Delft University of Technology

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Specialization:	Transport Engineering and Logistics
Report number:	2016.TEL.8040
Title:	Coupled DEM-MBD calibration for mixing sand.
Author:	M.C. van Etten

Title (in Dutch)	Gekoppelde DEM-MBD kalibratie voor het mixen van zand.

Assignment:	Computer/experimental assignment
Confidential:	no
Initiator (TUDelft):	Prof.dr.ir. G. Lodewijks
Initiator (TBS):	Prof.dr.ir. M. Jones
Supervisor (TUDelft):	Dr.ir. D.L. Schott
Supervisor (TBS):	Dr.ir. K. Williams
Supervisor (UoN):	Dr.ir. W. Chen
Date:	August 17, 2016

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Student:	M.C. van Etten	Assignment type:	Experimental Assignment
Supervisor (TUD):	Dr. ir. D.L. Schott	Creditpoints (EC):	15
Supervisor (TBS):	Dr. ir. K. Williams	Specialization:	TEL
Supervisor (UoN):	Dr. ir. W. Chen	Report number:	2016.TEL.8040
		Confidential:	No

Subject: **Coupled Discrete Element Modelling and Rigid Body Dynamics Calibration for Granular Materials**

Discrete element modelling requires calibration prior to its application into the real world scenarios. In some cases, the calibration process requires the involvement of the mechanical/hydraulic components of the entire system, such as rotary feeders and screw conveyors. This research aims to develop a calibration method for these special applications by coupling the discrete element modelling with the rigid body dynamics.

Essentially, a lab-scale calibration system will be initially designed and constructed. It is envisaged that the system will not only assess the granular material behaviours, the force/torque/energy information of the mechanical component will also be monitored. One granular material type will be nominated to participate in the investigation. TUNRA Bulk Solids has extensive lab scale systems which will be beneficial for facilitating this system in a timely fashion.

Additionally, the numerical simulations on the experimental system using the already established coupled discrete element modelling and rigid body dynamics will also be performed. The TUNRA DEM software is built on the LAMMPS & LIGGGHTS. The comparison between the experiments and numerical simulation will be carried out to determine the optimised DEM settings when modelling material – plant interactions.

A final internal report will be produced for this work.

Dr.ir. W. Chen

Preface

This report is the results of the Research Assignment and is a part of the final year of the master Transport Engineering and Logistics, a track of Mechanical Engineering. The project has been completed at the University of Newcastle in cooperation with the company TUNRA Bulk Solids. This opportunity gave me a broad insight into the possibilities of bulk handling and its research.
I want to thank Prof. Gabriel Lodewijks for the contact details to engage with TUNRA Bulk Solids and Dr.ir. Dingena Schott and Dr.ir. Kenneth Williams for their supervision during this project.
Special thanks to my supervisor Dr.ir. Wei Chen for assisting me with the tough work on the simulations and their results. This unique experience made me even more interested in the bulk handling environment and I am looking forward to making a contribution in this field of engineering.

Thank you,

Marc van Etten

Summary

In the bulk handling industry, a lot of components can be involved to carefully transport bulk material from place A to place B. Equipment has to be designed on several conditions to have a reliable system in different conditions. One of these parts of a conveying system can be a screw conveyor, by example. A change in moisture content can cause a lot of trouble since it can result in a big difference in shear stress in the bulk material. For example, when the moisture content in dry sand increases, the screw conveyor needs a lot more energy input to keep rotating. The better the change in performance or behaviour is known, the better the system can be designed and simulated to predict the performance under several circumstances.

In this work a calibration between experiments on sand with different percentage of moisture content being mixed by a single impeller and DEM-Rigid body input parameters was realised. This is done by having a closer look at the rotations of the shaft versus the energy input for the different values of moisture content. The expectation was that water bridges, due to the increase of the moisture content, caused an increase in shear strength and thus a drop in the measured rpm. The first part of the calibration and thus this report are the experiments. The second part will be the simulations and the calibration to match the results with the simulations.

Since medium grained sand is an easy drained material, increasing the moisture content to investigate the cohesion effect was only done up to 8% moisture content. A self-made setup was built to observe the change in behaviour. The available resources to create a setup for the experiments and the used medium grinded sand were provided by TUNRA Bulk Solids. The experimental plan was to insert batches of 1.25 kg to 2.5 kg of medium grained sand with a certain moisture content of 0, 2, 4, 6 or 8% into the 455 mm wide drum. By increasing the air pressure input up to 700 kPa using steps of 50 kPa, the 270 mm wide impeller started to mix the material. After each step of air pressure increase, the rotation of the shaft was measured during the steady state of mixing. Adding batches of material and increasing the moisture content were done until no rotation could be measured.

The experimental results show a linear relation between the measured air pressure input and the measured revolutions per minute of the shaft as an output. When increasing the added sand at the experiments at one constant moisture content, the linear resulting line dropped. The results show that the same happened when the amount of sand was kept constant and the moisture content was increased. Again, a linear relation almost parallel to the others was measured. This means that when increasing the moisture content of the samples or adding more sand into the drum, a drop in rpm of the shaft was the result. And so, more energy input was needed to realise the same amount or rotations when moisture content was increased. Thus the expectation of the drop in revolutions when adding more moisture or adding more sand was right. Finally, trendlines were created out of the results to be used in the calibration of this work.

These trendlines were calibrated to get a useful addition on simulating a change of moisture content in the bulk material. To realise this the simulations were done in Discrete Element Method software coupled with Rigid Body Dynamics software. The DEM software used was the TUNRA DEM software based on the LIGGGHTS and LAMMPS software. For the implementation of the shaft POEMS software was coupled. First, the initial state of the impeller and it motion was calibrated. This was done for three different points of the experimental results, known as the rotations of the shaft at 300 kPa, 400 kPa and 500 kPa air pressure input. To the initial energy adjusted to the shaft in DEM, a period of rotation was introduced. This way the initial state and the other results for the varied moisture content and added mass, were calibrated.

The result of this work is a configuration in parameters used to calibrate the coupled DEM-Rigid body model with the experiments. The calibration was done for three different moisture contents, for four different added mass per moisture content, and at three different points of air pressure input. The simulations used values of 0, 5000 and 9000 J/m^3 of cohesion energy density for their corresponding 0, 2 and 4 percent moisture content. The modelled results at the air pressure of 300, 400 and 500 kPa, are realised by decreasing the value of the period of rotation used in the simulation by 0.20, 0.15 and 0.11. The modelled values at the different air pressure input, match the experimental results, with exception of the initial state. The initial state of the experiments is a key issue in this work. Further on the slopes and the other results of the model are close to the experimental results. Only a slight under prediction of the model could be seen in the simulated results in comparison to the experiments. This could be caused by using a cohesion model which applies the cohesion in a homogeneous way to the mixture, while the moisture and so the cohesion in the experiments had a slightly more heterogeneous character.

Contents

1 Introduction

Bulk handling is widely used in different types of environments, from the food industry to the mining industry and much more. The transport of bulk material can be done by a chain of several types of conveyors in order to transport the material to the required place. Since it has influence on the performance of the process, each component in the system is equally important as all the other components in the chain. The performance of the process can be defined as the material flow through the system. A couple of factors has to be taken into account while designing a system in order to create a process with the desired performance. The quantity, the type and the condition of the transported bulk material are some of the factors. Therefore, every component of the system needs to have the proper specifications to handle the bulk material.

One of the possible components in bulk handling for feeding, discharging and conveying over a vertical distance is the screw conveyor. The screw conveyor can have a big difference in performance because of small changes in the material condition. For example, when the moisture content (MC) of the material will change, the shear stress of the bulk material will change as well. The cohesion shear force increases with the increase of moisture content till its saturated value. Different values in shear strength of the material can make a huge difference in performance. Higher shear strength can cause a slower rotation of the screw or even worse; it can block the screw conveyor and the entire operation. On the one hand the engine has to be powerful to process the demand and conversely on the other hand it has to be as small as possible in order to be cheap. It is important to know the performance range of the components to prevent a blockage from occurring.

Simulations are often used to investigate the performance of the process or a sub process. This could be the interaction of the used material and the equipment like the wear of a transfer chute or as in this case the force on a screw conveyor. For the granular material applications, Discrete Element Method known as DEM, can be used for simulations. To use the DEM and make it applicable to a real world application, calibration of the DEM has to be done. In some cases, the calibration process requires the involvement of the mechanical components of the entire system, like a screw conveyor. This research aims to develop a calibration method for the use of a mechanical component by coupling the discrete element modelling with the rigid body. In this research the focus will be on the use of an impeller mixing sand and to know more about the forces on and power needed of this component in different circumstances.

In this case medium sized sand will be used as the granular material type. Although sand is an easy draining and not a cohesive material, the water bridges between particles can increase the shear strength of the mixture at a very low moisture content percentage up to 8%. This free drain saturation moisture was measured by immersing the sand sample into water for half an hour, and monitor the water loss until a steady state was achieved. The moisture content of this sample was then measured. An investigation on the increase of moisture content and so the increase of shear strength can be done on a lower level of cohesion.

Because of simplicity and availability of resources in the workshop, the screw conveyor was changed into an impeller and a drum. Using an impeller for rotating the sand with different moisture content, the aim is to make a useful calibration for the application to know more about the resulting performance.

This research is about the calibration of the rotation force in terms of rotations per minute of the shaft, for mixing medium grained sand with moisture content up to 8%, rotated by an impeller. DEM software LAMMPS/LIGGGHTS coupled with POEMS will be used to model the particles, the shaft and impeller as a rigid body. The experimental and modelling results will be shown using Matlab and Paraview.

The experimental phase of this research assignment will be discussed in the first two following chapters. The setup of the experiments at chapter 2 and the results of the experiments in the **3**rd chapter. After that the calibration with the coupled DEM is introduced in chapter 4 DEM coupling. In chapter 5 Modelling results will be discussed. The report will end with the Conclusion and recommendations in chapter 6, the references and the appendix.

2 Experimental design

This research report starts with the experimental design of the experiments which will be the first part of the calibration in this research assignment. In order to realize this experimental investigation an experiment design and setup had to be made. Using the available resources and facilities at TUNRA Bulk Solids the following design and setup was created. The results are included in this chapter.

2.1 Impeller

For this research a different impeller was used than initially was attached on the shaft. To reduce the weight of the impeller as much as possible, the impeller was made out of aluminium. The design of the impeller is shown in Figure 1 and the manufactured result is shown in Figure 2. The impeller was designed to have a decent amount of contact area with the sand, 5.750 mm^2 surface area, and to have space to the side of the drum (100 mm). This way a small amount of sand could be moved to the sides of the drum and at the same time it did not take a lot of sand to get a steady state with contact between the impeller and the sand.

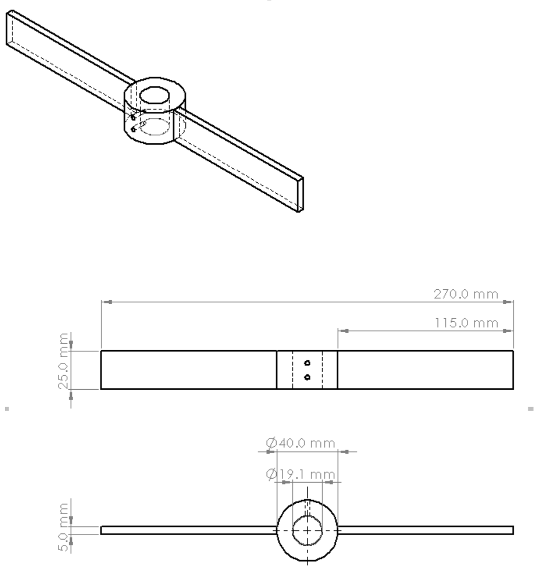

Figure 1. Solidworks Impeller drawing

Figure 2. Created and used impeller

2.2 Setup

In the Solidworks model as in Figure 3, the setup as modelled is shown. In this model an extra cylinder is placed over the shaft. This tube is added to hold the shaft in position and gives it the availability to rotate without falling down when it is simulated in LIGGGHTS. All these components are used in the coupled simulation.

