship does not make sense for application in a fluidized bed, but that is often what is used yet. Similarly, using a drag force from a packed bed also does not make sense since particle motion affects the drag force on the surrounding particles. Corrections to these drag models are available, but these corrections are empirically based.

Until recently, little attention has been focused on particle drag for the simulation of fluidized bed hydrodynamics. As a result, the commonly used drag force models used for modeling tend to over predict the entrainment rate and under predict the bed expansion, especially for Geldart Group A and C. The particles.

## 1.3 General theory

Due to computational limitations, the effective modelling approach used is usually considering the fluid and particle phases as continuous and interacting media governed by locally averaged equations

(Euler-Euler approach). For applications with a limited number of particles, or using the Monte-Carlo method, it is also possible to track the positions and the velocities of discrete particles by coupling with a continuous averaging approach for the fluid (Eulerian-Lagrangian approach). In those approaches, constitutive relations are used to take into account unknown terms appearing from the averaging, fluid-particle drag, etc. For gas-solid flows, the fluid-particle drag force has a dominant influence on the hydrodynamic behaviour of the flow and the simulation accuracy is strongly dependant on the fluid-particle drag constitutive relation.

It is important to describe the interaction between the particles and the momentum transfer between the phases. Different models are developed for this purpose. The kinetic theory of granular flow describes the interaction between particles and is based on the kinetic gas theory. In a bubbling fluidization bed there are regions with rather low volume fraction of particles and regions with high particle concentrations. The bed can be described by two flow regimes, the viscous regime and the frictional regime. In the viscous regime the kinetic and collisional stresses are dominating. The frictional regime occurs at high particle concentrations and in this regime the flow behaviour is described by friction and rubbing between the particles. The interaction between the particles and the continuous gas phase are described by a drag model, and several drag models are developed for this purpose. These models describe the momentum exchange between the phases. [3]

To model the gas-solid flow, the most commonly employed CFD simulation methods are the Eulerian-Eulerian two-fluid model (EE-TFM), Eulerian-Lagrangian discrete element method (EL-DEM), and hybrid multiphase particle-in-cell (MP-PIC). The disadvantage of DEM is that it is computationally intensive when the particle size becomes small. In such cases, the Euler-Euler approach is often preferred due to the less computational demand, in which both fluid and solid phases are treated as interpenetrating continua and show the flow dynamics by using averaged equations of motion. [4]

In EE-TFM approach kinetic theory of granular flow (KTGF) closure model are incorporated to simulate solid particle flow. EE-TFM model constitutive relationship contains solid-particle phase stress, inter-phase momentum transfer and particle interactions. Researchers have shown that the gravity and inter-phase drag force are the critical closure model to accurately predict the gas-solid flows and the solid phase stress contribution is insignificant, and it is crucial to accurately account for the solid particle clusters. [5]

Let's take the instance of the spherical solid particles in an incompressible Newtonian fluid, the key question is what is the dependence of the dimensionless drag coefficient  $C_D(R_e, \alpha_f)$  on both the local particle Reynolds number  $R_e$  and also on the local fluid volume fraction  $\alpha_f$ . If one adopts an Eulerian-Eulerian approach to solid-fluid multiphase flow in which the particle phase is modelled as a continuum, the question settles down to a choice between the various standard drag models that are part of commercial as well as open source CFD packages. The Wen and Yu, Syamlal and O'Brien, and the Di Felice models all make use of the classic Richardson-Zaki study of settling velocities. The Wen-Yu model equation follows the Richardson-Zaki prescription of modifying the

drag on an isolated sphere  $C_D(R_e)$  by a factor of the relative settling velocity  $v_r = \epsilon^{-\alpha}$  to account for the influence of neighbouring particles on the flow around it. Wen and Yu take the index  $\alpha = 2.65$  as constant whereas in Di Felice  $\alpha = \alpha(R_e)$  is fitted. Syamlal and O'Brien build in settling data more intimately via  $C_D(R_e/v_r)/v_r^2$ . If one instead adopts the Eulerian-Lagrangian approach one is generally left with a choice between an isolated particle drag model and that of Gidaspow. The use of the isolated particle drag model is appropriate to the traditional application of Eulerian-Lagrangian modelling for small solids concentration where collisions are relatively unimportant and collective effects should arise out of the simulation rather than being built into the particle-fluid coupling via the drag force. [6]

Provided the above general theory underpinning our project, We will emphasize on the implementation of simulation with the open-sourced and commercial applications in the following sections.

## 2 Geometry

In this section, we demonstrate several geometric models we have built for simulation in accordance with the scales and structures of the extant products.

We first did measurement for the powder chamber of the Handy 3 as shown in the cover page. And then given the data, we built the simplified chamber geometry in the SOLIDWORKS 2021 as follows:

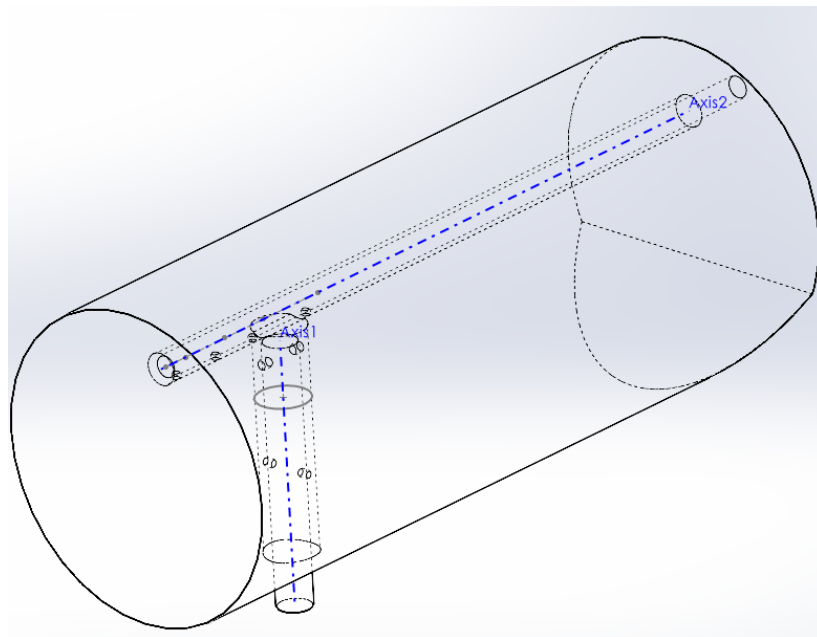


Figure 2: Simplified powder chamber model for the Handy 3

Then the above geometry was divided into the half of the original one to facilitate the setting of symmetry in the numerical models as follows.

