THE DISPERSAL BEHAVIOUR OF ENGINEERED NANOMATERIALS (ENMs) USING CFD APPROACH

By

MUHAMMAD QAEYYUM HIFFNIE B MAHADZIR

14846

Dissertation submitted in partial fulfilment of

The requirement for the

Bachelor of Engineering (Hons)

Chemical

JANUARY 2015

Universiti Teknologi PETRONAS

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CERTIFICATION OF APPROVAL

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A project dissertation submitted to the
Chemical Engineering Programme
Universiti Teknologi PETRONAS
In partial fulfilment of the requirement for the
Bachelor of Engineering (Hons)
(Chemical Engineering)

Approved by,

____

(Dr. Risza binti Rusli)

UNIVERSITI TEKNOLOGI PETRONAS

BANDAR SERI ISKANDAR, PERAK

JANUARY 2015

CERTIFICATION OF ORIGINALITY

This is to certify that I am responsible for the work submitted in this project, that the original work is my own except as specified in the reference and acknowledgement, and that the original work contain herein have not been undertaken or done by unspecified sources or persons.

____

Muhammad Qaeyyum Hiffnie Bin Mahadzir

ABSTRACT

Use of powders in the nm-range such as ENM in the industrial settings has increased due to the unique properties exhibited by these materials. This increase in demand for nanopowders in industry lead to more associated hazard as ENM has its own potential hazard that may harm people and environment. However, very few known and aware about the explosion risk of ENM. Therefore, this project will focus on developing a dispersion model to study the dispersion behaviour of ENM that lead to the explosion. The project use ANSYS FLUENT CFD simulation software to develop the model. In this project, the time-averaged Navier-Stokes equation was used since it is most reliable in order to study on the fluid flow and the simulation was based on an Eulerian-Lagrange approach to study the behaviour of dispersion of ENM particles inside a 20L spherical explosion chamber.

ACKNOWLEDGEMENT

First and foremost, praise to God for giving me this opportunity to complete this Final Year Project II after struggling with all the problems and challenges faced for the past several weeks. There were about 13 weeks which have been given to me in completing this Final Year Project II.

Next, I would like to pass my gratitude to Dr. Risza Rusli who is my supervisor. It is only under her keen supervision that I am able to complete this project successfully. She had been a very supportive supervisor and willing to share her knowledge in order to ensure that I could learn and understand everything in this project.

After that, my appreciation is given to my beloved friends. Thank you for all supports and motivations which help me a lot when I was facing a hard time when completing this project. Lastly, not to forget those who are directly or indirectly involved in supporting me when designing my Final Year Project II.

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CHAPTER 1

INTRODUCTION

1.1 Background

Particles in the nano-sized range have been present on earth for millions of years and have been used by mankind for thousands of years. Soot for instance, as part of the Black Carbon continuum, is a product of the incomplete combustion of fossil fuels and vegetation; it has a particle size in the nanometere micrometer range and therefore falls partially within the ‘nanoparticle’’ domain. Recently, however, nanoparticles (NP) have attracted a lot of attention because of our increasing ability to synthesize and manipulate such materials.

Today, nanoscale materials find use in a variety of different areas such as electronic, biomedical, pharmaceutical, cosmetic, energy, environmental, catalytic and material applications. Because of the potential of this technology there has been a worldwide increase in investment in nanotechnology research and development. The forecasted huge increase in the manufacture and use of NP makes it likely that increasing human and environmental exposure to NP will occur (Nowack & Bucheli, 2007).As a result NP are beginning to come under scrutiny and the discussion about the potential adverse effects of NP has increased steadily in recent years; in fact it has become a top priority in governments, the private sector and the public all over the world.(Nowack & Bucheli, 2007)

1.2 Problem Statement

Nowadays the usage of nanoparticle in the industries such as biomedical, pharmaceutical, energy and etc increased due to uniqueness of the materials. Besides that, the advancement in science and technology has resulted in a corresponding increase in the number of nanoscale products.

Most manufacturing units that process nanoparticles faces a threat from fires and explosion. According to (Wu, Chang, & Hsiao, 2009), there have been 11 cases of Taiwan occupational accidents due to dust explosion between the years 1991 and 2003. So far, literature studies concerning the evaluation of explosion and flammability hazard of powders were essentially carried out on micro-sized powder. (Pritchard,2004 ; Mittal, 2014)

But after the incident at the Taiwan, “nano-safety” has emerged as a new area of concern especially for nm-metal powder. So, this study is focus on the accidental nanoparticle factors affected to the dispersal behaviours produced by engineered nanomaterial.

1.3 Objective

The objectives of study for the project entitled of “Accidental Nanoparticle Factors Affected to the Dispersal Behaviour produced by ENMs using CFD approach” are as following:

1. To develop a dispersion model for nanoparticles using Computational Fluid Dynamic (CFD) simulation software
2. To study the differences in dispersion behaviour of microparticles and nanoparticles

1.4 Scope of Study

The scopes of study for the project entitled of “Accidental Nanoparticle Factors Affected to the Dispersal Behaviour produced by ENMs using CFD approach” are as following:

1. The type of ENM used in this study is aluminium nanopowder.The reason of choosing aluminium nanopowder because it is one of the explosive material that widely used in the industries such as paint industry, paper industry and etc.
2. This project uses the ANSYS FLUENT to model the dispersion of ENM with an Euler-Lagrange approach.