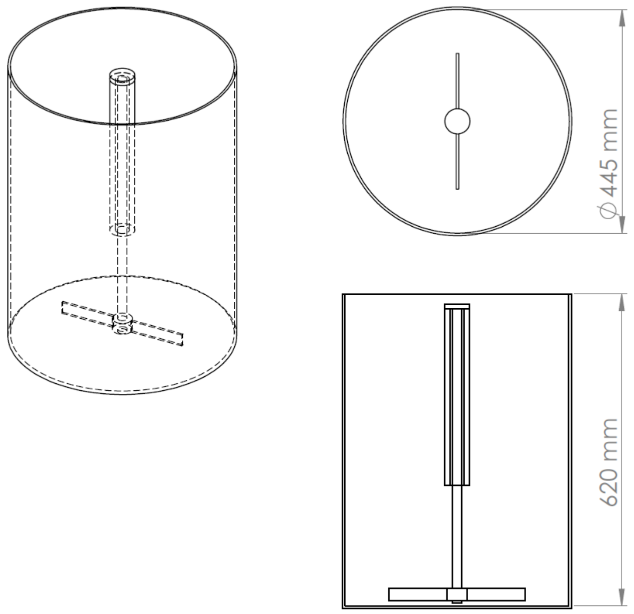

Figure 3. Solidworks 2D drawing of the experimental setup

Connecting a regulator to the general air supply gave the opportunity to regulate the air input into the hose with steps of 50 kPa to a maximum amount of 700 kPa. Although the air pressure input had a range till 1000 kPa, the air supply was limited at 720 kPa to 750 kPa. Because of the variation in maximum air supply, the maximum air pressure was rounded down to 700 kPa. This way for every experiment the results were measured at the same maximum air pressure input.

The compressor hose was connected to the pneumatic engine mounted onto the drum and turning the air input into a rotation of the shaft. At the end of the attached shaft connected to the pneumatic engine is the aluminium impeller assembled.

The input of air pressure, as shown in Figure 4, can be read from the air regulator and the rounds per minute of the shaft will be measured by a laser tachometer. This photo tachometer used is shown in Figure 5. A 5 mm wide reflecting strip was attached on the shaft so the rpm of the shaft could be measured by the tachometer using a horizontal line.


Figure 4. Air pressure regulator

Figure 5. Photo Tachometer


Figure 6. Used pneumatic engine


Figure 7. View inside the drum


Figure 8. Drum

2.3 Material samples

Adding the sand into the drum was initially done by steps of 2.50 kilograms. In a later stadium this changed to two different steps. During the first experiments a free rotation of the impeller in steady state was noticed. The impeller was capable to rotate the sand to the sides with a free rotation of the impeller and no contact with the sand as a result. This was the case till a certain amount of added sand. For 0% moisture content sand will be collected at the side of the drum till 10.0 kg of sand. For the other experiments with different moisture content this happens up to 5.0 kg of sand.

As said, the first tests this critical amount was reached at adding 10.0 kg of sand. The decision to change the steps of 2.50 kg to 1.25 kg was made in order to have a better insight of the results between the 2.50 kg steps. During a later stadium the critical point of free rotation was reached at 7.50 kilograms. An extra step of 1.25 kg to measure the rpm at a level of 8.75 kg was not made because the difference was noticed in a late stadium and because of the critical period of time.

2.3.1 Particle size distribution

The sand used in the experiments was facilitated by TUNRA Bulk Solids. To investigate the particle size distribution a sieve test was done. The results of two sieve tests can be found in Figure 9 and Figure 10.

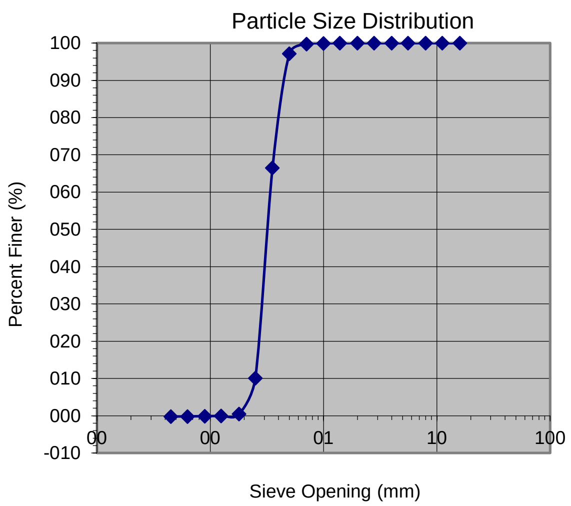

Figure 9. Sand PSD test 1

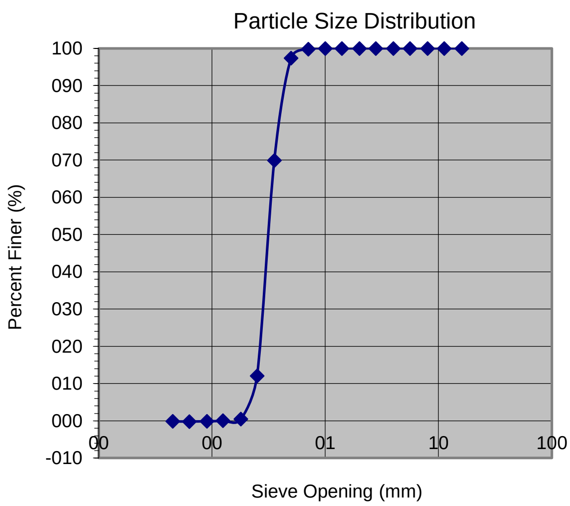

Figure 10. Sand PSD test 2

The results of the sieve tests show a steep and almost vertical line which means a uniform particle size distribution for the samples. The particle sizes of the samples will be for 99.3% between 0.180 mm and 0.500 mm and for 85.4% between 0.250 mm and 0.355 mm. The samples for these experiments can be taken directly from the batch. A variation in the ending results because of a difference in particle size will not happen because of the uniform particle size of the used material.

2.3.2 Moisture content

The range of moisture content was set to 0% to 8%. Since sand is an easy drained material it is not capable of holding the moisture and therefore it is not a cohesive material for a big range of moisture content. Since the maximum stable air pressure input was 700 kPa, the increase of moisture content while getting useful results was limited.

Therefore, the experiments were done for moisture contents of 0%, 2%, 4%, 6% and 8%. Steps of two percent moisture content were used to eliminate process errors like for example weighing. Later in the report big ranges between similar experiments were found but the same slopes did occur. Each experiment is done in a continues timeframe, this means without a break and each process time step after the other. This is to prevent the sand to decrease in moisture content. The outside temperatures when doing the experiments vary from 25 to 35 degrees Celsius. To avoid the samples with a higher moisture content than zero to dry out, the samples were quickly mixed by hand for a couple of minutes. This way the mixture was as homogenous as possible without a decrease in in moisture content or drying out.

2.4 Margin of error

In the whole process of experimenting a lot of measurements are done. All the measurements have a certain margin of error. This margin of error determines how reliable the measurements and the experimental results are.

The used photo tachometer has an accuracy of 0.1 rpm. So it has a ±0.05 % accuracy.
For measuring the 2.50 kg, 1.25 kg samples and the added water, scales down to 0.01 gram and so ±0.005 % accuracy were used for measuring the 2.50 kg, 1.25 kg samples and the added water. Since the air pressure input is measured by an analogue instrument with 50 kPa between the readable lines, the accuracy of these measurements are 25 kPa. This is clearly the biggest error in these measurements. The experimental results in the following chapters have their margin of error but this is not shown to keep the graphs clear. In Figure 11. a zoomed-in part of one of the results is used to show the margin of error on the results.

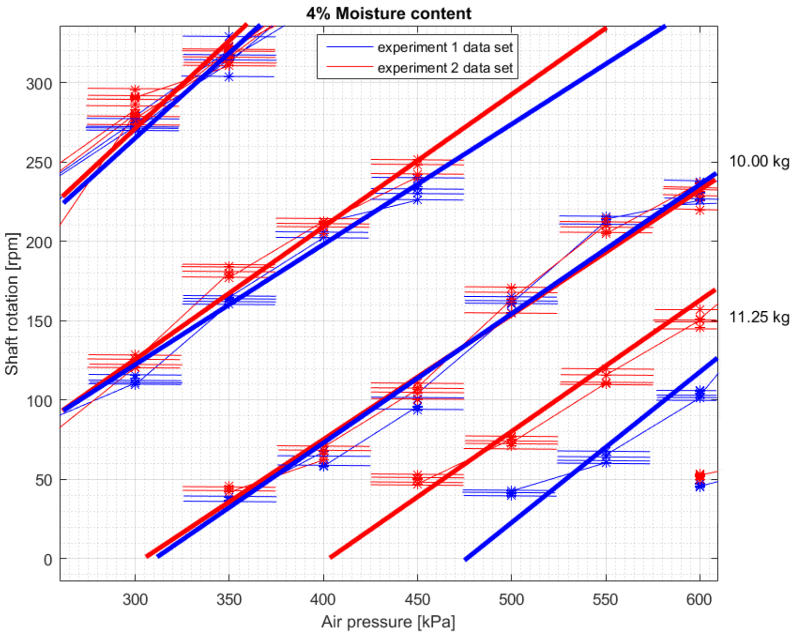

Figure 11. Margin of error on the results

On this scale the margin of error of the shaft rotation and the weight of the sample, respectively 0.1 and 0.01, are neglected in comparison to error of margin of the air pressure.

Besides the error by reading accuracy using an analogue instrument such as the air pressure regulator, there is also the error of measuring. During the experiments each measurement is repeated five times and each experiment has been done twice.

2.5 Experimental plan and process steps

For this assignment experiments were done up to 8% moisture content while increasing the added material and the air pressure to the pneumatic engine. The plan of the experiments is shown in Table 1,Table 2 and Table 3. In Table 1, the moisture content and the added mass is constant while increasing the air pressure input. In Table 2, the added mass increases including the increase of the air pressure like in Table 1. Finally, the Table 3 shows the increase of the moisture content including the increase of air pressure and the increase of added mass. All the input was tested to its maximum to the point that there was no change in result. The regulator was able to control the air pressure input up to 700 kPa and both the maximum values for the moisture content and the added mass caused a blockage of the impeller. A further increase of the two last parameters was not found useful.

Table 1. Experiments: increasing the air pressure per moisture content and added mass

# Test	*Moisture Content [%]*	*Added mass [kg]*	*Air Pressure [kPa]*
1	0	0	0
2			50
3			100
4			150
5			200
6			250
7			300
8			350
9			400
10			450
11			500
12			550
13			600
14			650
15			700

Table 2. Experiments: increasing the added mass per moisture content

# Test	*Moisture Content [%]*	*Added mass [kg]*	*Air Pressure [kPa]*
16	0	0	0 to 700 [steps of 50]
31		2.5	0 to 700
46		5.0	0 to 700
61		7.5	0 to 700
76		10.0	0 to 700
91		11.25	0 to 700
106		12.50	0 to 700
121		13.75	0 to 700
136		15.0	0 to 700
151		16.25	0 to 700

Table 3. Experiments: increasing the moisture content to 8% while increasing the added mass and air pressure for each step.

# Test	*Moisture Content [%]*	*Added mass [kg]*	*Air Pressure [kPa]*	*Amount of measuring points*
1	0	0 to 16.25	0 to 700	151
152	2	0 to 13.75	0 to 700	121
273	4	0 to 12.50	0 to 700	106
379	6	0 to 11.25	0 to 700	91
470	8	0 to 10.0	0 to 700	76
				546 total amount

Measurements are done five times at each point in the experiments. For example, a resulting rotation speed at 2% MC, at 10.0 kg of added mass and at an air pressure input of 500 kPa, is measured five times with the tachometer. Since all the experiments were done twice, this means that this was done at 1092 points (two times the 546 points).

The experimental process steps of the experiments done can be found on the next page as Figure 12. These steps were maintained during the experiments.