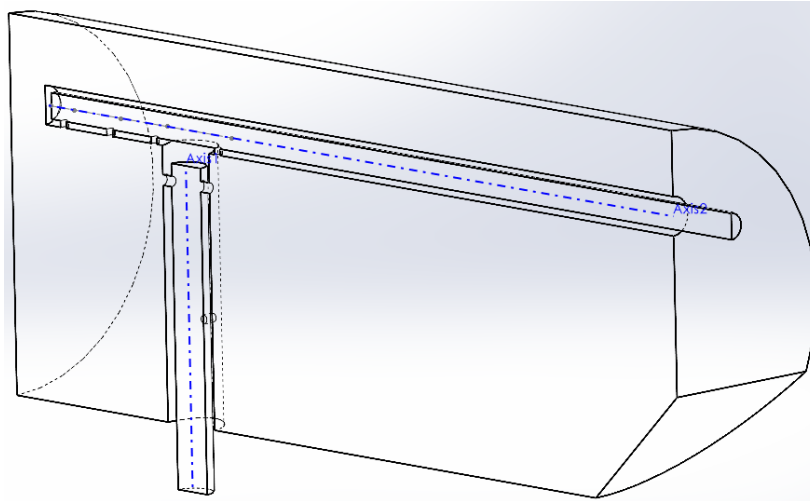


Figure 3: Half of the simplified powder chamber model for the Handy 3

### 3 MFiX Multiphase Flow Simulation Software

MFiX as known as Multiphase Flow with Interphase eXchanges software, was developed over two decades by the National Energy Technology Laboratory. It includes the following set of complementary modeling tools that can be brought to bear on multiphase flow technologies that will be detailed in the next few sections.

Since MFiX is a open-sourced software, it regularly releases the updated versions and fixes the reported bugs. It is very useful to browse and create the discussion topics in the Q&A forum [7]. The user account "Ju.Wu" was created during this intern, and all of the project-oriented questions I have submitted and the corresponding answers can be found at [8].

#### 3.1 Implementation

There are main CFD-TFM, CFD-DEM and its variants solvers in the software. It is essential to first build the simple models and projects to be familiar with the implementation procedure. The user tutorials and example projects can be found out in [9]. The general procedure for "segregated mesher/solver" is:

- Select solver/physics between MFiX-TFM/DEM/PIC, configure the gravity, drag model and momentum formulation(kept as defaults in trials). Inspect the .stl file to see whether there exists any collapsed triangle, duplicate edge/vertex, missing triangles. For instance, the Blender software can be used to eliminate the duplicate entities. And then import the "cleaned" .stl file as geometry and make sure its normals' direction pointed to the flow to decide whether to flip that.
- Configure the regions to set the inlet, outlet, boundaries, powder bed, monitor slices for the models. It is important to cut off the inlet and outlet tubes with the settled planes so that the inlet and outlet slices will be automatically generated as the intersecting plane.



- There is only cut-cell meshing method provided, so we have to set the background mesh with either uniform or control-point methods for each direction of X-Y-Z. As for the uniform method, the uniform cell size for each direction will be computed itself provided the total number. As for the control point method, it can set the local meshing resolution for each direction. The regional mesh needs to be smaller than the geometric details near it. And then fine-tune the parameters of cut-cell method such as small cell/area tols, snap tol, and intersection/facet angle/dot product tols.
- Set the density, viscosity, molar weight and the reference pressure of the fluid as the continuous phase and keep other parameters as defaults for further configuration in the future. And then set parameters of the solid as the dispersed phase like diameter, density and viscosity, and it is possible to set particle distribution for DEM and its variants.

We first built a simple model that contained inlet, outlet, internal tubes and chamber with the provided "implicits" in the software. Do not forget to convert an implicit function to polydata with "sample\_implicit" function. As we have tried, it was hard to assemble a geometry with delicate structures like nozzles with the built-in implicits due to the insufficient sampling resolution of the "sample\_implicit" function.

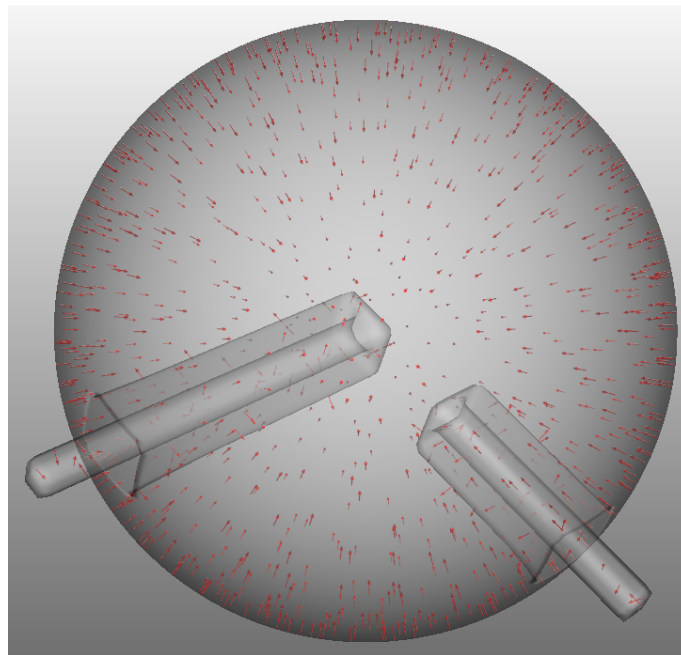


Figure 4: Test chamber model built in the provided implicits

Then we built another simple model with inlet, outlet, chamber and internal tubes of  $\varnothing 2.4mm$  in the SOLIDWORKS 2021, then exported the .stl file of ASCII format and imported it to the software as Fig. 13.

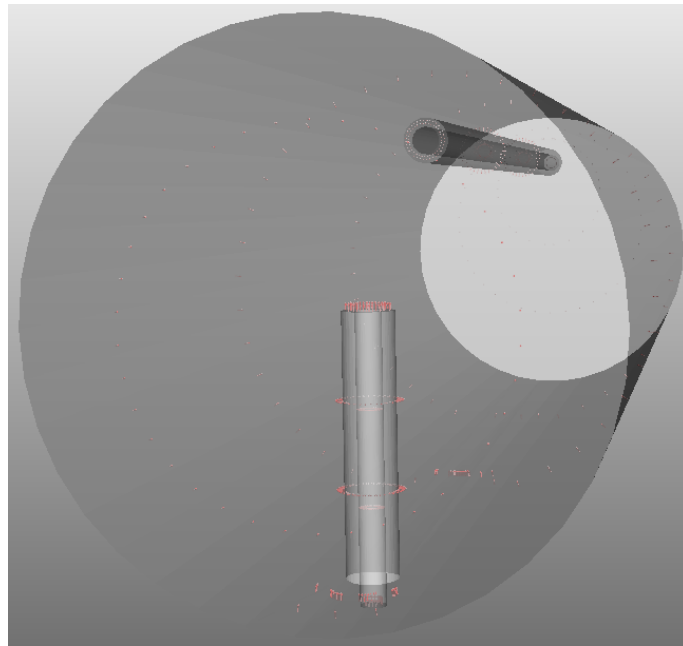


Figure 5: Test chamber model built in the imported .stl file

Finally we imported the Handy 3.0 .stl file in which the duplicate elements have been removed and set up the following meshing parameters as shown in Fig. 6 to obtain mesh with relatively good quality.

Background
**Mesher**

**Mesher** cutcell ▼

**Options**

Reset all tolerances to default

☐ Enable array re-indexing

Small cell tolerance 0.1

Small area tolerance 0.1

Merge tolerance 0.0

Snap tolerance X 0.2 Y 0.2 Z 0.2

Allocation factor 1.0

Maximum iterations 10000

Intersection tolerance 1.0000e-16

Facet angle tolerance 1.0000e-06

Dot product tolerance 1.0000e-07

Max facets per cell 10

Normal distance tolerance 0.2

**Mesh**

Figure 6: A set of appropriate meshing parameters

### 3.1.1 MFiX-TFM method

To set up MFiX-TFM method, we need to first switch the solver to "MFiX-TFM", and then configure the details of parameters according to [9]. We get the simulation regions as Fig. 7.