CHAPTER 2

LITERATURE REVIEW

2.1 Engineered Nanomaterial

2.1.1 Definition

Nanomaterials are defined as materials with at least one external dimension in the size range from approximately 1-100 nanometers. Nanoparticles are objects with all three external dimensions at the nanoscale (NIOSH,2009). Nanoparticles that are naturally occurring (e.g., volcanic ash, soot from forest fires) or are the incidental byproducts of combustion processes (e.g., welding, diesel engines) are usually physically and chemically heterogeneous and often termed ultrafine particles. Engineered nanoparticles are intentionally produced and designed with very specific properties related to shape, size, surface properties and chemistry. These properties are reflected in aerosols, colloids, or powders. Often, the behavior of nanomaterials may depend more on surface area than particle composition itself. Relative-surface area is one of the principal factors that enhance its reactivity, strength and electrical properties. (Stanford University,2009)

Engineered nanoparticles cannot be considered as a uniform group of substance. ENMs are produced from many substances, in many forms and sizes and with variety of surface coatings (Savolainen et al., 2010).ENMs may be bought from commercial vendors or generated via experimental procedures by researchers in the laboratory (e.g., CNTs can be produced by laser ablation, HiPCO (high-pressure carbon monoxide, arc discharge, and chemical vapor deposition (CVD)). Examples of engineered nanomaterials include: carbon buckeyballs or fullerenes; carbon nanotubes; metal or metal oxide nanoparticles (e.g., gold, titanium dioxide); quantum dots, among many others.

2.1.2 Hazard from Engineered Nanomaterial

The recent development in nanotechnology opened new perspectives for many application both industry and society. As nanomaterial production and use are going to increase, there can be more associated hazard (Vignes et al., 2012). However, knowledge of the exposure to, or effects of ENM on human health and safety in occupational environment is limited and does not allow reliable assessment of risks of ENM on workers' health(Savolainen et al., 2010). A hazard that received significant attention is exposure to skin or inhalation in the lungs.(Marry Kay)

Based on (Fouqueray et al., 2012), the ENM also cause effect on freshwater organism and this study known as ecotoxicological. Exposure to the ENM caused decrease of growth and reproduction of daphnia (genus of small, planktonic crustaceans)

2.1.3 Factors Affected the Dispersal Behaviour

Combustion of solid materials, especially dust explosions, is particularly influenced by the dispersion characteristics of the particles in the combustion air. As highlighted by Eckhoff (2009), the most important properties of the dust dispersion are: (i) the particle shape, (ii) the particle size distribution (PSD), (iii) the agglomeration degree, (iv) the dust concentration within the cloud and (v) the degree of turbulence of the suspension.According to Carlos etc. al (2013) The effect of the particle size distribution on dust explosion has already been extensively studied. It is generally considered that, by reducing the particle size, the dust ignitability increases as well as its explosivity.

Next is the degree of agglomeration of the powder, defined as the ratio between the collision diameter of the agglomerates and the diameter of the primary particles. Based on research by Eckhoff, (2003) if the agglomerates are not broken by the dispersion process, they tend to behave as a large single particle of the size of the agglomerate, burning with the same combustion regime. As particle diameter is decreased, attractive force (Van der Waals forces) become more dominant and powder exhibit higher propensity to coagulate. This behaviour lead to decrease of Minimum Ignition Temperature (MIT) (Paul,2014). The anticipated significant increase in explosion severity (overpressure and rate of pressure rise) for nano dusts has not been observed in recent laboratory studies. Particle agglomeration is believed to be the major factor for this explosion severity behaviour, since inter-particle forces are much stronger for fine dusts.

In addition, turbulence can affect the properties of the initial dust cloud and the flame propagation. Turbulence can both have a promoting effect on the dust explosivity or a quenching effect on the flame kernel growth (Carlos etc. al ,2013) It has obviously an impact on the mixing of fuel and oxidizer, on the efficiency of the heat transfer, but also on the dust concentration distribution in the cloud as well as on the agglomeration degree of the powder.

2.2 Experiment to Determine Characteristic of Dust Explosion

2.2.1 Characteristic of Dust Explosion

The three requirements for combustion are a fuel, an oxidizer (usually air) and adequate heat or ignition source. This is often called the "fire triangle". The fuel can be any material capable reacting rapidly and exothermically with an oxidizing medium. In this case, the fuel is a combustible dust. For dust explosion, the dust must be dispersed in the air at the same time that the ignition source is present. The resulting rapid oxidation of the fuel dust leads to rapid increase in temperature and therefore pressure. Generally they are deflagrations.

Based on study by Vahid (2009), he stated that dust is divided into categorise which Group A and Group B. For Group A the dusts which ignite and propagate away from the source of ignition are considered explosible. The dust which do not propagate flame away from the ignition source are considered non-explosible and this dust fall under Group B. Group B powders are known to present a fire hazard and may be explosible at elevated temperatures (e.g. in dryers).

Another important characteristic of dust is based on minimum ignition energy (MIE). The MIE of a dust cloud depends on various factors including particle size, dust concentration, humidity, turbulence, oxygen concentration and chemical composition. The graphs below show the effect of dust concentration and particle size.