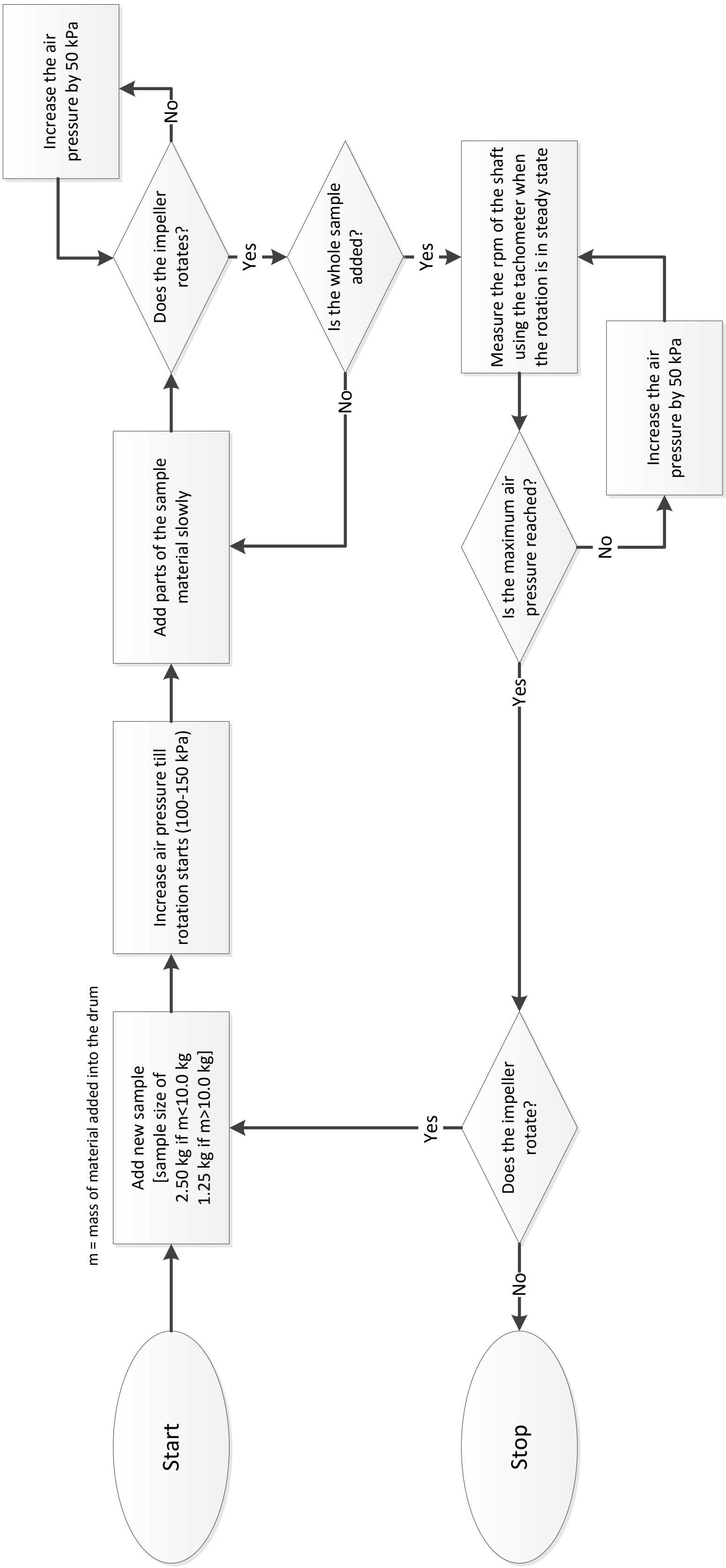

Figure 12. Process flow

Finally after all the steps and work done, the results have to be processed and prepared for analyzation. This is done using Matlab and the results will be shown in the next chapter.

3 Experimental results

In this chapter the results of the experiments for mixing sand with 2%, 4% and 6% will be given. First the raw data will be shown in graphs and in the second subchapter the trendlines which are used for calibration will be shown. The figures in this chapter show the results of the experiments. On the right side, next to the graph, the amount of added sand is written down. This weight of 0 kg up to 16.25 kg is written next to the end of the line and is the corresponding weight of the added sand of that particular line. So as can be seen the rpm of the shaft drops per added material.

3.1 Resulting data for increasing moisture contents

In the following graphs the resulting data is shown for the 0% moisture content experiments. The blue dots and lines corresponds with the results of the first experiment done for that certain moisture content. The red dots and lines correspond with the second time the experiments were done.

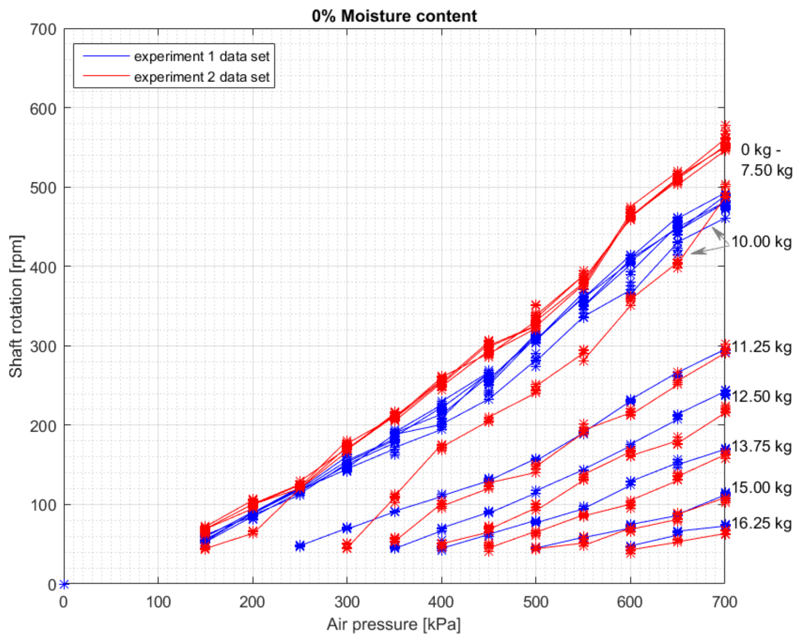

Figure 13. Results for the experiments at 0% moisture content

On the right side of the graph at the end of each line, the corresponding added mass is written. As in all the graphs, the top line is the initial state since it has not any sand added yet. In Figure 13, multiple lines are close to this initial state line. Since there is free rotation for the experiments done up to 7.50 kg, the results are the same as the initial state. This causes that the lines for the added mass of 0, 2.5, 5.0 and 7.5 kg are very close to each other. Therefore, these value of the added sand close to the corresponding lines is written as 0 kg – 7.50 kg. This is again clarified in Figure 14, using a close up of the results.

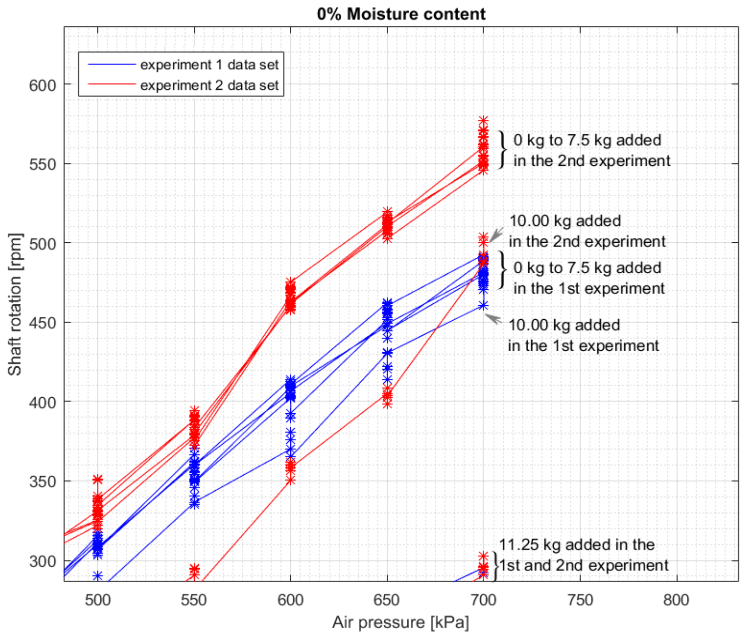

Figure 14. Results with the corresponding amount of added value

In Figure 13. Results for the experiments at 0% moisture content, one line surprises. The second experiment of adding 10.0 kg into the drum has a different slope to the other lines and therefore is not parallel to the other resulting lines. Besides that, the resulting line of the same experiment but done for the first time (the blue line) is parallel to the others and much closer to the initial state lines. Of all of the lines in the results, this one is not like the others. This might have been caused of the unknown difference in loading the sand in the drum.

As can be seen in the resulting graphs, the initial state of the engine can be different for each experiment. In every experiment the initial state has been determined by doing the experiment without any added material. The rpm of the shaft during the initial state of the experiments can have a big variation. This difference in measured rpm increases linear with the increase of the air pressure input and can get up to a difference of 160 rpm at 700 kPa. Therefore, the performance of the pneumatic engine is different every day. In order to prevent fluctuations in the results as much as possible, the whole experiment had to be done at once and continuous, meaning that the experiments were done during one period of one day. This way the fluctuation in initial state of the engine is excluded and the moisture content will not change over that time period.

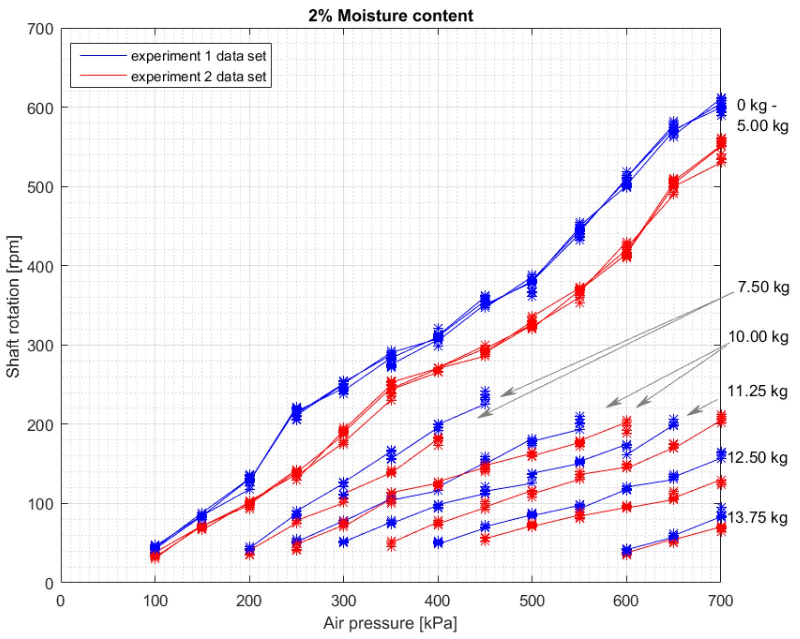

Figure 15. Results for the experiments at 2% moisture content

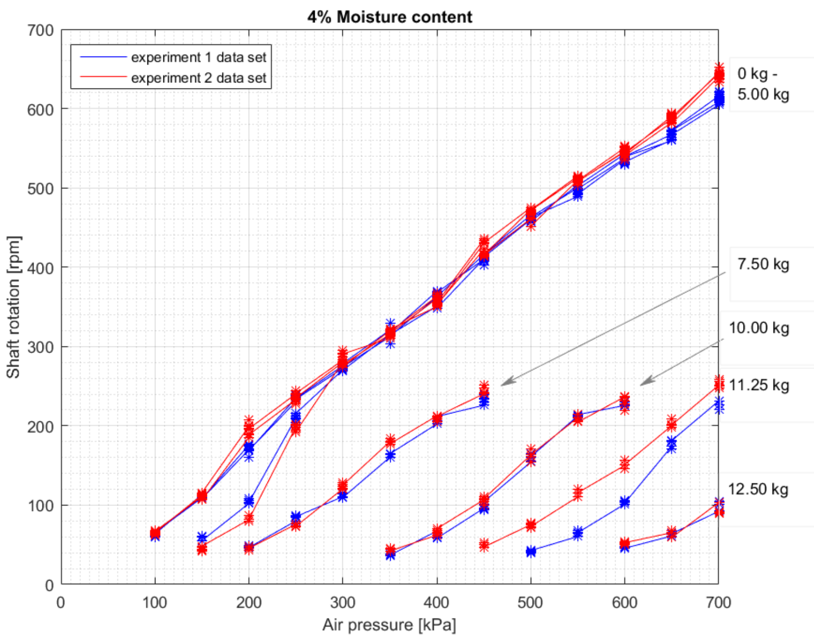

Figure 16. Results for the experiments at 4% moisture content

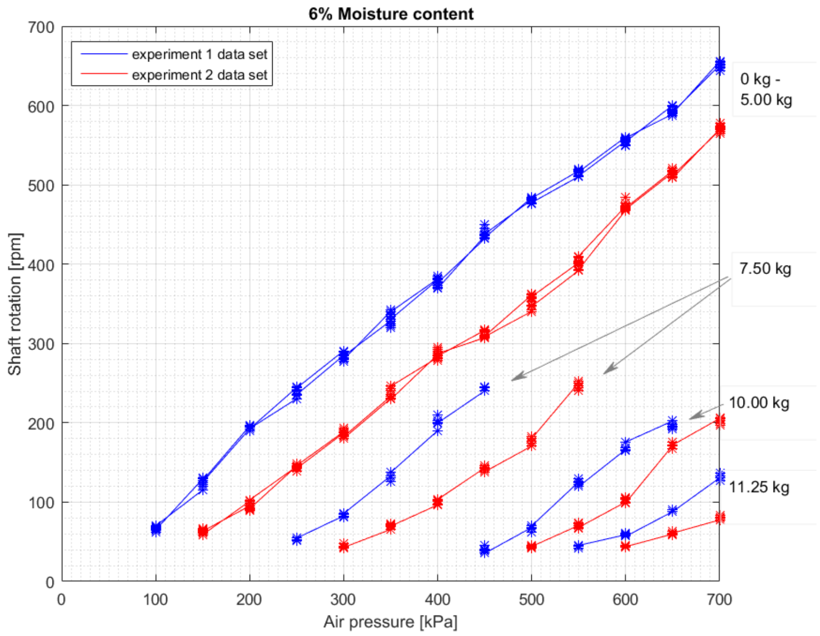

Figure 17. Results for the experiments at 6% moisture content

Something else that can be noticed in the graphs with a level of moisture, is the abrupt stop of some of the results. For example, at the results of the experiments for a moisture content of 6% as in the grey box with the black outline in Figure 18, there is a limited amount of RPM output. At a level between 200 and 300 RPM the rotation will reach a steady state at free rotation of the impeller, like the initial state rotation. When the rpm of the impeller increases as a result of increasing the air pressure, the sand can get the same brighter colour of a 0% moisture content sample. In addition, the brighter sand is moved around easily over the edges like the 0% moisture content sample. It is likely that the sample will decrease in moisture content and will behave like dry sand at that level of rotations. This step in a decrease in moisture content and increase of revolutions up to initial state is shown in the oval in Figure 19, below.