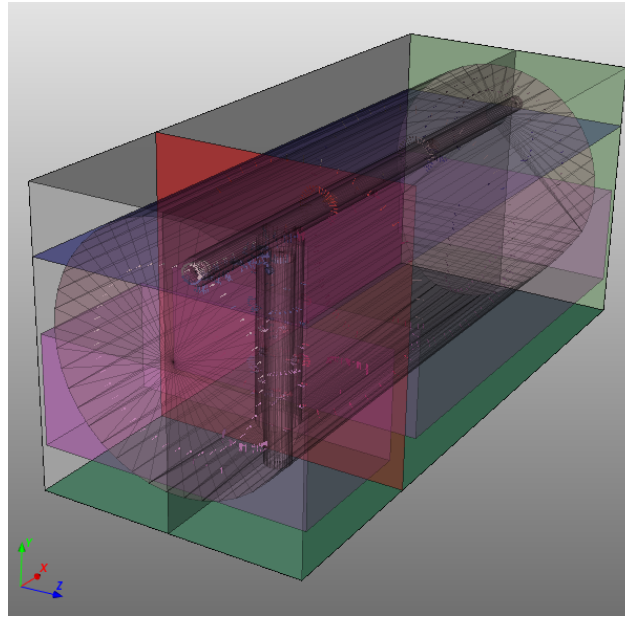


Figure 7: Set-up regions of powder chamber of Handy 3.0

It would take hundreds of days to get 5 seconds simulation results even with HPC computer, so we dismissed this method.

### 3.1.2 MFiX-PIC method

To set up MFiX-PIC method i.e., a variant of DEM method, we need to first switch the solver to "MFiX-PIC", and then apart from normal set-up procedure, we need to care about the parameters "statistical weights", "number of particles per parcel" and "mesh cell size" in each direction to trade off the simulation accuracy and time cost. We got 0.1s simulation result as Fig. 8.

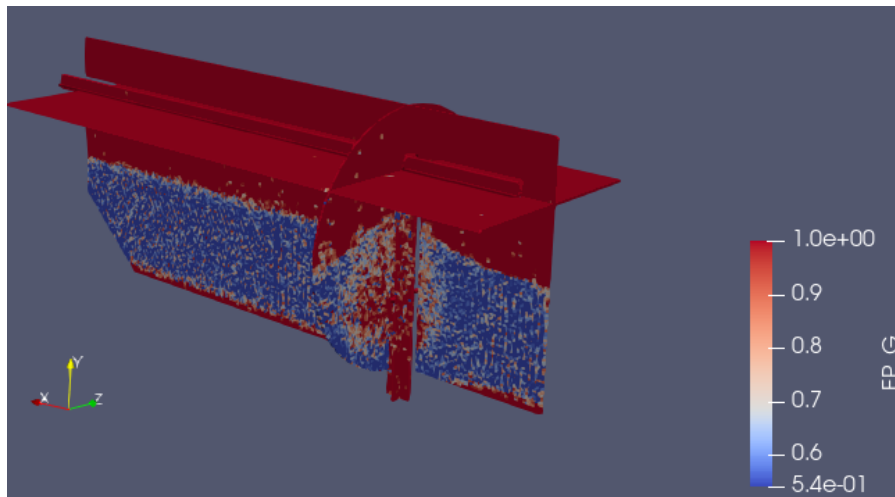


Figure 8: Volume fraction of powder in 0.1s via PIC method

### 3.2 Connection with computing cluster SCITAS

To connect the MFIX to computing cluster, debug/submit the simulation tasks to the queue and transfer simulation and project data bidirectionally, the convenient and state-of-art way is to use the Linux OS. We installed the MFIX in one of computing clusters in SCITAS and used ssh command to log in and transfer the files bi-directionally. We used sbatch to run the tasks. One of the .sh file is as shown in Fig. 9.

```
#!/bin/bash
#SBATCH --nodes 2
#SBATCH --ntasks-per-node 2
#SBATCH --cpus-per-task 18
#SBATCH --mem 20G
#SBATCH --time 01:00:00

export OMP_NUM_THREADS=$SLURM_CPUS_PER_TASK

set -e

module purge
module load gcc mvapich2

DATA_DIR=$HOME/miniconda3/envs/mfix-21.3.2/share/mfix/templates/tutorials/tfm/fluid_bed_2d
[ -d $DATA_DIR ] || ( echo "$DATA_DIR not found!" && exit 1)

srun ./mfixsolver -f $DATA_DIR/fluid_bed_tfm_2d.mfx NODESI=2 NODESJ=2
```

Figure 9: Configuration of sbatch file

### 3.3 Pre/post processing

The MFIX needs other open-sourced software to pre-process imported geometry and visualize the obtain result data in .vtu format.

#### 3.3.1 Blender to clean duplicate entities

Blender is a open-sourced software, we used it to remove the duplicate elements in the .stl file. The command path is "Mesh¿cleanup¿merge by distance". We need to adjust the merge distance and make sure all faces/vertices are selected.

There is no universal value for the "merge distance". It depends on the scale and unit of the .stl file. If the .stl file coordinates are expressed in meters and we want to merge points or remove details less than  $0.1\text{mm}$ , then the distance will be 0.0001. If the unit is in millimeters, the the distance would be 0.1. It is common to start with small values and then gradually increase it. If it is too large, it begins losing details in the geometry. The ideal procedure is to generate the cleanest .stl file possible with few elongated triangles and do the clean-up to remove duplicates and the few bad triangles. The model ready to remove the double elements from in Blender is shown as Fig. 10.