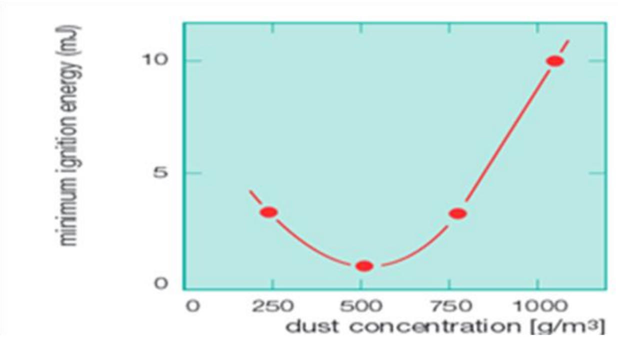


Figure 1: MIE vs Dust Concentration

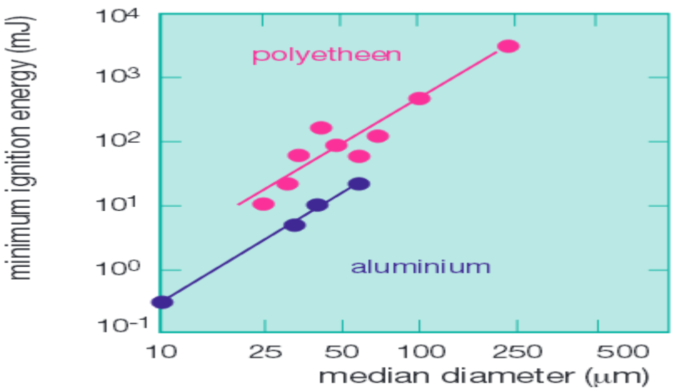


Figure 2: MIE vs Particle Size

In general, dust with particle size above 400microns will not ignite. As the size particle decrease, the MIE also decrease. As the temperature increase, the particle will disperse more vigorously hence this increase the surface area of the particle. Thus, this leads to the decrease of MIE value.

2.2.2 Type of Experiment

The scientist or researches usually will conduct experiment in order to determine the parameters of dust explosion. There are a few standardized apparatus that are being used such as “Hartmann Tube”, “20-L sphere” and “Mike 3”. But the most common apparatus that are often used for dust explosibility studies are the “20-L sphere” and “Hartmann Tube”.

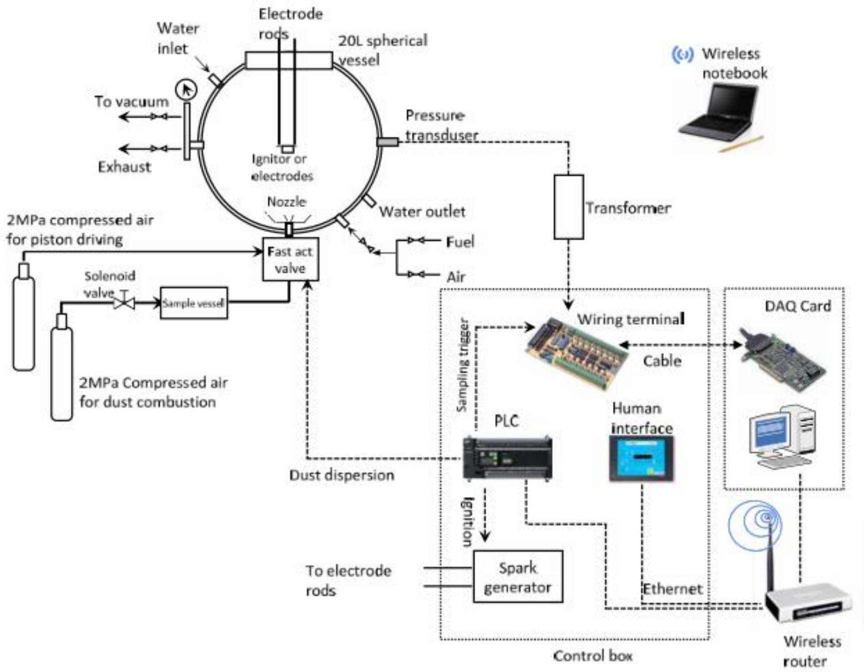


Figure 3: Schematic diagram of 20 L explosion test system

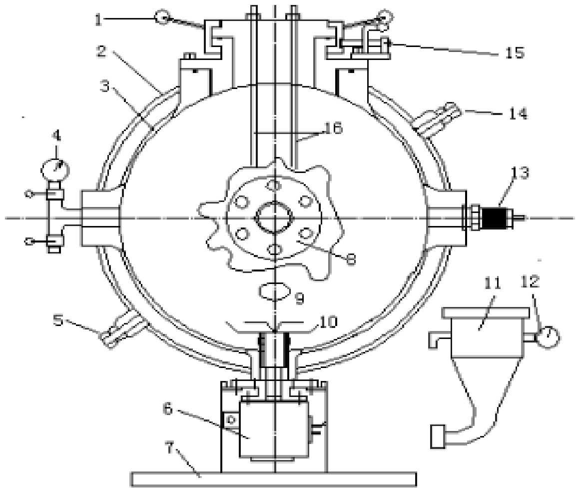


Figure 4 : The 20 L spherical explosion chamber

No	Description	No	Description
1	Handles	9	Inlet of fuel gas/air
2	Outside layer	10	Dispersion valve
3	Inside layer	11	Dust sample vessel
4	Vacuum gauge	12	Gauge with signal output
5	Inlet of recycling water	13	Pressure sensor
6	Dust/air multiphase valve	14	Outlet recycling water
7	Stand	15	Safety interlock
8	Inspect window		

Table 1: Part of 20L spherical explosion chamber

The test system consist 20 L spherical explosion chamber, control and data acquisition system (**Figure 3**). The explosion chamber is a double-layered stainless steel vessel (**Figure 4**). Water or other fluid media can be used to maintain initial temperature of explosion test. On the vessel wall there are different connections: vacuum, exhaust, fuel inlet and air inlet. A glass window can be used to observe the light of ignition and explosion flames.