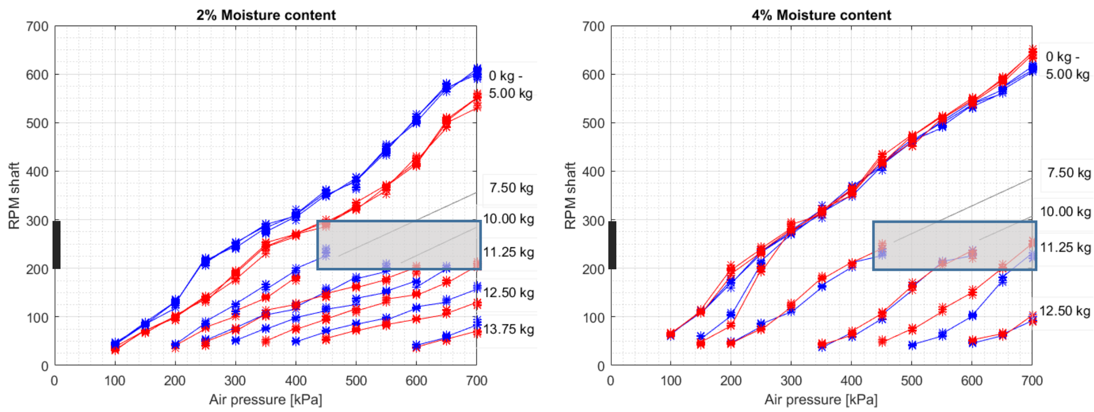

Figure 18. Boxed area where the rotation of the impeller dries the sand for moisture content 2 and 4%

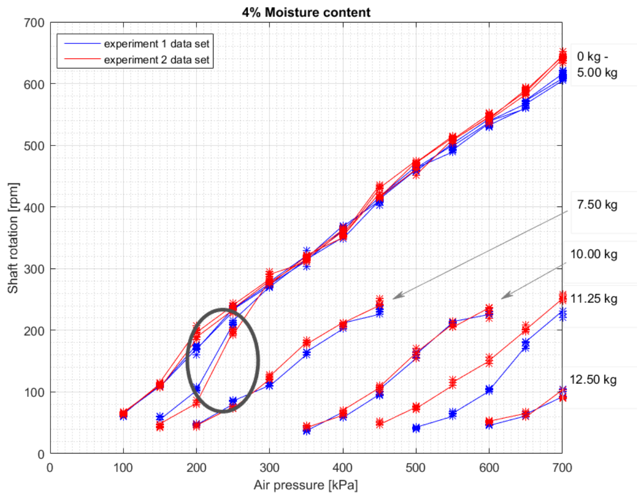

Figure 19. The change from a dropped result to an initial state result

For the moisture content 0, 2, 4 and 6% the results are shown above but not for the experiments with 8% moisture content. The experiments at the highest tested moisture content did not gave a gradient in the results. Either the shaft was rotating in its initial state since there was no contact with the added sand, or the shaft was not moving as a result of the contact with the sand. Therefore, the experiments with 0, 2, 4 and 6 moisture content will be investigated further down this report.

3.2 Trendlines

The linear trendlines of the results are shown in the following figures. These trendlines will be used as the data to calibrate the DEM simulation to. The trendlines for all the experiments have a R-squared value bigger than 0.915. This means that the lines are fitted to the exact data for at least 91.5%. As can be seen in the previous chapter in Figure 11, the trendlines cross all the margin of error. This combined with the R-squared value of at least 0.915 makes the lines usable. Figure 20, Figure 21, Figure 22 and Figure 23 show the resulting trendlines.

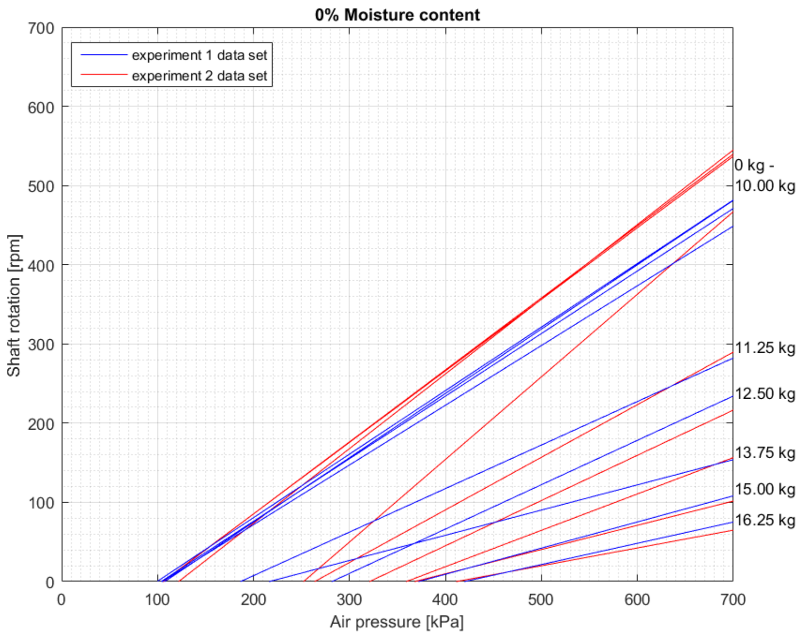

Figure 20. Trendlines for the experiments at 0% moisture content

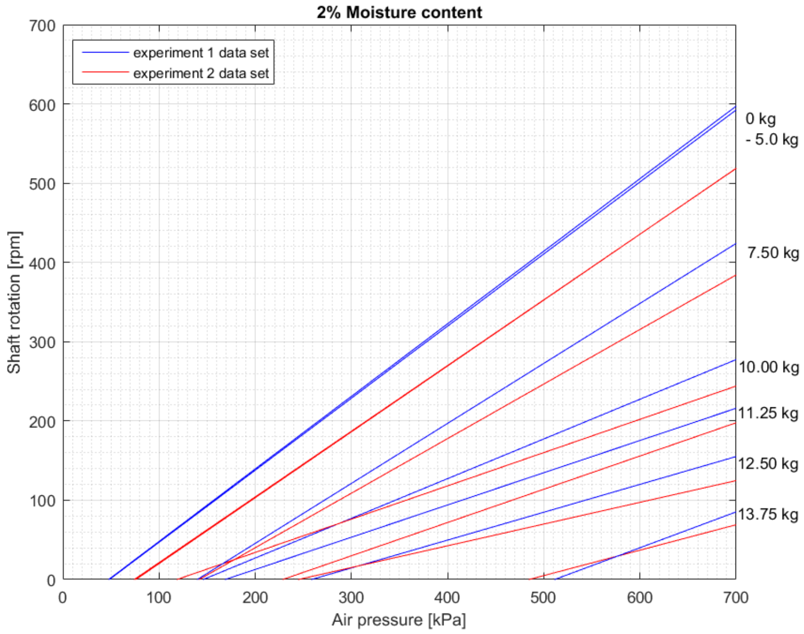

Figure 21. Trendlines for the experiments at 2% moisture content

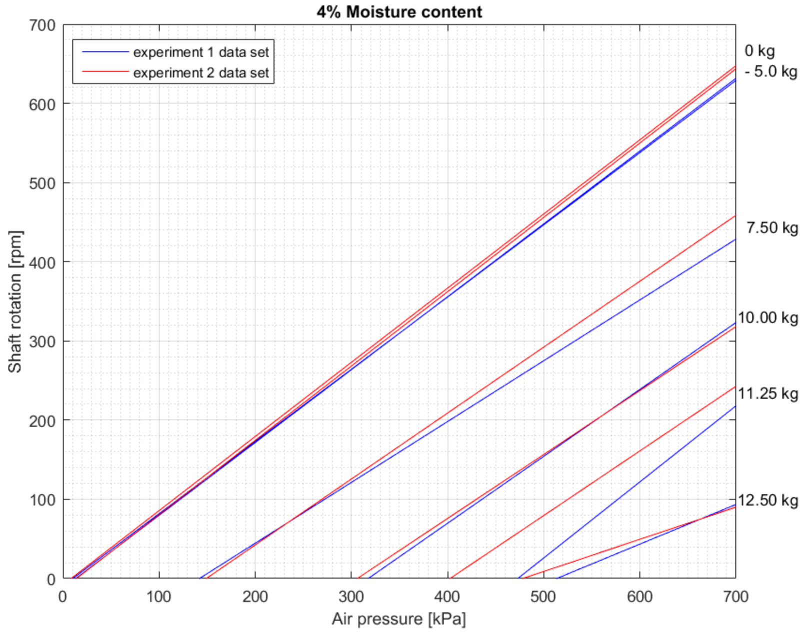

Figure 22. Trendlines for the experiments at 4% moisture content

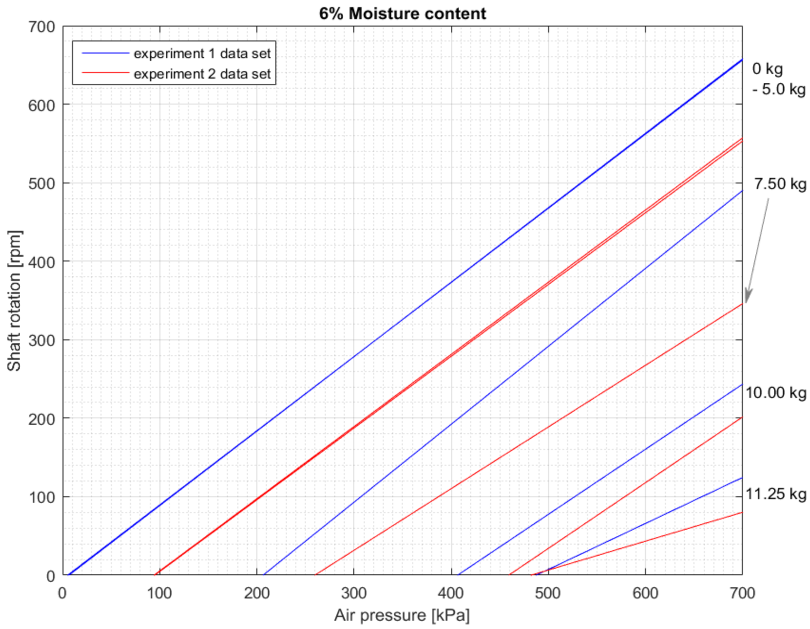

Figure 23. Trendlines for the experiments at 6% moisture content

In the figures above, the logical result of a decrease in rotation of the shaft when more sand is added is shown. Due to the higher shear stress, the engine needs more power per added sample to keep rotating. This decrease in rotation while increasing the moisture content is also shown in Table 4.

Table 4. Rpm per MC% at 700 kPa air pressure input

Added mass [kg]	Rpm 0% Moisture C.	Rpm 2% Moisture C.	Rpm 4% Moisture C.	Rpm 6% Moisture C.
0-5.00	*500*	*550*	*650*	*600*
7.50	*500*	*400*	*650*	*400*
10.00	*500*	*260*	*435*	*225*
11.25	*280*	*200*	*225*	*100*
12.50	*225*	*130*	*100*	-
13.75	*150*	*75*	-	-
15.00	*110*	-	-	-
16.25	*75*	-	-	-
17.50	-	-	-	-

Also, these trendlines show that the amount rotations decreases when the moisture content increases. This is clarified in Figure 24, where the trendlines are shown for the various moisture content at and addition of 11250 and 12500 gram of sand. These amounts of added sand were chosen because they have comparable results for each experiment done.