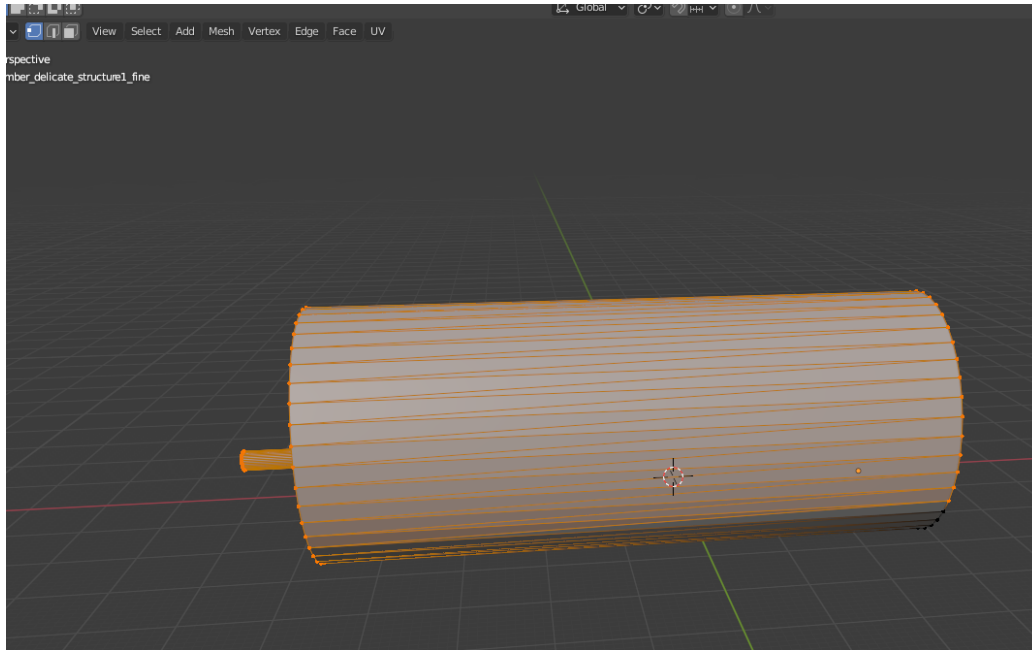


Figure 10: Model to remove double elements from in Blender

### 3.3.2 Visualization with ParaView

ParaView is an universal open-sourced software for .vtu file visualization and processing, and it is widely acceptable in FEM computation community. We used ParaView to make animation, select desired regions and do math operation like integral. The generated videos has been saved in my personal folder "JU2021" and one static instance is shown in Fig. 8.

## 4 COMSOL

The COMSOL is a commercial multi-physics simulation software. Towards multi-phase flow problem for fluidization like systems, it provides "Euler-Euler Model" and "Mixture Model" i.e., a simplified Euler-Euler method that uses one momentum equation to represent all phases. We tried the best to test them and tune the solver parameters, but in the end it did not work for both of the methods.

### 4.1 Mixture Model

The problem for the this method is

- It requires the continuous and dispersed phases are both liquid and have similar density. But in our case the density of the solid powder particle has much more larger density than that of the air gas.
- It took too short time (near 2 seconds) to clear all of powder inside the chamber.

## 4.2 Euler-Euler Model

It was quite hard for us to tune the solver parameters to make the task in this method converge. The following solver error is persistent.

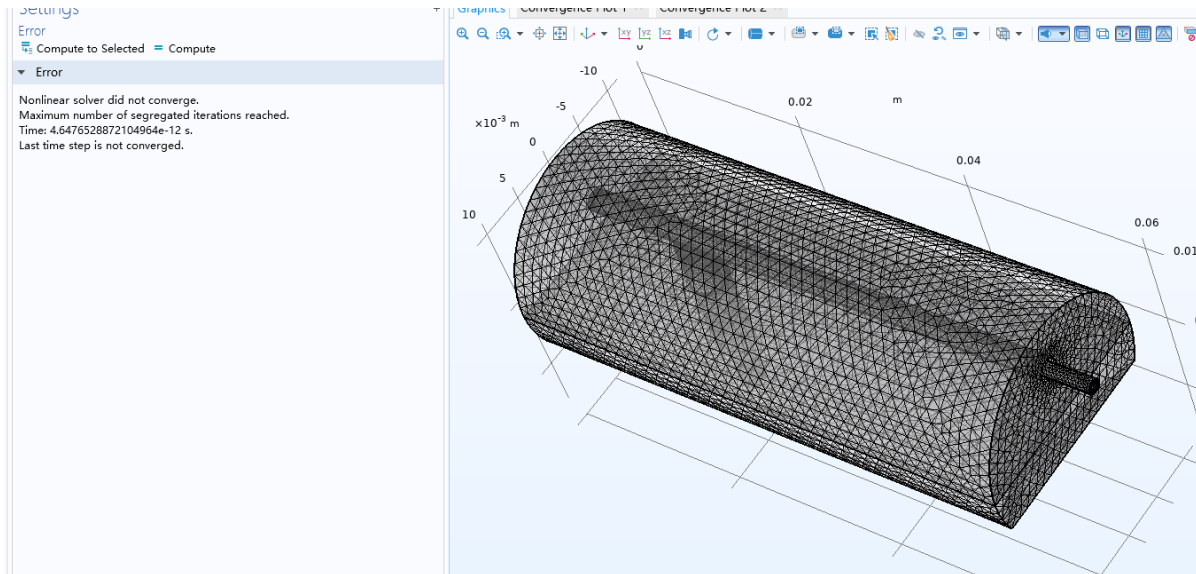


Figure 11: Persistent unstable solver

## 5 Cradle

In this section, we used the Cradle software dedicated to CFD simulation developed by Hexagon AB company.

### 5.1 Initial specifications

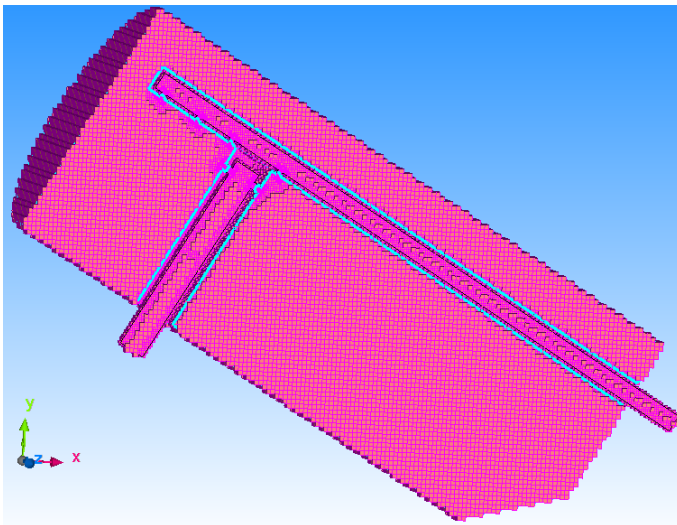
We selected the dispersed multi-phase flow analysis type based on Euler-Euler model, the continuous phase was chosen as incompressible gas, and there is no option of solid particles for the dispersed phase.

The detailed specifications of **experiment 1** for the numerical models are as:

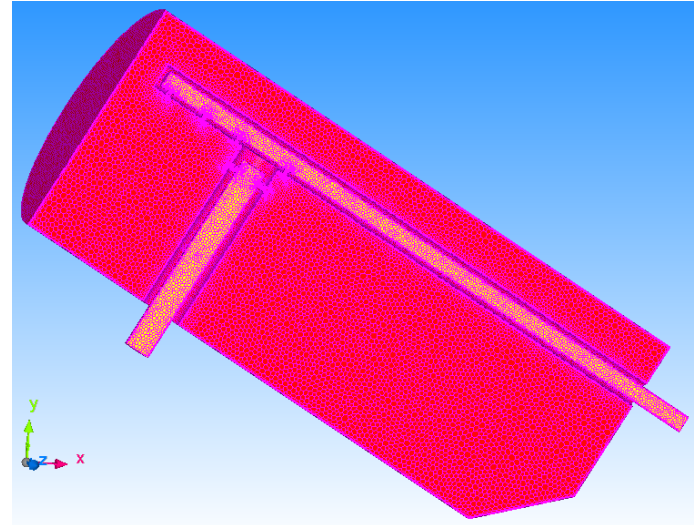
- Material for the dispersed multi-phase flow:
  - a). Air modelled as incompressible air at 3 bars ( $\rho = 3.57 \text{ kg/m}^3$ ).