A fast act valve is mounted under the bottom of the vessel, which driven by compressed air. A sample with volume by 0.6 L is connected to the fast act valve. The dust sample can be dispersed to the chamber by compressed air through the dispersion nozzle. The value of Kst and maximum overpressure, Pmax, are often determined using this apparatus.

2.2.3 Previous study on Experiment of Dust Explosion

The dust explosion hazard continues to represent a recognized threat to process industries that manufacture, use or handle powders and dust of combustible materials (Eckhoff,2005), which presents urgent need for knowledge and technology in explosion mitigation and prevention. Many studies were carried out on this field and current substantial articles focus on influences of dust concentration, particle size, oxidant concentration, moisture content and turbulence (Kuai et al., 2013).

Dust explosion research involving nano-materials has been limited, but some research groups have performed test with various materials to better understand the properties of nano-size powders. One of the experiment was conducted by (Boilard, Amyotte, Khan, Dastidar, & Eckhoff, 2013) using standard dust explosion equipment which are Siwek 20-L explosion chamber, MIKE 3 apparatus and BAM oven. The purpose of the experiment to determine the explosibilty of micron- and nano-titanium and compared according to explosion severity and likelihood. The results show a significant increase in explosion severity as the particle size decreases. The likelihood of an explosion increases significantly as the particle size decreases into the nano rage. These results had been agreed by Mittal (2013);(Yuan, Amyotte, Hossain, & Li, 2014).

In another study did by Tasneem (2006), she states that a dust cloud would explode only if the dust concentration is within the certain limit. A certain stoichiometric concentration of volatiles in air of the solid phase fuel must be generated for a flame to propagate rapidly through the mixture before more fuel volatiles produced. This indicates that the lower concentration limit is determined by the minimum quantity of fuel particles that must exist in order to sustain combustion. A near parabolic relationship exists between dust concentration and ignition energy. A further decrease in dust concentrations results in an increase in the ignition energy.

2.3 CFD Simulation

2.3.1 Previous Study on Dust Explosion using CFD

Dust explosion is dangerous hazard. There are basically two ways to study dust explosion and their dangers. One is to use different device in laboratories and real equipment from industry in large scale test sites to carry out small and large dust explosion tests. Another one is to use computational fluid dynamic simulation (CFD) method to stimulate dust explosions (Shi etc al. 2012). CFD can be useful for theoretical studies which in some cases could not be carried out under real industrial conditions. Based on Carlos (2013), CFD has been developed in order to describe the dispersion of a confined gas-solid flow in a typical test designed for the determination of dust cloud flammability.

Mostly the behaviour of the nanoparticles such as dispersion, explosion and etc. is being tested using experimental method. There are only a few researches on nanomaterial behaviour using computational fluid dynamic (CFD) simulation. One of it is study by Carlos etc. al (2013) on CFD modelling of nanoparticles dispersion. The simulation was based on an Euler-Lagrange approach and performed with ANSYS FLUENT TM 13.0. The material use in this research was aluminium.

In this study the researcher wants to determine the zones where turbulence causes variations on the particles size distribution (agglomeration/fragmentation dynamics). The higher pressure that increase the velocity of the fluid phase and induce an annular flow along the vertical tube and cause the immediate expansion of gas in the vessel

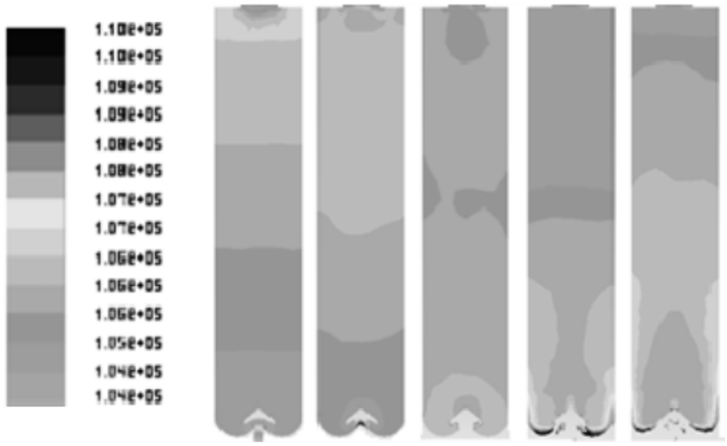


Figure 5 : Pressure inside the Hartmann tube in a dispersion process (Pa). Profiles at a) 5 ms b) 20 ms c)80 ms d) 100 ms e) 120 ms (Carlos et. al,2013)

The results evidence zone near the tube walls with high pressure and velocities near the walls that promote higher concentrations of solid which are attributed to the distribution of gas and particles collision.

On the other paper by Skjold et al. (2006), they were developed a new CFD-code which is Dust Explosion Simulation Code (DESC) for the assessment of accidental hazard arising from dust explosion in complex geometries. The approach followed entails the estimation of the laminar burning velocities of dust cloud from standardized laboratory-scale tests, and its subsequent use as input to the combustion model incorporated in DESC.

2.4 Case histories of ENM and dust explosion

Dust explosion have been a recognized threat to humans and property for a long time. A series of sugar dust explosion occurred on February, 2008 at the Imperial Sugar manufacturing facility in Port Wentworth, Georgia, resulted in 14 workers fatalities. Eight workers died at the scene and six others eventually succumbed to their injuries at the Joseph M. Thirty six workers were treated for serious burns and injuries – some permanent, life altering condition. The explosion and subsequent fires destroyed the sugar building and other parts of sugar refining process area. Based on investigation by CSB, there were some causes that this explosion happened such as sugar and cornstarch conveying equipment was not designed or maintained to minimize the release of sugar and sugar dust into the work area. Besides that, inadequate housekeeping practices resulted in significant accumulations of combustible granulated and powdered.