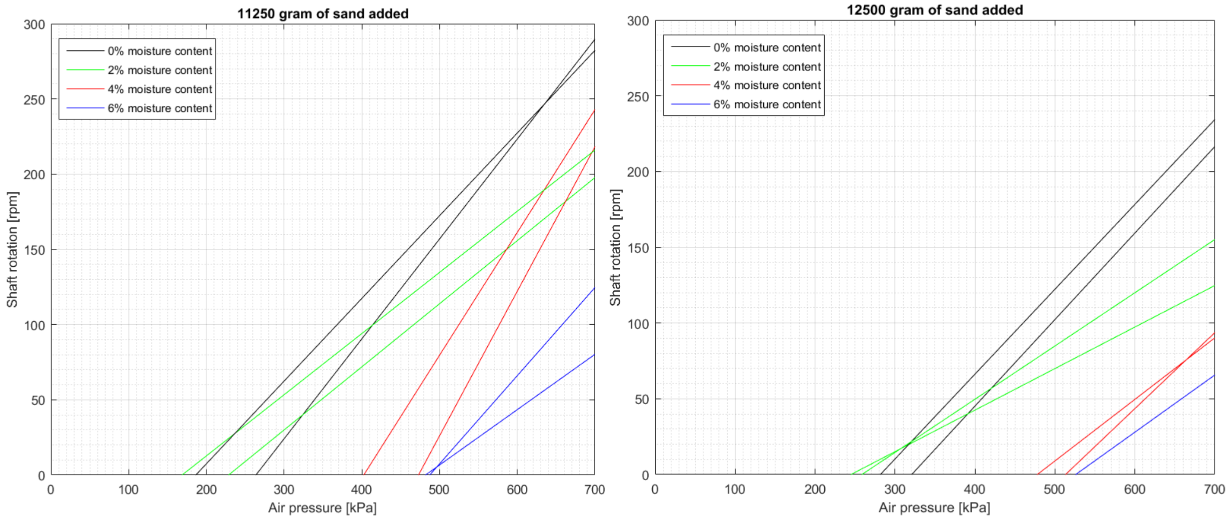

Figure 24. Trendlines for 11250 gram and 12500 gram added sand per moisture content

3.3 Initial state

The trendlines of the initial states of each experiment are compared in Figure 25. A difference in initial state of at least 150 rpm and a difference in slope can be seen.

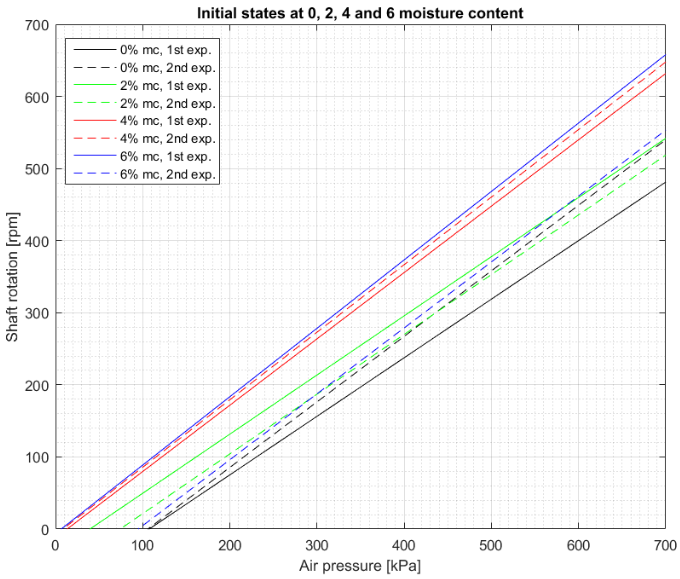

Figure 25. Initial states shown per moisture content

The first experiment of the two 2% moisture content experiments was done at 38 degrees Celsius on January 12th. The second experiment was done at 24 degrees Celsius on the 13th of January. These two experiments have the biggest difference in temperature but not the biggest difference in values for the initial state. So the difference in engine performance due to the difference in temperature cannot be said.

4 DEM coupling

To measure force and impact on the rigid body, in this case the impeller and the shaft, a coupling has to be made to create the interaction between particles and the rigid body during rotation. In the first part of this chapter the DEM software will be introduced. In the second part of the DEM coupling the POEMS software will be explained.

4.1 LAMMPS and LIGGGHTS contact models

The Discrete Element Method software used for this calibration is LAMMPS and LIGGGHTS. LAMMPS stands for Large scale Atomic or Molecular Massively Parallel Simulator. LIGGGHTS stands for LAMMPS Improved for General Granular and Granular Heat Transfer Simulations. As the full name of LIGGGHTS says, it is based on the LAMMPS software. Both open source DEM codes software for numerical simulations of granular systems are used to simulate the behaviour of the used sand in the experiments.

To make the simulation useful contact models need to be attached to them in order to react like the real world environment in term of for example angular velocity and torque. A number of particle-particle and particle-wall models are used in this simulation. These contact models [1] compute the resulting torque and forces of the particle-mesh element and particle-particle interaction. Since a granular material is used in this research, a simulation of a granular model is built. For the use of a granular model there are a couple of contact models needed. In the script the following input is used.

```
pair_style gran model hertz tangential history cohesion sjkr2 rolling_friction epsd2
```

Model value
Main contact model for determining reaction by compression or overlap of the particles is the Hertz model. The determination of the friction force in particle-particle contact is done by using the following formula. This is only applicable when the particles are in contact with each other.

$$F = (k_n \cdot \delta n_{ij} - \gamma_n \cdot vn_{ij}) + (k_t \cdot \delta t_{ij} - \gamma_t \cdot vt_{ij}) \tag{1}$$

The left side after the equal sign in the first equation is the normal force. Within that normal force, k_n is the elastic constant for normal contact, δn_{ij} is the normal overlap (the spring force) and vn_{ij} is the normal relative velocity (the damping force).

$$k_n = \frac{4}{3} \cdot Y^* \cdot \sqrt{R^* \cdot \delta_n} \tag{2}$$

$$\gamma_n = -2\sqrt{\frac{5}{6}} \cdot \beta \cdot \sqrt{S_n \cdot m^*} \tag{3}$$

$$S_n = 2 \cdot Y^* \cdot \sqrt{R^* \cdot \delta_n} \tag{4}$$

$$\beta = \frac{\ln(e)}{\sqrt{ln^2(e) + \pi^2}} \tag{5}$$

$$\frac{1}{Y^*} = \frac{(1 - v_1^2)}{Y_1} + \frac{(1 - v_2^2)}{Y_2} \tag{6}$$

$$\frac{1}{R^*} = \frac{1}{R_1} + \frac{1}{R_2} \tag{7}$$

$$\frac{1}{m^*} = \frac{1}{m_1} + \frac{1}{m_2} \tag{8}$$

With e as the coefficient of restitution, v as the Poisson ratio, Y as the Young's modulus.
The part between the right brackets of the friction force formula (1) shows the tangential force. This tangential force has the same components as the normal force but for the tangential side.

The tangential part of the granular model has a spring part involved. This will take care of the tangential displacement when particles have a tangential overlap. Added to this tangential value is the history. The history will take the duration of the contact of the two particles into account and is a product of the relative tangential velocity times the size of the time step.

$$k_t = 8 \cdot G^* \cdot \sqrt{R^* \cdot \delta_t} \tag{9}$$

$$\gamma_t = -2\sqrt{\frac{5}{6}} \cdot \beta \cdot \sqrt{S_t \cdot m^*} \tag{10}$$

$$S_t = 8 \cdot G^* \cdot \sqrt{R^* \cdot \delta_t} \tag{11}$$

$$\frac{1}{G^*} = \frac{2(2-v_1)(1+v_1)}{Y_1} + \frac{2(2-v_2)(1+v_2)}{Y_2} \tag{12}$$

With G as the shear modulus.

Cohesion value
During the simulations the sjkr2 cohesion contact model is used. This is a contact model based on the Johnson-Kendall-Roberts model. In this simplified contact model there is a normal force added to provide the cohesion of the material. To following force is added to realise the so called cohesion force.

$$F_2 = k_{ced} \cdot A \tag{13}$$

Now k is known as the cohesion energy density in J/m^3 and A is the contact area of the two particles, determined as followed.

$$A = 2 \cdot \pi \cdot \delta_n \cdot (2R) \tag{14}$$

Rolling friction value
For the rolling friction is the EPSD2 (elastic-plastic spring-dashpot) used [1]. This is a rolling friction contact model based on the EPSD but knows a difference in the rolling stiffness and in the viscous damping torque. The rolling stiffness k_r is in the EPSD contact model defined as

$$k_r = 2.25 \cdot k_n \cdot \mu_r^2 \cdot R^{*2} \tag{15}$$

In the EPSD2 the contact model if defined as

$$k_r = k_t \cdot R^{*2} \tag{16}$$

With k_t as the tangential stiffness and R^* is the effective radius. The other change comparing both rolling friction contact models is the viscous damping torque. In the EPSD2 this M_r^d is not taken into account. So the torque will only will be depended by the spring torque M_r^k, known as

$$M_r^k = -k_r \cdot \theta_r \tag{17}$$

With θ_r as the relative rotation between two particles.
These contact models were used in the simulation to implement the moisture content and so the cohesion is involved in the system.

4.2 POEMS

For the implementation of the rigid body dynamics to determine the output of the system, the use of POEMS is introduced. POEMS stand for Parallelizable Open Source Efficient Multibody Software. At the Rensselaer Polytechnic Institute this software package was developed by Prof Kurt Anderson et al. and Rundranarayan Mukherjee created the interface for LAMMPS and POEMS [2]. In this application the set of spheres created are treated like one rigid body. Like in DEM, at every time step the properties are computed and updated. This software package computes the torque and force on the equipment each time step. Then the location and properties are updated so the spheres representing the equipment moves as a whole piece. The coupling, associated motion constraints, and time integration is performed by POEMS computes the constrained rigid-body motion of articulated multibody systems [3].

More information about the interface and coupling of LAMMPS and POEMS can be found in the paper ‘Substructured molecular dynamics using multibody dynamics algorithms’ [4]

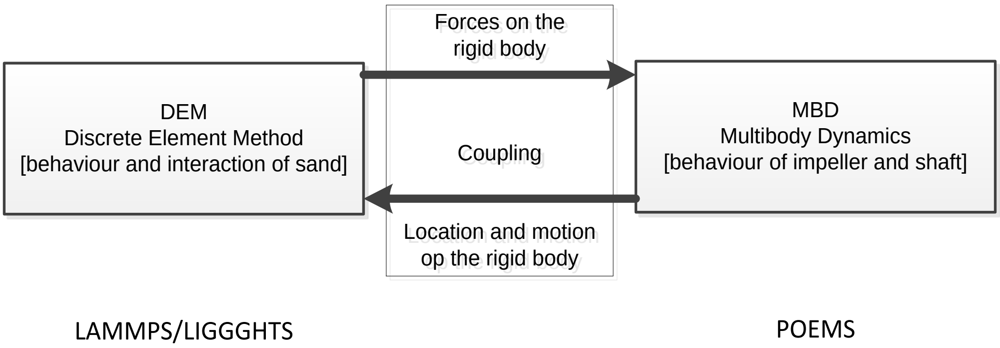

Figure 26. Coupling DEM with POEMS

Using POEMS, the impeller can be coupled as a rigid body. As can be seen in the next figures, the impeller is simulated as it is made out of particles. The contact with the sand will now be simulated as particle-particle interaction.