- b). Powder modelled as incompressible water of the density  $\rho = 1450 \text{ kg/m}^3$  and the viscosity  $1.85 \text{e-}5 \text{ Pa} \cdot \text{s}$ .
- Full Eulerian multiphase flow solver.
- The long axis of the chamber model is at a 30 degree angle to the horizontal ground.
- Fixed time step of constant  $1 \text{e-}5 \text{ s}$ .
- Boundary conditions: a). Air mass flow rate at  $6.5 \text{e-}5 \text{ kg/s}$  at Inlet b). Pressure outflow at outlet with static pressure of 3 bars.
- Numerics:
  - a). Under-relaxation of the equations for helping the loop process i). Momentum: 0.4 ii). Energy: 0.6 iii). Pressure: 0.4 iv). Density: 0.2 v). Volume Fraction (multiphase): 0.3
  - b). Avoidance of Divergence (Elements): Stability oriented
  - c). Matrix Solver: Accuracy/stability oriented
- Output:
  - a). FPH files every 25 cycles
  - b). RPH files each 0.002s

And then we generated the octree and mesh of the imported .SLDPRT model as follows:



Octree of the imported model



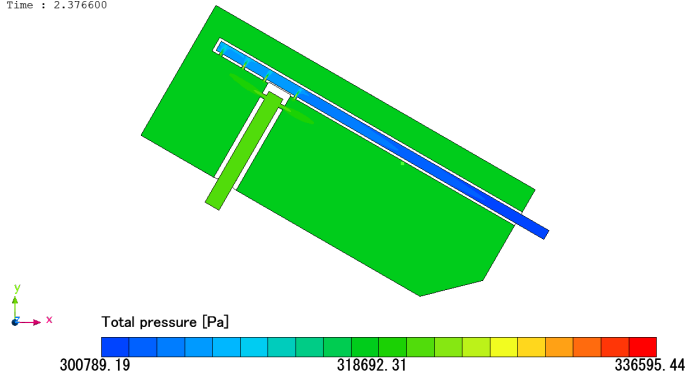
Mesh of the imported model

## 5.2 Initial results

We demonstrated the contours of the variables "total pressure", "magnitude of velocity of the continuous phase (air)", "magnitude of velocity of the dispersed phase (powder)" and "volume fraction of the dispersed phase (powder)" of the experiment 1 at  $T_s = 2.3766 \text{ s}$  as follows:

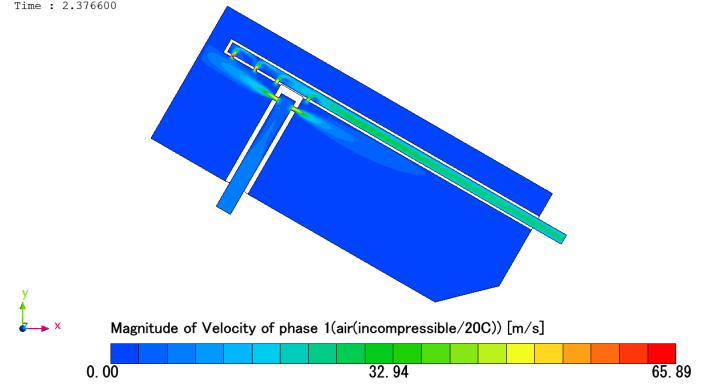


Cycle: 237660  
Time : 2.376600



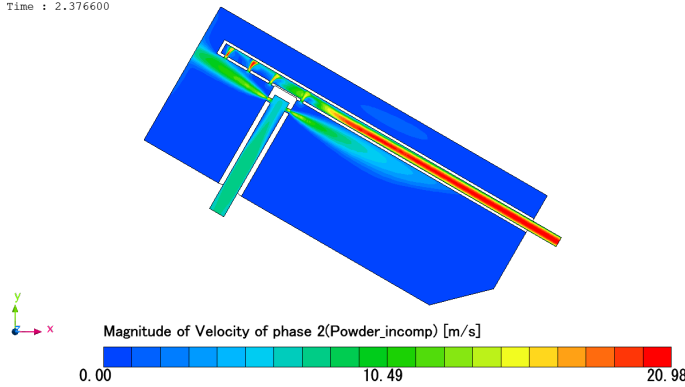
Contour of the total pressure at  $T_s$

Cycle: 237660  
Time : 2.376600



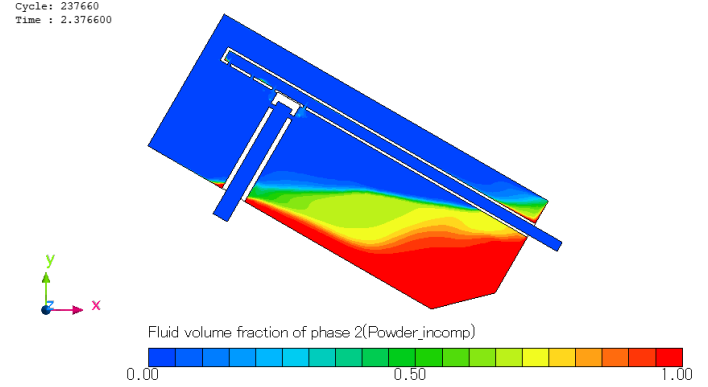
Contour of the magnitude of air velocity at  $T_s$

Cycle: 237660  
Time : 2.376600



Contour of the magnitude of powder velocity at  $T_s$

Cycle: 237660  
Time : 2.376600



Contour of the powder volume fraction at  $T_s$

### 5.3 Self-defined functions

To better capture the transient behaviors and approximate boundary conditions i.e., inlet velocity and outlet pressure to the reality. We built a full model that comprised of outer nozzle and external environment.

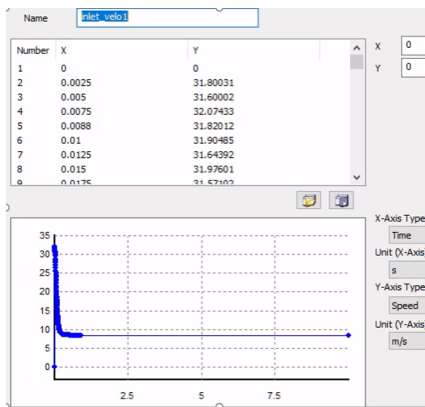
The detailed specifications of **experiment 2** for the numerical models are as:

- Material for the compressible flow:
  - a). Air modelled as compressible air.
- Flow and heat transfer solvers.
- Pressure based solver.
- Fixed time step of constant 1e-5s.
- Boundary conditions: a). Air mass flow rate at 6.5e-5 kg/s at Inlet b). Pressure outflow at outlet with static pressure of 1 bars.
- Numerics:
  - b). Avoidance of Divergence (Elements): Stability oriented
  - c). Matrix Solver: Accuracy/stability oriented

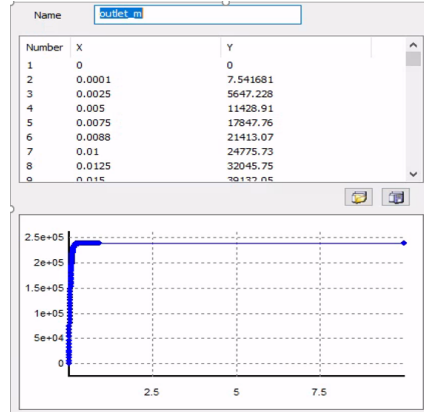


- Output:
  - a). FPH files every 50 cycles
  - b). RPH files each 0.002s

Then we extracted the inlet velocity and total pressure of the monitored outlet slice and obtained the self-defined function tables for the final experiment as follows:



Inlet velocity input table



Outlet static pressure input table

## 5.4 Final specifications

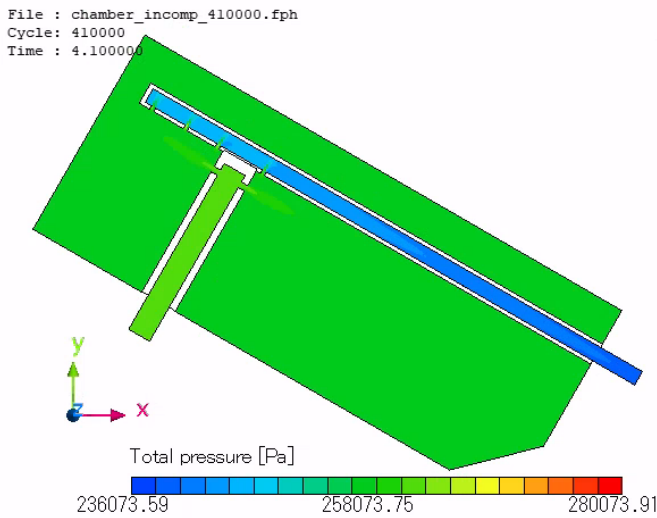
With the self-defined function tables as input, the detailed specifications of **experiment 3** for the numerical models are as:

- Material for the dispersed multi-phase flow:
  - a). Air modelled as incompressible air at 3 bars ( $\rho = 3.57kg/m^3$ ).
  - b). Powder modelled as incompressible water of the density  $\rho = 1450kg/m^3$  and the viscosity  $1.85e-5Pa \cdot s$ .
- Full Eulerian multiphase flow solver.
- The long axis of the chamber model is at a 30 degree angle to the horizontal ground.
- Fixed time step of constant  $1e-5s$ .
- Boundary conditions: a). Air inlet flow velocity defined by input table b). Pressure outflow at outlet with static pressure defined by table input.
- Numerics:
  - a). Under-relaxation of the equations for helping the loop process i). Momentum: 0.4 ii). Energy: 0.6 iii). Pressure: 0.4 iv). Density: 0.2 v). Volume Fraction (multiphase): 0.3
  - b). Avoidance of Divergence (Elements): Stability oriented
  - c). Matrix Solver: Accuracy/stability oriented

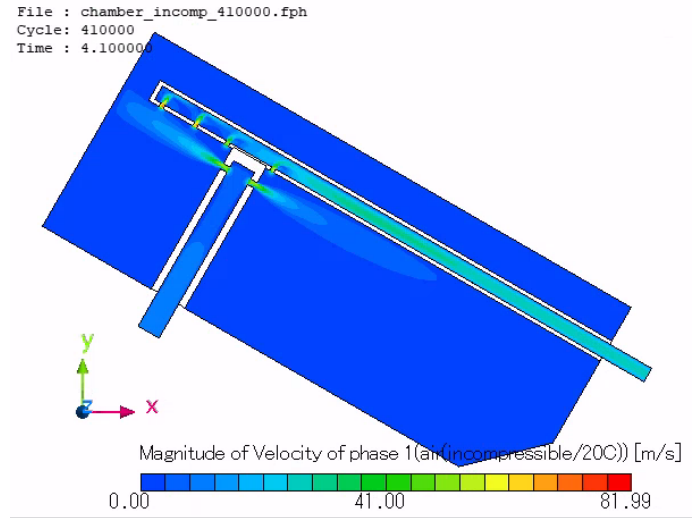
- Output:
  - a). FPH files every 25 cycles
  - b). RPH files each 0.002s

## 5.5 Final results

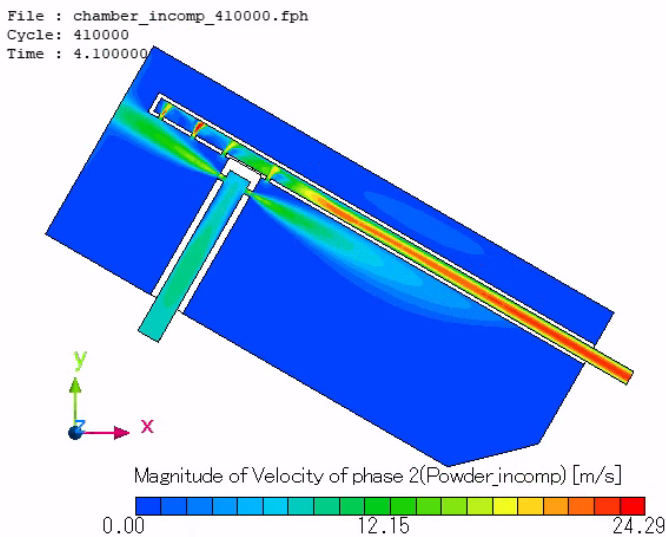
We demonstrated the contours of the variables "total pressure", "magnitude of velocity of the continuous phase (air)", "magnitude of velocity of the dispersed phase (powder)" and "volume fraction of the dispersed phase (powder)" of the experiment 3 at  $T_{s3} = 4.1s$  as follows:



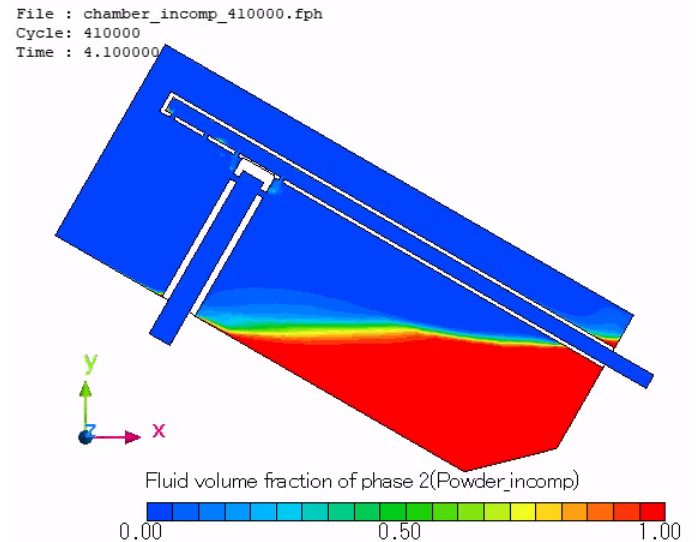
Contour of the total pressure at  $T_{s3}$