Based on studies by (Joseph, 2007), on February 2003, a combustible dust explosion occurred at the CTA Acoustics facility in Corbin, Kentucky. The impact of this incident, 7 workers was killed and 37 others were injured. CSB found that the fuel for the explosion was phenolic resin used to produce insulation and acoustic materials for automotive industry. The explosion began near a curing oven, where routine cleaning lofted accumulated resin dust that was ignited by fire in an oven on which the doors were left open.

According to Nowack et.al (2014), to date, no major accidents with ENM are known, therefore, they do not have any experience with the dissipation behaviour of ENM after an accident. Also, models are not yet available that is able to stimulate the distribution of ENM in the environment on a local scale. However they assume that ENM has higher potential for major accident especially when ENM present as powder, because they are easier dispersible than suspended ENM.

CHAPTER 3

METHODOLOGY

3.1 Project Workflow

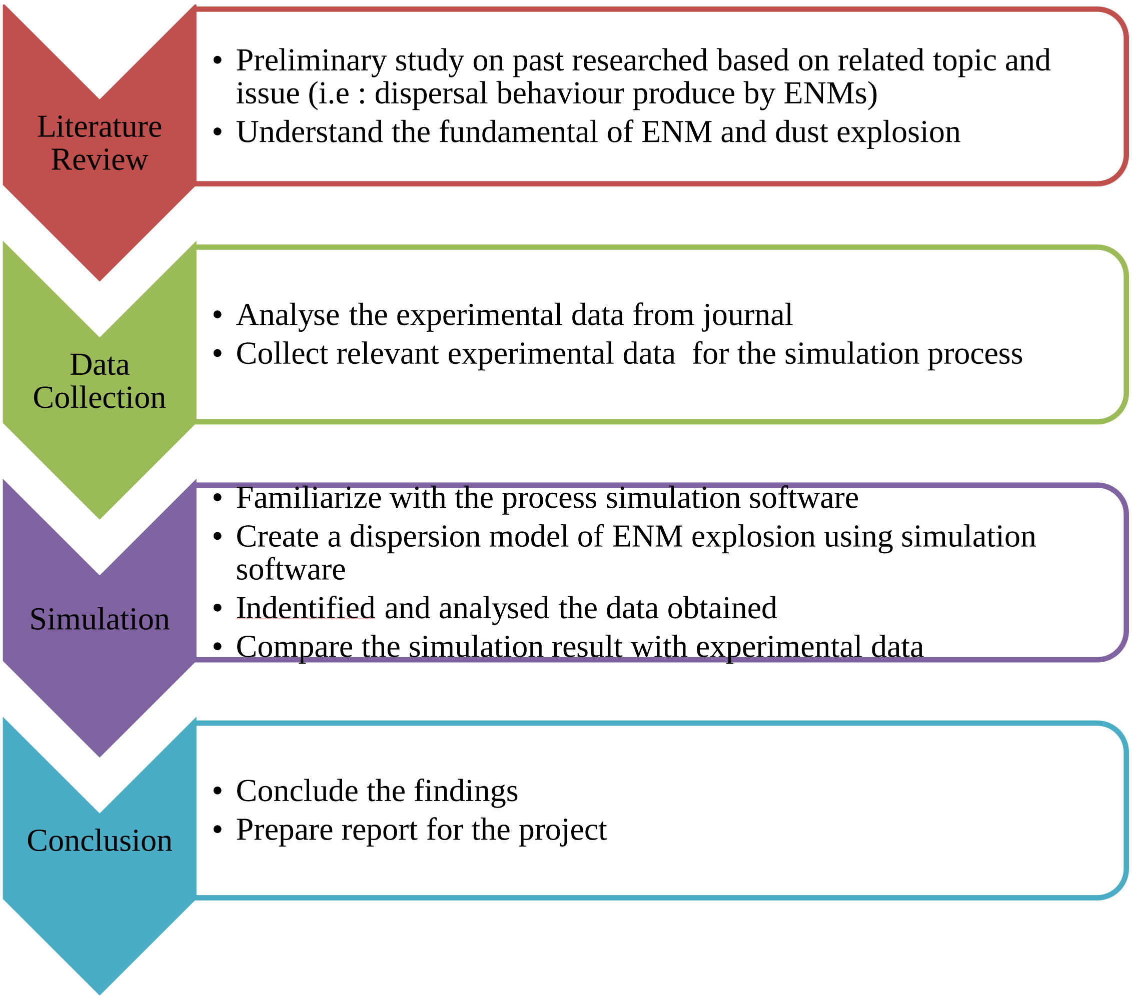


Figure 6: Project Workflow

For all project, usually the first step need to be done is collection of information. So for this project the literature review was conducted as the first step in order to obtain data regarding the ENM. Mostly the information related to ENM, properties of dust explosion and simulation of dust explosion using computational fluid dynamic (CFD) were obtained from the books, journals, reports and websites. It is crucial to understand the basic concept of the ENM and dust explosion, so that the project can be conducted efficiently and effectively.

A list of data consisting parameter for explosion must be available before dispersion model can be developed using CFD as it will be the input data in the simulation software. This data obtained through the analysis of experimental data of explosion from past journal and research. Then, the collection of the data will be used as the input in the modelling.

Tutorial need to be done in order to understand the concept of process simulation software. After that, a dispersion model is to be built to study the dispersion behaviour of ENM using simulation software. Because the input data were taken from experimental data of dust explosion, therefore, the results from the modelling using simulation software shall be validated and compared with the result of the experimental dust explosion before make a conclusion.