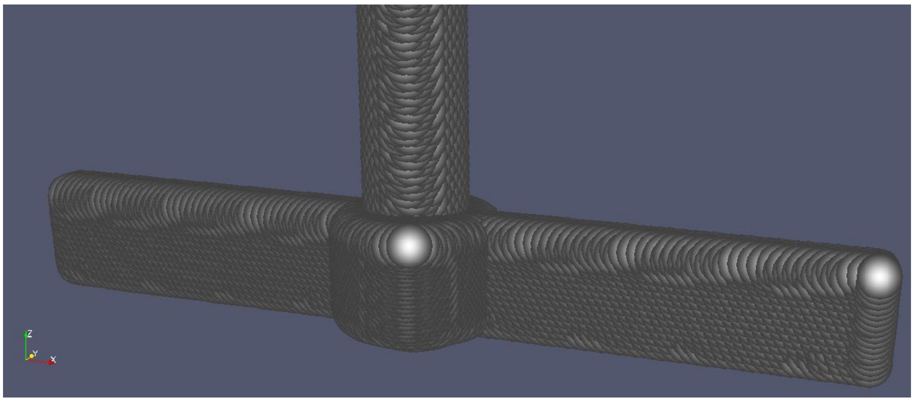

Figure 27. Impeller simulated as spheres

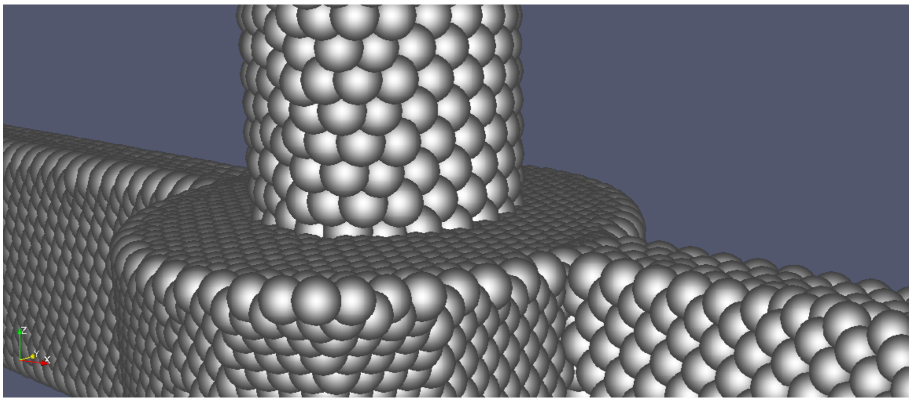

Figure 28. Rigid body formation of the impeller using spheres

4.3 Parameters

The particle to particle contact and particle to equipment contact knows several parameters which has influence on the behaviour. When particles collide the output motion of the particles will be computed using the given parameters. This configuration of parameters has to be fitted to the experimental results in order to create a good calibration. The used parameters used in the simulation are as followed:

```
# Variables - Timestep & Dumpstep
variable dt           equal  5e-6         # Time step
variable factor       equal  1/${dt}      # Steps per second
variable dumpstep     equal  0.01*${factor} # save results every dumpstep

# Variable - Particle size distribution
variable r1 equal 0.003      # d=10mm
variable r2 equal 0.003      # d=12mm
variable r3 equal 0.003      # d=14mm
variable r4 equal 0.003      # d=18mm
variable r5 equal 0.003      # d=20mm

variable frac1 equal 0.2     # particle size fractions
variable frac2 equal 0.2
variable frac3 equal 0.2
variable frac4 equal 0.2
variable frac5 equal 0.2
variable cutoff equal 2*${r1}

# Variables - Particle and wall properties
variable cor          equal  0.3    # coefficient of restitution
variable dens         equal  2700   # Particle density (bulk density * porosity)
variable poiss        equal  0.3    # Poissons ratio
variable youngmod     equal  1e7    # Young modulus
variable youngmod_steel equal 1e7   # Young modulus
variable ff           equal  0.5    # Particle particle friction
variable wf           equal  0.4    # Particle wall friction
variable rf           equal  0.1    # Rolling friction
variable CED          equal  0.     # Coh.Energy Density
variable AED          equal  0.     # Adh.Energy Density
# Variables - Mass flow rate
variable m       equal 10           # Mass [kg] of particles to be generated
variable tfill   equal 2            # Time for generating particles [s]
variable Q       equal ${m}/${tfill} # Mass flow rate for generating particles
```

All the DEM parameters for the medium grained sand are known from previous research at TUNRA Bulk Solids. The parameter of the above list with difference values during the simulations for the different moisture contents is the Cohesive Energy Density.

5 Modelling results

First the initial state of the results will be calibrated. After the calibration of the initial state the rpm drop at different moisture content can be calibrated. Three points per calibration will be used each time.

5.1 The DEM-Rigid body model

The general computational process of the DEM-Rigid body modelling was demonstrated in Figure 29. General computational process of the DEM-Rigid body modellingFigure 29. The calibration process was illustrated in Figure 32Figure 29. When no material was present in the experimental drum, a rotational motion at a fixed angular velocity was applied to the impeller rigid body. During the rotation of the impeller, the stress experienced by the spheres forming the impeller was exported to a VTK file at the pre-defined time step. A Python script was then designed to extract the stress list on all the spheres in the impeller, after which the stress profile applied on the impeller from previous time step was introduced to the current computation. The net stress to be applied on the impeller was then calculated and applied to the impeller so the impeller would rotate at a new angular velocity.

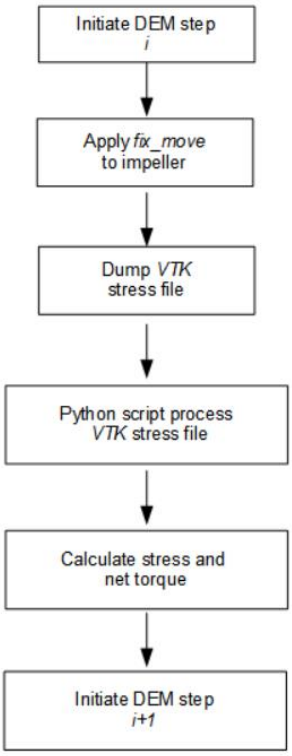

Figure 29. General computational process of the DEM-Rigid body modelling

The first phase of the DEM-Rigid body modelling was to calibrate the rotation of the impeller to the experimental condition. This calibration will be a one-point calibration since all the parameters already have been calibrated values for the use of DEM in LIGGGHTS by TUNRA Bulk Solids. Therefore, only the applied energy will change of value and when the moisture content will be increased the cohesion energy density (CED) will be changed as well.
The first step for calibration is to calibrate the initial state. This initial state as can be seen in the experimental results is the line of free rotation of the shaft and impeller. A *fix_move* command was used to apply the rotational motion to the impeller. This command performs updates of position and velocity for atoms in the group each time step using the specified settings or formulas, without regard to forces on the atoms. This can be useful for boundary or other atoms, whose movement can influence nearby atoms.

The input format of this command is

- `fix ID group-ID move style args keyword values`
- `rotate args = Px Py Pz Rx Ry Rz period`
- `Px,Py,Pz = origin point of axis of rotation (distance units)`
- `Rx,Ry,Rz = axis of rotation vector`
- `period = period of rotation (time units)`

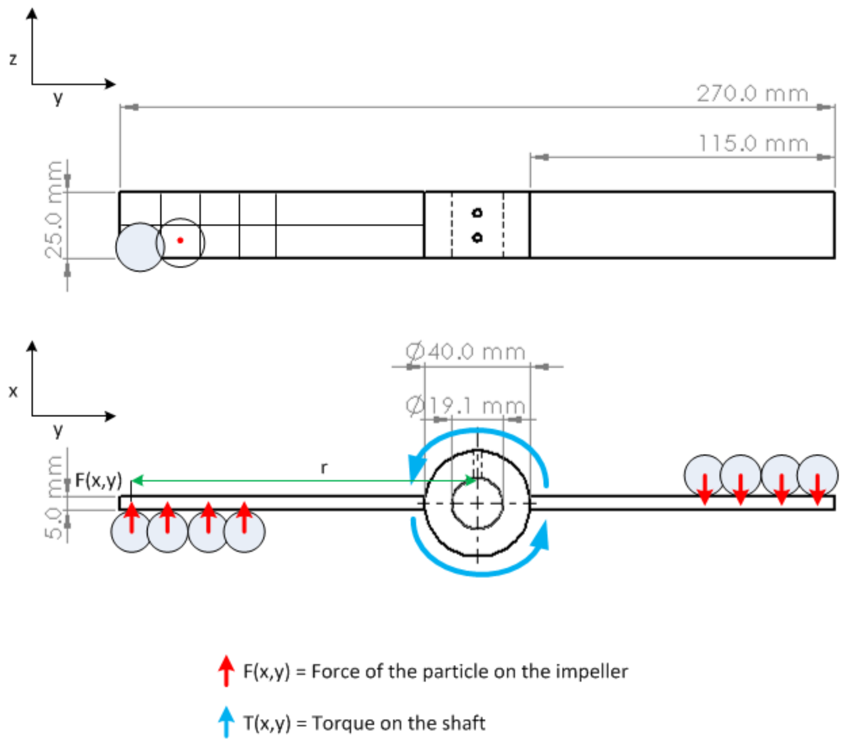

Figure 30. Particles and impeller interaction resulting in torque

The resulting torque on the shaft as a rigid body is shown in Figure 30 and is as followed:

$$T_{(x,y)} = F_{(x,y)} \cdot r_{(x,y)} \tag{18}$$

$$T_{tot.resistance} = \sum_{x=1,y=1}^{n} T_{(x,y)} \tag{19}$$

$$T_{result} = T_{applied} - T_{tot.resistance} \tag{20}$$

The $T_{(x,y)}$ is a product of the normal force $F_{(x,y)}$ of the particles on the mesh, in this case the impeller particles, and the distance of that point of contact to the centre of the shaft $r_{(x,y)}$. The total resistance on the shaft $T_{tot.resistance}$ is the sum of all these individual torques $T_{(x,y)}$. The difference in the applied torque on the shaft $T_{applied}$ and the total resistance torque $T_{tot.resistance}$ will give a resulting torque T_{result}. This resulting torque will be compared to the output torque or resulting rpm. A difference in output and input will cause a change in the input energy, known as $T_{applied}$. This way the right amount of $T_{applied}$ results in the right amount of rpm output.

For the calibration of the initial state a factor on the applied force on the shaft is introduced. This factor is a correction on the simulation to generate the experimental results. This calibration for the initial state is done at 300 kPa, 400 kPa and finally at 500 kPa. Each point has a different applied rotational velocity as specified in the unit of period of rotation to realise the experimental steady state values. Figure 31 shows the period of rotation for the three different point during the calibration of the initial state.

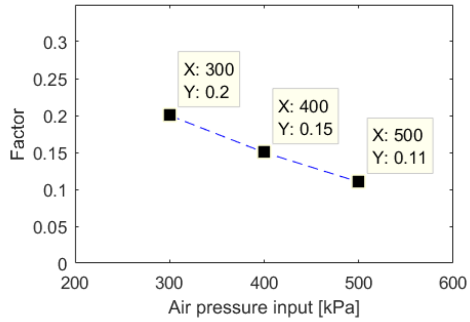

Figure 31. Period of rotation for initial state calibration

Now that the calibration for the initial state has been done, the first calibration for the first experiments can be done. This will be investigated in the next subchapters.

5.2 RPM drop 0% MC adding 10.0 kg

One of the initial simulations is shown in Figure 32. This is a screenshot of the simulation for the initial state calibration of 0% moisture content adding 10.0 kg into the drum.

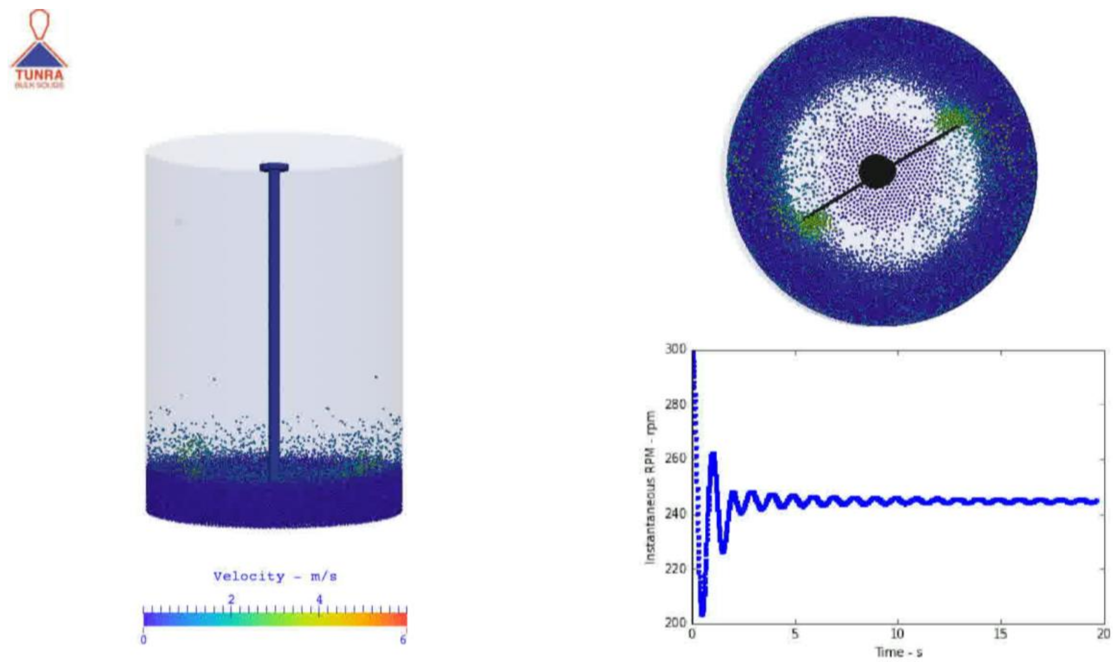

Figure 32. Screenshot simulation initial state 0%MC, 10.0 kg, 300 rpm

In the right bottom corner of the graph in Figure 32 the rpm of the shaft is shown. The initial state, at the begin of the simulation when no material is added. The energy added to the shaft and so impeller, results in an initial rpm of 300 rpm for 0% moisture content. A fluctuation appears in the rpm of the shaft in the following seconds, with a steady state to approximately to 245 rpm. Both simulations for the initial state and the rpm drop can be seen in Figure 33. As expected, the results show a drop in rpm due to adding the material. Comparing this drop of steady state about 55 rpm to the experimental results as in **Error! Reference source not found.**, a similar drop can be seen.