Contour of the magnitude of air velocity at  $T_{s3}$



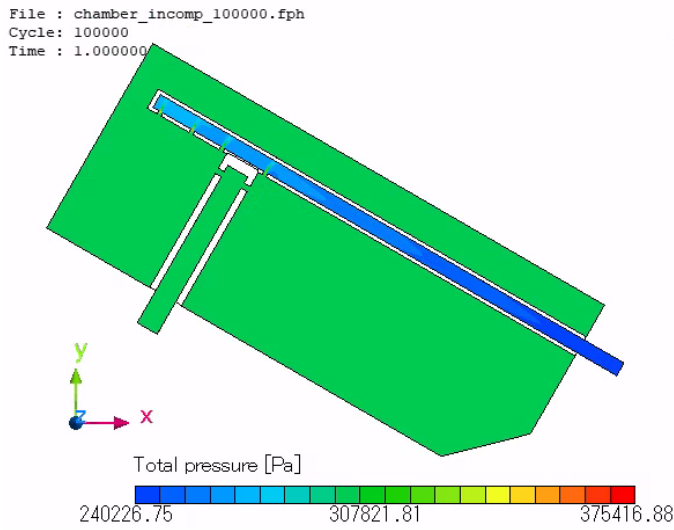
Contour of the magnitude of powder velocity at  $T_{s3}$



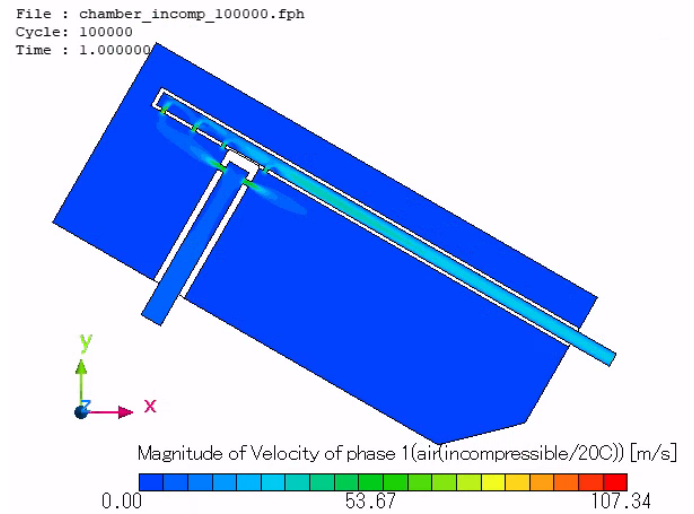
Contour of the powder volume fraction at  $T_{s3}$

To compare with the behaviors of the last cycle and visualize the condition inside the chamber near the peak of the transient phase in one paddle cycle, we selected the .fph file of the experiment 3 at

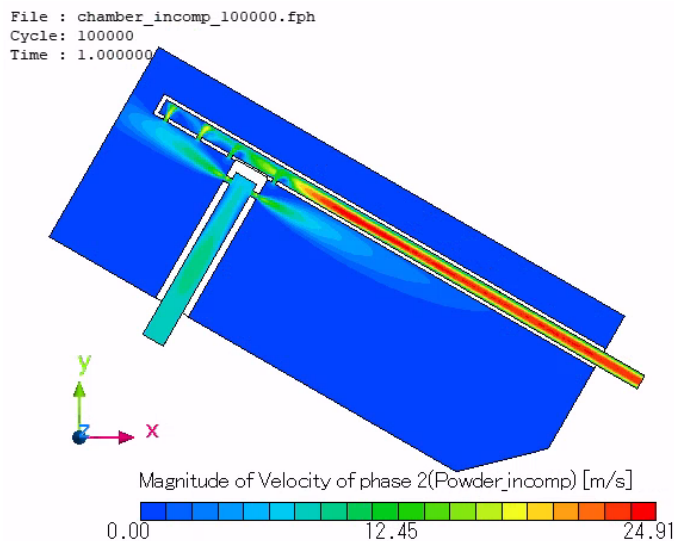
$T_m = 1.0s$  and demonstrated the contours of the variables "total pressure", "magnitude of velocity of the continuous phase (air)", "magnitude of velocity of the dispersed phase (powder)" and "volume fraction of the dispersed phase (powder)" as follows:



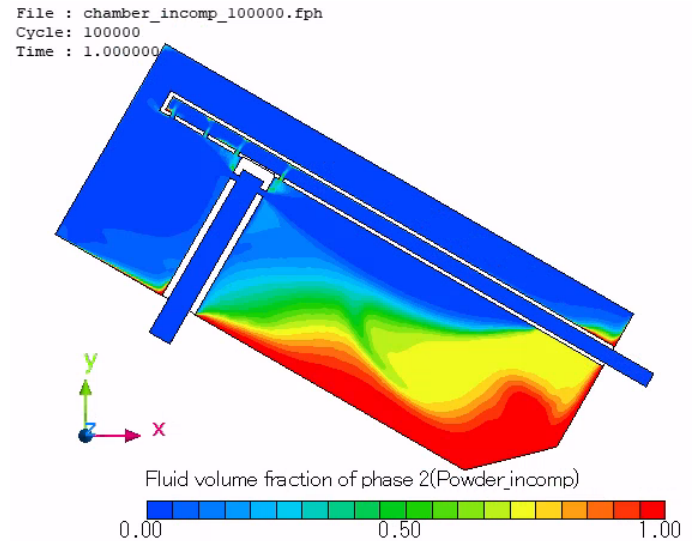
Contour of the total pressure at  $T_m$



Contour of the magnitude of air velocity at  $T_m$

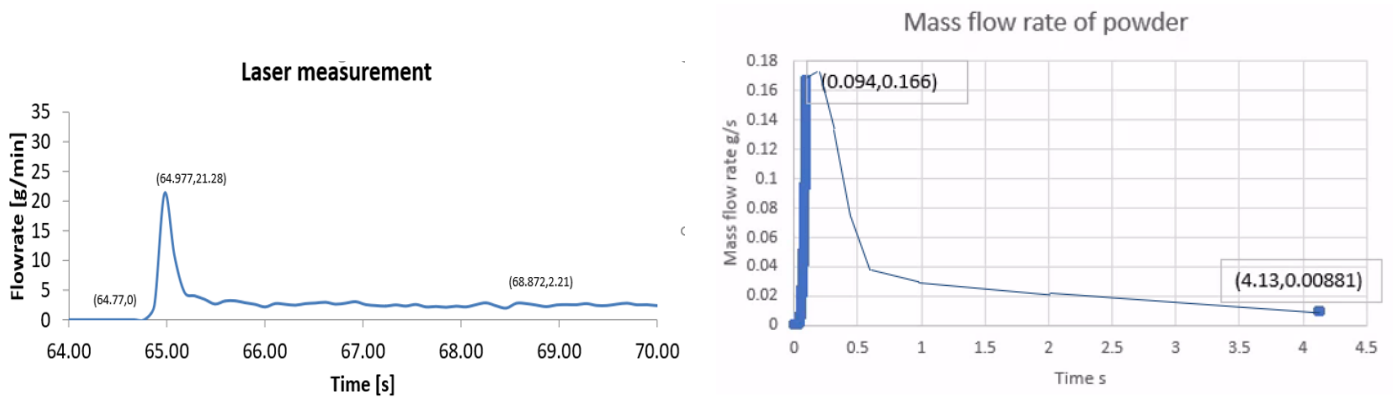


Contour of the magnitude of powder velocity at  $T_m$



Contour of the powder volume fraction at  $T_m$

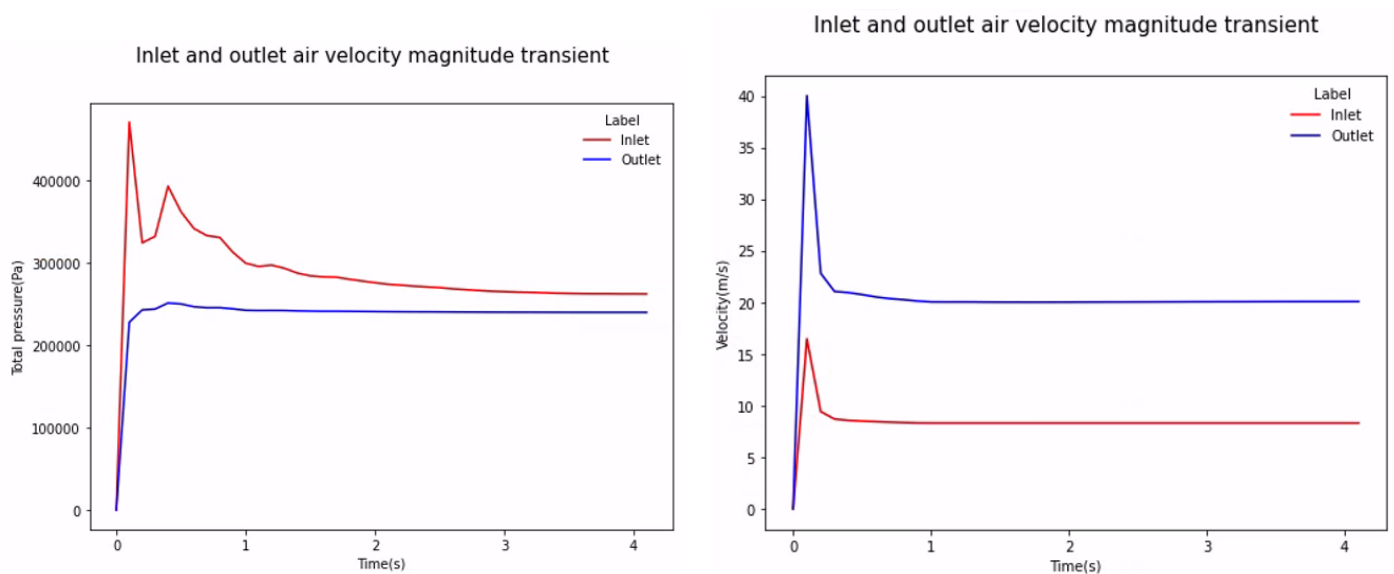
We can observe that both of the experimental and simulation data share the same ratio (near tenfold) of peak and stable mass flow rate shown as follows:



Experimental transient curve for one paddle cycle

Simulated transient curve for part of one paddle cycle

We plots inlet/outlet air velocity magnitude and inlet/outlet total pressure as follows:



Inlet/outlet air velocity magnitude evolution

Inlet/outlet total pressure evolution

## 5.6 Connection to HPC cluster servers

We have two available remote desktop HPC computers shown as follows:

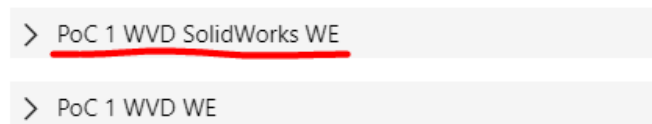


Figure 12: Test chamber model built in the imported .stl file

Where the red-highlighted one is with GPU and the blue-highlighted one is the classic without GPU for simulation. We installed the MFIX and Cradle on both of the remote computers.

## 6 Conclusion

We can list the brief performance table for the three software as follows:

Criteria Software	Accuracy	Flexibility	Easy-to-use	Price	Stability	Speed
Cradle scFLOW	High	Middle	High	20K CHF/Y & rent	High	High
MFiX	Middle	High	Middle	Free	Middle	Slow
Comsol	N/A	Low	N/A	20K CHF/Y	Low	Middle

Figure 13: Performance table for the three software

We know that COMSOL can not work for our tasks, MFiX is too slow, unstable and needs to be reinstalled regularly, Cradle can capture interesting features from experimental results and provide flexible purchase options.

We have the following outlooks for future work:

- Model verification: we ought to further fine-tune the physical parameters of material in the Cradle to fit the simulation results to the experimental data better. At the same time, we have to consider how to avoid the generated simulation data exceeding the limits of computer memory and how to use the overclocking desktop computer and remote server with 64 cores together to speed up progression of simulation.
- Sensitivity analysis: we can set meshes with rougher resolutions, increase solver step interval, and decrease input table density to see the robustness of results against these changes. If the results are robust enough against these parameter changes within predefined tolerance, the time cost can be significantly reduced.
- Codes development: we can develop codes to accompany the main software to do automatic post-processing and results analysis such as files extraction according to time stamps and machine learning to recognize patterns from a large number of variables,
- Software rent options: after the first three steps complete, we can rent the Cradle for a period of time to test the prototype models before manufacture and real experiments, which is more cost balanced.

## 7 Acknowledges

Thanks to the guidance and help of Dr.Marcel Donnet. Thanks to Dr.Sebastian Gautsch for his supervision and provided access to the computing resources in EPFL. Thanks to Mr.Etienne Orliac for his professional instruction on how to use SCITAS computing cluster. Thanks to Mr.Magnus Björkman for his professional instruction on how to fine-tune parameters for the computationally expensive projects in COMSOL.

## References

- [1] Dechsiri, C. (2004). Particle Transport in Fluidized Beds: Experiments and Stochastic Models.
- [2] Simonin, Olivier and Chevrier, Solène and Audard, François and Fede, Pascal Drag force modelling in dilute to dense particleladen flows with mono-disperse or binary mixture of solid particles. (ICMF 2016)
- [3] Ramesh, P., Ramesh, L., Raajenthiren, D.M. (2010). A REVIEW OF SOME EXISTING DRAG MODELS DESCRIBING THE INTERACTION BETWEEN THE SOLID-GASEOUS PHASES IN A CFB Paladi.
- [4] Karunarathne, S.S., Tokheim, L. (2017). Comparison of the influence of drag models in CFD simulation of particle mixing and segregation in a rotating cylinder.
- [5] Upadhyay M, Kim A, Kim H, Lim D, Lim H. An Assessment of Drag Models in Eulerian–Eulerian CFD Simulation of Gas–Solid Flow Hydrodynamics in Circulating Fluidized Bed Riser. ChemEngineering. 2020; 4(2):37.
- [6] Tupper, G.B., Govender, I., Mainza, A.N. (2014). An Inertial Cell Model for the Drag Force in Multi-phase Flow. arXiv: Fluid Dynamics.
- [7] NETL, MFiX online forum. (2021). <https://mfix.netl.doe.gov/forum/c/mfix/5>
- [8] NETL, MFiX user profile page. (2021). [https://mfix.netl.doe.gov/forum/u/Ju\\_Wu/activity](https://mfix.netl.doe.gov/forum/u/Ju_Wu/activity)
- [9] NETL, MFiX user tutorial. (2021). <https://mfix.netl.doe.gov/doc/mfix/21.3.2/html/tutorials/index.html>
- [10] COMSOL, CFD user guide. (2021). <https://doc.comsol.com/5.4/doc/com.comsol.help.cfd/CFDModuleUsersGuide.pdf>
- [11] Azure, Remote desktop web client. (2021). <https://rdweb.wvd.microsoft.com/arm/webclient/index.html>