3.2 Research Methodology

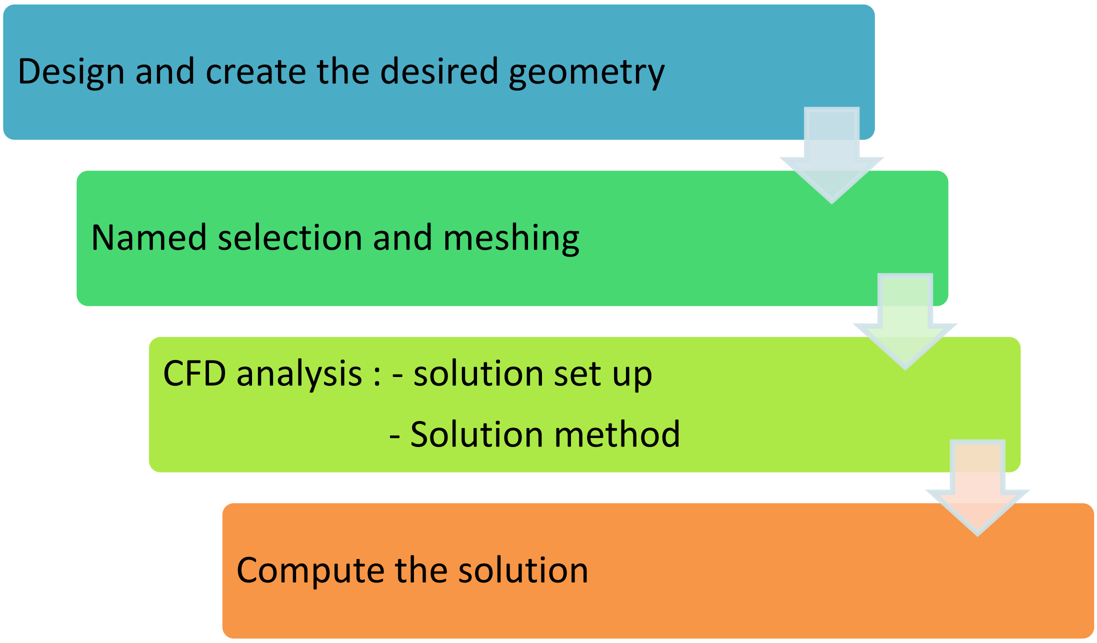


Figure 7: Research Methodology

3.2.1 Design and create desired geometry

Based on the experiment, the equipment use to conduct dust dispersion is inside a 20L explosion vessel. The apparatus is hollow sphere made of stainless steel and is rated to resist up to 30 bar. There is a small cylindrical tube connecting the vessel to a dust chamber at the bottom of the vessel. The dust will be injected trough the cylindrical tube from the dust chamber and the dust-air cloud dispersion is formed inside the vessel.

The three dimensional computational domain were created using ANSYS Design Modeler in this project because it is easier to monitor the dust-air dispersion inside the vessel. For this project, two domains were created which are sphere and cylindrical tube. The sphere has a volume 20 L (0.02 m^3) while the length and diameter of the cylindrical tube is 4 cm and 2cm respectively. The main equipment in the dust dispersion experiment is the spherical vessel while the cylindrical tube acts as an inlet for injecting dust into the vessel. The figure below shows the geometrical details of the computational domain.

In order to create spherical shape geometry, primitive tool was used and sphere was selected as shown in **Figure 8**. The advantage of this tool in ANSYS Design Modeler is the user can create models quickly by selecting desired 3D shape. After that, the user need to determine the origin and the radius of the sphere in three directions (x,y and z).

In this project, the selected origin of the sphere is (0, 16.84, 0) while the radius is 16.84cm, which is the calculated based on the formula of volume of sphere. The primitive tool also being used to create cylindrical tube which is attached at the bottom of the sphere.

$$V = \frac{4}{3}\pi r^3$$

$$20000cm^3 = \frac{4}{3}\pi r^3$$

$$47774\ cm^3 = r^3$$

$$r = 16.84cm$$

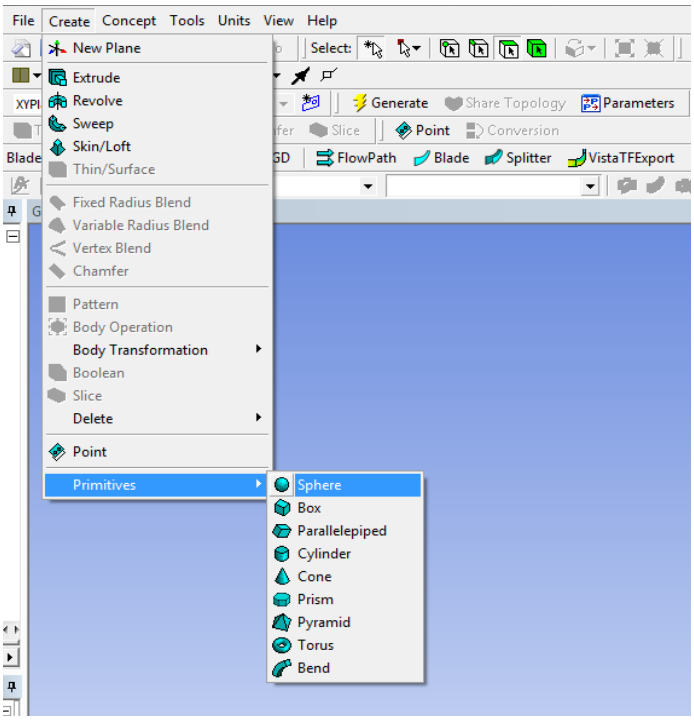


Figure 8: Primitives feature in ANSYS DesignModeler

Details of Sphere1	
Sphere	Sphere1
Base Plane	XYPlane
Operation	Add Material
Origin Definition	Coordinates
FD3, Origin X Coordinate	0 m
FD4, Origin Y Coordinate	16.84 m
FD5, Origin Z Coordinate	0 m
FD6, Radius (>0)	16.84 m
As Thin/Surface?	No