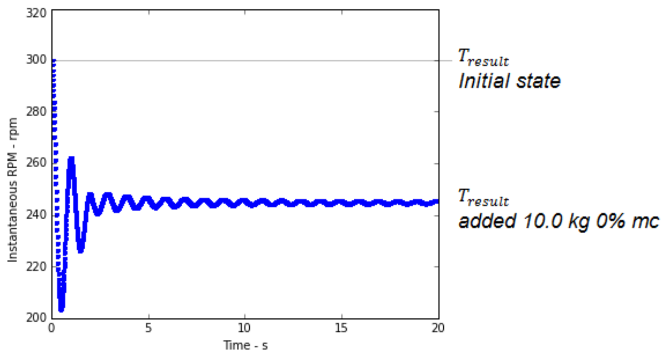

Figure 33. Rpm drop in the steady states at 10.0 kg 0% mc

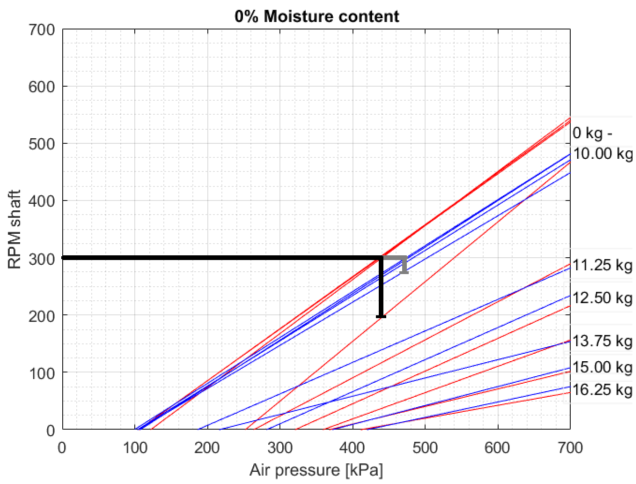

Figure 34. The rpm drop on the trendlines at 300 rpm

The rpm drops for experiment data set 1 (blue) and data set 2 (red) have a remarkable difference. Data set 1 has a drop about 80 rpm and data set 2 a drop of 35 rpm. This gives an average of 57.5 rpm in rotation decrease when 10.0 kg of dry sand is added. For the trendlines the differences in data set 1 the rpm drop is 100 rpm and for the second data set it is about 50 rpm. The average rpm drop using the trendlines is 75 rpm. Since the situation of adding 10.0 kg in the drum with 0% moisture content knows a big difference in the two data sets, this point of calibration is a difficult one to realise. Further results of the calibration using the values of the period of rotation will show if these are correct and useful.

5.3 Modelling 0% moisture content

For the 0% moisture content, the average modelling results generated, the average experiment results and the difference between both are shown in Table 5. These results are compared with the experimental results in Figure 35.

Table 5. Results for 0% moisture content at 0.20, 0.15 and 0.11 period of rotation

Moisture content	***0%***			
Period of rotation	*0.20 (300 kPa)*			
Mass [kg]	*0*	*10.0*	*12.5*	*15.0*
Steady state model [rpm]	*198*	*167*	*0*	*0*
Steady state exp. [rpm]	*166*	*99*	*0*	*0*
Difference [rpm]	*32*	*68*	*0*	*0*
Period of rotation	*0.15 (400 kPa)*			
Mass [kg]	*0*	*10.0*	*12.5*	*15.0*
Steady state model [rpm]	*289*	*228*	*46*	*0*
Steady state exp. [rpm]	*252*	*191*	*56*	*8*
Difference [rpm]	*37*	*37*	*10*	*8*
Period of rotation	*0.11 (500 kPa)*			
Mass [kg]	*0*	*10.0*	*12.5*	*15.0*
Steady state model [rpm]	*377*	*309*	*91*	*23*
Steady state exp. [rpm]	*338*	*278*	*112*	*41*
Difference [rpm]	*39*	*31*	*-21*	*-18*

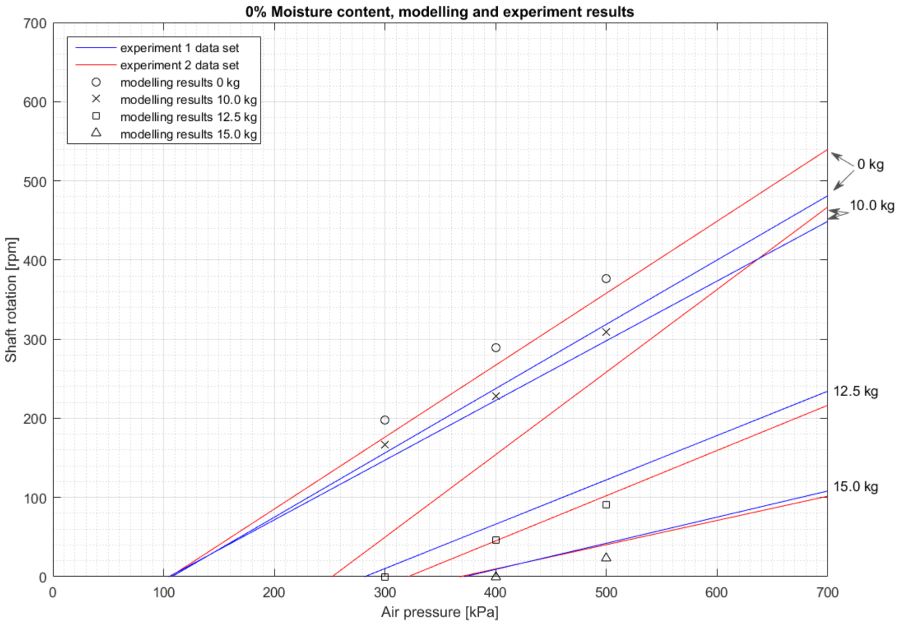

Figure 35. Comparing modelling and experiment results for 0% moisture content

5.4 Modelling 2% moisture content

Table 6 includes the generated average modelling results, the average experiment results and the difference between both for the 2% moisture content. These results are compared with the experimental results in Figure 36.

Table 6. Results for 2% moisture content at 0.20, 0.15 and 0.11 period of rotation

Moisture content	***2%***			
Period of rotation	*0.20 (300 kPa)*			
Mass [kg]	*0*	*7.5*	*10.0*	*12.5*
Steady state model [rpm]	*198*	*101*	*76*	*0*
Steady state exp. [rpm]	*209*	*115*	*77*	*15*
Difference [rpm]	*-11*	*-14*	*-1*	*-15*
Period of rotation	*0.15 (400 kPa)*			
Mass [kg]	*0*	*7.5*	*10.0*	*12.5*
Steady state model [rpm]	*289*	*187*	*117*	*65*
Steady state exp. [rpm]	*296*	*187*	*123*	*46*
Difference [rpm]	*-7*	*0*	*-6*	*19*
Period of rotation	*0.11 (500 kPa)*			
Mass [kg]	*0*	*7.5*	*10.0*	*12.5*
Steady state model [rpm]	*377*	*275*	*181*	*78*
Steady state exp. [rpm]	*384*	*260*	*169*	*77*
Difference [rpm]	*-7*	*15*	*12*	*1*

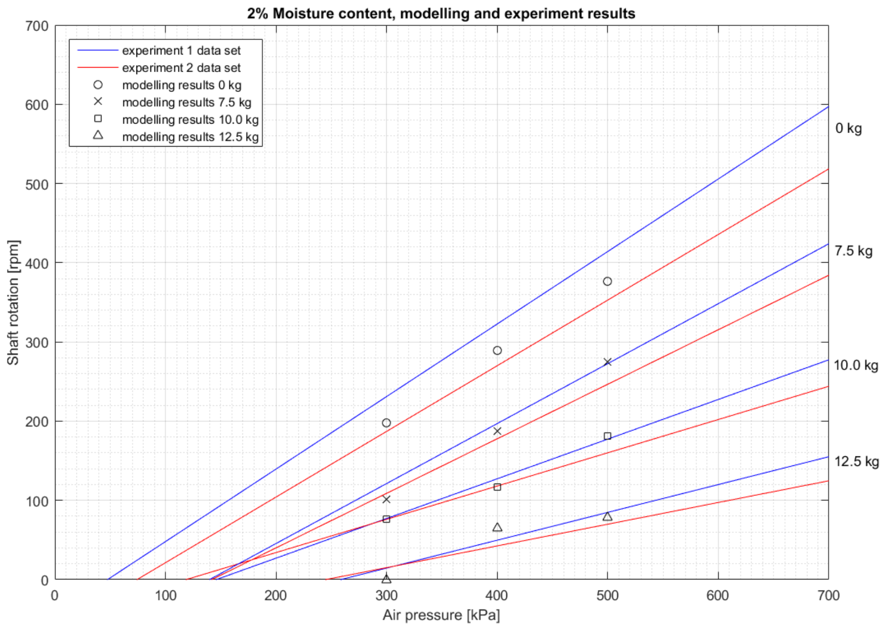

Figure 36. Comparing modelling and experiment results for 2% moisture content

5.5 Modelling 4% moisture content

The average modelling results generated for the 4% moisture content, the average experiment results and the difference between both are shown in Table 7. These results are compared with the experimental results in Figure 37.

Table 7. Results for 4% moisture content at 0.20, 0.15 and 0.11 period of rotation

Moisture content	***4%***			
Period of rotation	*0.20 (300 kPa)*			
Mass [kg]	*0*	*7.5*	*10.0*	*12.5*
Steady state model [rpm]	*198*	*101*	*0*	*0*
Steady state exp. [rpm]	*268*	*124*	*0*	*0*
Difference [rpm]	*-70*	*-23*	*0*	*0*
Period of rotation	*0.15 (400 kPa)*			
Mass [kg]	*0*	*7.5*	*10.0*	*12.5*
Steady state model [rpm]	*289*	*178*	*53*	*0*
Steady state exp. [rpm]	*361*	*204*	*73*	*0*
Difference [rpm]	*-72*	*-26*	*-20*	*0*
Period of rotation	*0.11 (500 kPa)*			
Mass [kg]	*0*	*7.5*	*10.0*	*12.5*
Steady state model [rpm]	*377*	*287*	*128*	*0*
Steady state exp. [rpm]	*454*	*283*	*155*	*0*
Difference [rpm]	*-77*	*-4*	*-27*	*0*

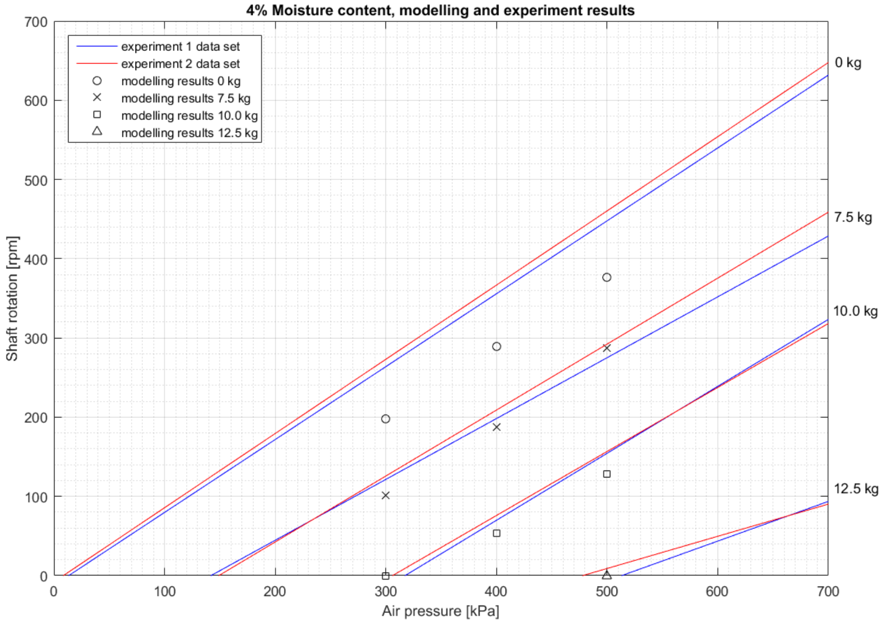

Figure 37. Comparing modelling and experiment results for 4% moisture content

5.6 Results

The period of rotations used at the calibration in combination with the change of CED per moisture content give the results as shown above. The configuration for the certain points are as shown in Table 8. The difference in rpm between the experiments and the simulations increases more while increasing the moisture content. This is shown in the tables at the corresponding moisture content as the difference between the modelled result and the experiment result. The points have a small under prediction but the lines of the modelled results have a similar slope to their corresponding experiment results. The period of rotation is independent of the moisture content and only set according to the different air pressure.

Table 8. Modelling configuration per point

Moisture content [%]	CED [J/m^3]
0	*0*
2	*5000*
4	*9000*

Air pressure [kPa]	Period of rotation
300	*0.22*
400	*0.15*
500	*0.11*

6 Conclusion and recommendations

During the simulation a parameter called the period of rotation must be added and set to the configuration corresponding with the energy input. In this assignment and setup, using a pneumatic engine to rotate medium grained sized sand with an impeller with 5.750 mm^2 surface area moving the sand, values of the period of rotation are 0.20, 0.15 and 0.11 respectively to 300, 400 and 500 kPa. The moisture content is only adjusted by the change in cohesion of density.

As can be seen the DEM model under predicts the revolutions per minute to the experiments when the moisture content increases. This happens also at the points of the initial state, when 0.0 kg of the medium grained sand has been added. This under prediction of the model could be explained by the fact that the cohesion model applies the cohesion to the material homogeneously, where in reality the cohesion force is not fully homogeneous in the system but heterogeneously. This is also in line with the resulting increase of difference between the model and the experiment results, when increasing the moisture content. As said in chapter 2.3, the preparation of the sample is done by mixing the sand and the water by hand. By measuring the moisture content during or after the experiments and to make sure of using a homogenous mixture, the level of moisture content and the distribution of the moist through the mixture could be maintained better.

Other recommendations on this work and further work start at the setup of the experiments. Resources will be always limited but there are some recommendations on the setup and the process steps.

To limit the fluctuation in engine performance, the use of a pneumatic engine with a steady performance or an electric engine is recommended. This can have less fluctuation in initial state and in the other steady states as a result. This can cause more comparable results with for example, less difference in slopes.
Another recommendation on the setup is the use of a digital energy input regulator. The used analogue air pressure input regulator causes a 25 kPa margin of error. When this margin of error could be limited, the position and the slope of results and so trendlines could be more accurate. Also experiments could be done in a temperature constant environment to neglect the influence of temperature, although the biggest difference in temperature does not cause the biggest difference in initial state values.

A recommendation on the process steps is about the material input flow. This time the material was added slowly by hand. This way of filling the drum could have caused a difference in the sand orientation in the drum and in the end the difference in measured output RPM. This is one non consistent factor in the filling process. A steady input flow like a chute and a steady input by using a small conveyor could prevent this to happen.
The data sets for each moisture content experiments know a difference in initial state and so a difference in further measurements. This fluctuation in initial state can be, like in the case of the 6% moisture content, as big as around 150 RPM. This of course has influence on the calibration as the simulation values must be compared to data values in a bigger range. More experiments should be done to get more results and so, to know more about the accuracy and precision of the current and further results and the interrelated relation between the trendlines. Especially the behaviour of the 10.0 kg at dry sand needs further inspection on its behaviour.

During the calibration, an interesting thing that could be seen is the line of the period of rotation. This line is the result of the values of the period of rotations at the 300 kPa, 400 kPa and 500 kPa points. The thing here is that the values of these points of calibration do not make a linear line. Interesting to know if this line really is linear over multiple point or if there is an asymptotic line. Further investigation on the calibration of the results at for example 600 kPa and more points can be useful.

References

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Appendix: in_file

```
#variable NTHREADS equal 8
#package omp ${NTHREADS} force/neigh thread-binding verbose                        # Openmp threading

# Variables - general
variable pi        equal    3.141592654       # PI
variable a         equal    1                          # Test number

# Variables - Timestep & Dumpstep
variable dt          equal    5e-6              # Time step
variable factor      equal    1/${dt}                    # Steps per second
variable dumpstep equal  0.01*${factor}                  # save results every dumpstep


# Variable - Particle size distribution
variable r1 equal 0.003     # d=10mm
variable r2 equal 0.003     # d=12mm
variable r3 equal 0.003     # d=14mm
variable r4 equal 0.003     # d=18mm
variable r5 equal 0.003     # d=20mm

variable frac1 equal 0.2    # particle size fractions
variable frac2 equal 0.2
variable frac3 equal 0.2
variable frac4 equal 0.2
variable frac5 equal 0.2

variable cutoff equal 2*${r1}


# Variables - Particle and wall properties
variable cor         equal  0.3      # coefficient of restitution
variable dens        equal  2700     # Particle density (bulk density * porosity)
variable poiss       equal  0.3      # Poissons ratio
variable youngmod equal 1e7                   # Young modulus
variable youngmod_steel equal 1e7             # Young modulus
variable ff                 equal 0.5# Particle particle friction
variable wf                 equal 0.4# Particle wall friction
variable rf                 equal 0.1# Rolling friction
variable CED                equal 0.  # Coh.Energy Density
variable AED                equal 0.  # Adh.Energy Density
# Variables - Mass flow rate
variable m           equal 10           # Mass [kg] of particles to be generated
variable tfill       equal 2    # Time for generating particles [s]
variable Q           equal ${m}/${tfill} # Mass flow rate for generating particles

# Variables - Definition of times (points when simulation behaviour changes)
variable t1       equal   ${tfill}       # [s] until filling of the hopper should be finished
variable t2       equal   0.5              # [s] until material should settle in the top box
variable t3       equal   20       # [s] start rotating

variable steps1   equal   ${t1}*${factor}    # calculation step number to reach a certain time
variable steps2   equal   ${t2}*${factor}
variable steps3   equal   ${t3}*${factor}

######################################################################################################################
#########################

# General setting
atom_style         granular            # Granular style for LIGGGHTS

atom_modify        map array           # The map keyword determines how atom ID lookup is done for molecular
problems.
                                          # When the array value is used, each processor stores a lookup table of
length N,
                                          # where N is the total # of atoms in the system. This is the fastest
method for most simulations,
                                          # but a processor can run out of memory to store the table for very large
simulations.

boundary  f f f                 # Boundary definition in x y z (f=fixed bound., particles will be deleted,
                                          #                                m=modified bound., boundaries will be
extended,
                                          #                                p=periodic bound.)

newton             off                 # This command turns Newton's 3rd law on or off for pairwise and bonded
interactions.

communicate        single vel yes         # This command sets the style of inter-processor communication that occurs
each timestep as atom coordinates
                                          # and other properties are exchanged between neighboring processors and
stored as properties of ghost atoms.
```

```
units             si                       # [s] [m] [kg] [N]

read_restart      restart.restart
region            reg block -0.3 0.3 -0.3 0.3 -0.02 1 units box   # Defines rectangular boundaries in x y z [m]
#create_box       2 reg  # Numbers of atome (particle / wall) types
# type 1: inserted particles
# type 2: impeller rigid body
# type 3: walls

neighbor ${cutoff} bin      # Defines parameter for contact searching
neigh_modify      delay 0

# Material properties required for new pair styles
fix               m1 all property/global youngsModulus peratomtype ${youngmod}  ${youngmod}
fix               m2 all property/global poissonsRatio peratomtype ${poiss} ${poiss}
fix               m3 all property/global coefficientRestitution peratomtypepair 2 ${cor} ${cor}&
                                                                                              ${cor} ${cor}
fix               m4 all property/global coefficientFriction peratomtypepair 2 ${ff} ${wf}&
                                                                                          ${wf} ${ff}
fix               m5 all property/global coefficientRollingFriction peratomtypepair 2 ${rf} ${rf}&
                                                                                                ${rf} ${rf}
fix               m6 all property/global cohesionEnergyDensity peratomtypepair 2 ${CED} 0&
                                                                                                0 0
#fix              m7 all property/global k_finnie peratomtypepair 2 1.0 1.0 1.0 1.0  # for wear analysis


# New pair style
pair_style gran model hertz tangential history cohesion sjkr2 rolling_friction epsd2 # Defining contact models
options:
                                                                                 # rolling_friction typeA cohesion
sjkr
pair_coeff        * *

# Set time step = always constant
timestep ${dt}

# Set gravity
fix               gravi all gravity 9.81 vector 0.0 0.0 -1.0

# Load Balancing Setting
partitioner_style     zoltan OBJ_WEIGHT_DIM 1

# Define granular walls
fix               drum all mesh/surface file CAD/drum.stl type 2
fix               impeller all mesh/surface/stress file CAD/impeller_body.stl type 2 stress on reference_point 0 0 0
fix               ins_mesh1 all mesh/surface/planar file CAD/gen_new.stl type 2 move -0.2 -0.2 0
fix               wall all wall/gran model hertz tangential history cohesion sjkr2 rolling_friction epsd2 mesh
n_meshes 2 meshes & drum impeller

# particle insertion
# distributions for insertion
fix               pts1 all particletemplate/sphere 1 atom_type 1 density constant ${dens} radius constant ${r1}
fix               pts2 all particletemplate/sphere 1 atom_type 1 density constant ${dens} radius constant ${r2}
fix               pts3 all particletemplate/sphere 1 atom_type 1 density constant ${dens} radius constant ${r3}
fix               pts4 all particletemplate/sphere 1 atom_type 1 density constant ${dens} radius constant ${r4}
fix               pts5 all particletemplate/sphere 1 atom_type 1 density constant ${dens} radius constant ${r5}

# Definition of particle fractions
fix               pdd1 all particledistribution/discrete 1.  5 pts1 ${frac1} pts2 ${frac2} pts3 ${frac3} pts4
${frac4} pts5 ${frac5}

# Definition of generation surface

#region           insert_reg block -0.15 0.15 -0.15 0.15 0.06 1 units box

# Definition of mass flow rate
#fix              ins1 all insert/stream seed 5330 distributiontemplate pdd1 &
                  maxattempt 100 mass ${m} massrate ${Q} overlapcheck yes vel constant 0. 0. -1.0&
                insertion_face ins_mesh1 extrude_length 0.5

#apply nve integration to all particles that are inserted as single particles

fix               integr all nve/sphere

#output settings, include total thermal energy
fix               ts all check/timestep/gran 1000 0.1 0.1
compute           rke all erotate/sphere
#compute fc all pair/gran/local pos id force
thermo_style      custom step atoms ke c_rke f_ts[1] f_ts[2] vol
thermo            1000
#thermo_modify    lost ignore norm no
#compute_modify   thermo_temp dynamic yes


shell rm post                  # deleting existing link to a virtual post directory
```

```
shell mkdir post_300_${m}      # creating a directory for the simulation results (LINUX bash command)
post_${os}_${ff}_${rf}_${wf}
shell ln -s post_300_${m}  post # create a symbolic link to the saving directory for the file watcher makro in
Paraview

fix             rotate_vane all move/mesh mesh impeller rotate origin  0 0 0 axis 0 0 1  period 0.2
# Saving all walls as a single stl file: for static only 1x needed, every dumpstep for movable walls
dump              dumpstl1 all mesh/stl 1 post_300_${m}/static*.stl &
                                      drum
dump              dumpstl2 all mesh/stl ${dumpstep} post_300_${m}/impeller*.stl impeller

# Writing particle information in a file
dump              dmp_m all custom ${dumpstep} post_300_${m}/dump_*.liggghts id type x y z ix iy iz vx vy vz fx fy fz
omegax omegay omegaz

dump              dumpstress all mesh/gran/VTK ${dumpstep} post_300_${m}/dump*.vtk output face stresscomponents area
impeller #

#dump             dmpfc all local ${dumpstep} post_300_${m}/fc*.dump c_fc[1] c_fc[2] c_fc[3] c_fc[4] c_fc[5] c_fc[6]
         c_fc[7] c_fc[8] c_fc[9] c_fc[10] c_fc[11] c_fc[12] #[x,y,z],[x,y,z],id1,id2,periodic_flag,Fx,Fy,Fz

#dump             dmp_rigid vane_rigid custom ${dumpstep} post_300_${m}/vane*.liggghts id type x y z vx vy vz fx fy
fz omegax omegay omegaz

#dump_modify       dmp_m    sort     id


run               1         # run simulation for 1 step --> file "static.stl" is written
undump            dumpstl1  # no further saving of the "static.stl" file needed
run               ${dumpstep}
write_restart     restart.restart
```