Details of Cylinder2	
Cylinder	Cylinder2
Base Plane	XYPlane
Operation	Add Material
Origin Definition	Coordinates
FD3, Origin X Coordinate	0 m
FD4, Origin Y Coordinate	2 m
FD5, Origin Z Coordinate	0 m
Axis Definition	Components
FD6, Axis X Component	0 m
FD7, Axis Y Component	-6 m
FD8, Axis Z Component	0 m
FD10, Radius (>0)	2 m
As Thin/Surface?	No

Figure 9: Details of sphere and cylinder

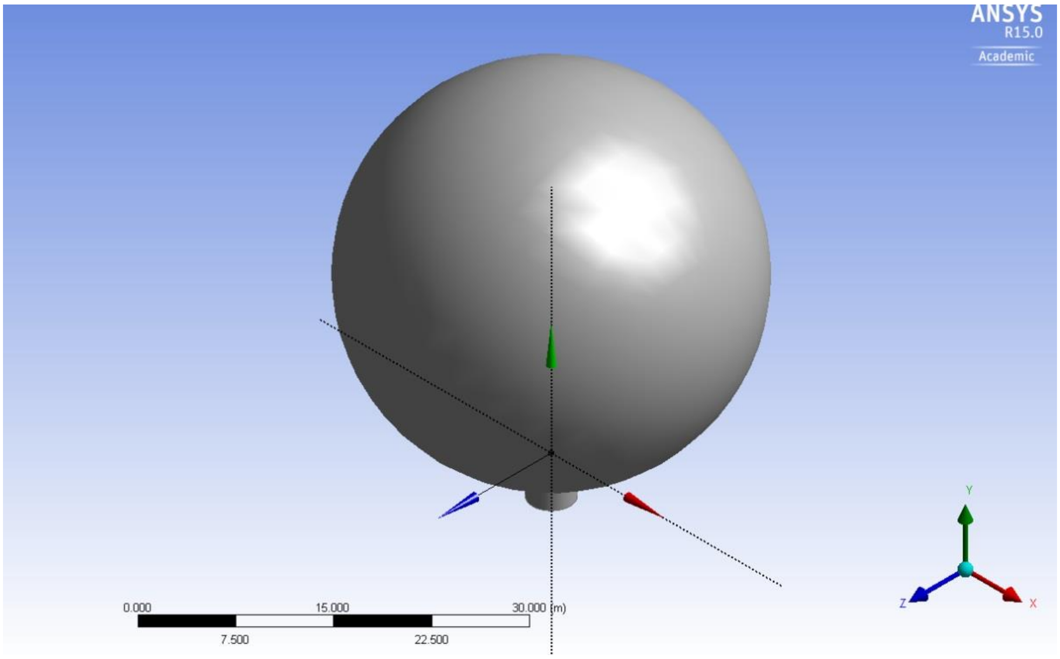


Figure 10 : Original Computational Domain

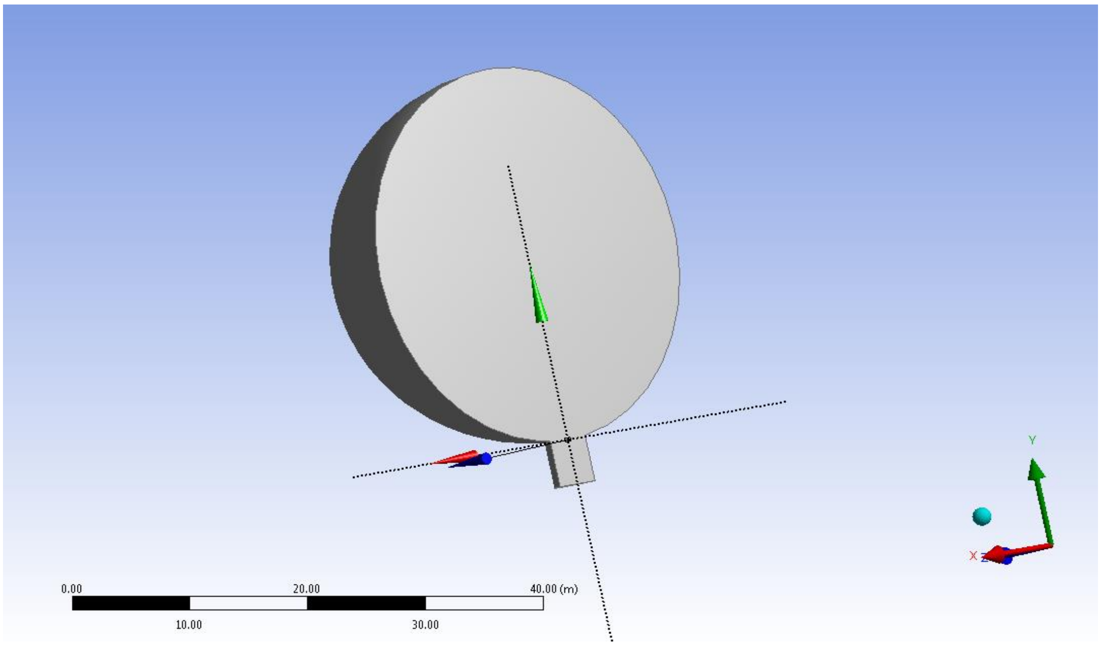


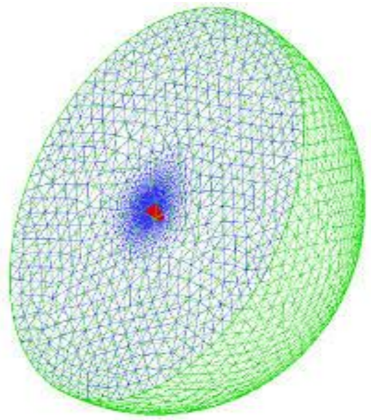
Figure 11: Computational Domain after Applying Symmetry

The symmetry tools is used to sliced the three dimensional computational domain in **Figure 10** into half at its symmetry plane (XY Plane), shown in **Figure 11**. The computational domain was renamed to fluid so that ANSYS Fluent will detect that the volume fluid zone and treat it accordingly.

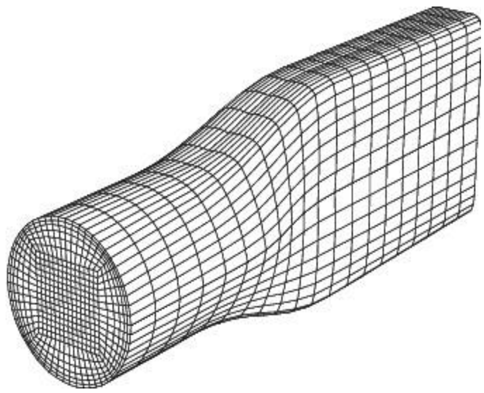
3.2.2 Named Selection and Meshing

After the computational domain had been generated, now it comes to the most importance step in CFD Fluent which is meshing using ANSYS Meshing application. Before that, the user need to label the boundary in the geometry by creating named selection for the necessary parts such as velocity inlet and the symmetry surface. The outer boundaries are automatically detected by ANSYS Fluent.

After named selection had been created, the computational domain need to undergo meshing process. This procedure consumed a quite sometimes in order to obtain the best quality of domain. It is important to make sure the domain is high quality so that the result obtained from the simulation will be more accurate. There are 2 types of mesh which are structured and unstructured. For this project, unstructured mesh is used because it is simpler compared to structured mesh. Parameter such as physical preference, relevance centre, assembly method meshing, inflation and etc. plays significant role to obtain the desired mesh. The quality of mesh can be checked at the Mesh Metric tab. There are 7 types of mesh quality checking and the common type that being used are Orthogonal Quality and Skewness. For this project the Orthogonal Quality is selected as mesh quality checking. The range of Orthogonal Quality are from 0 to 1 with 0 correspond to low quality and 1 correspond to high quality mesh. Generally if the value of minimum Orthogonal Quality above 0.1 is already acceptable.



Unstructured Mesh



Structured Mesh

Figure 12: Type of Mesh

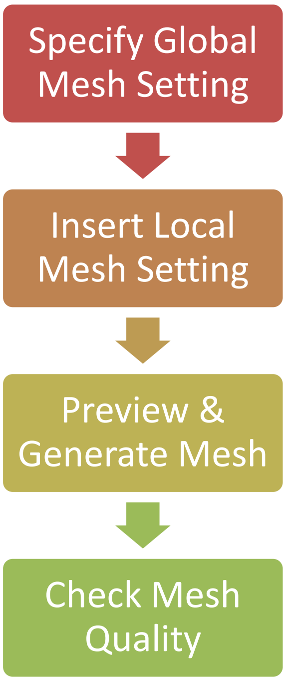


Figure 13: Meshing process

In the Default tab, make sure CFD and Fluent were selected for 'Physic Preference' and 'Solver Preference' so that the assembly meshing is active. The component that being adjusted in the Sizing tab were 'Use Advanced Size Function (ASF)', 'Relevance Centre', and 'Smoothing'.

There are three type of relevance centre which are coarse, medium and fine. Based on Baker (2006), the main source of error in meshing process is the mesh is too coarse and that the reason why fine relevance centre is chosen in this project. The number of smoothing iterations selected is high. Besides that, inflation is also important element need to be considered in order to get high quality mesh because inflation is used to generate thin cells adjacent to boundaries. So in this project the inflation selected is program controlled.

The assembly meshing is the shape of mesh cells which consists of three different methods which are None, Cut Cells and Tetrahedrals. Each methods will produce different number of nodes and element. The number of element for domain should not too high to avoid longer the simulation process. In this project, 'None' is chosen as the assembly meshing method as it yield highest minimum orthogonal quality compared with other method. After all the meshing parameters had been defined, the next step is to generate mesh by clicking 'Update' button at the mesh tab or simply click 'Generate Mesh'.

Meshing Parameter	Components
1) Default	→ Physic Preference : CFD → Solver Preference : Fluent
2) Sizing	→ Use Advanced Size Function : Curvature → Relevance centre : Fine → Smoothing : High
3) Inflation	→ Use auto Inflation : Program Controlled
4) Assembly Meshing	→ Method : None

Table 2: Meshing Parameter Table

As stated previously, the meshing process consumed quite sometimes because requires several trial and error in order to get high quality mesh. The user need to adjust the basic meshing parameter as indicated in **Table 2**. The number of nodes, elements and mesh quality can be obtained at Statistic under mesh tab.

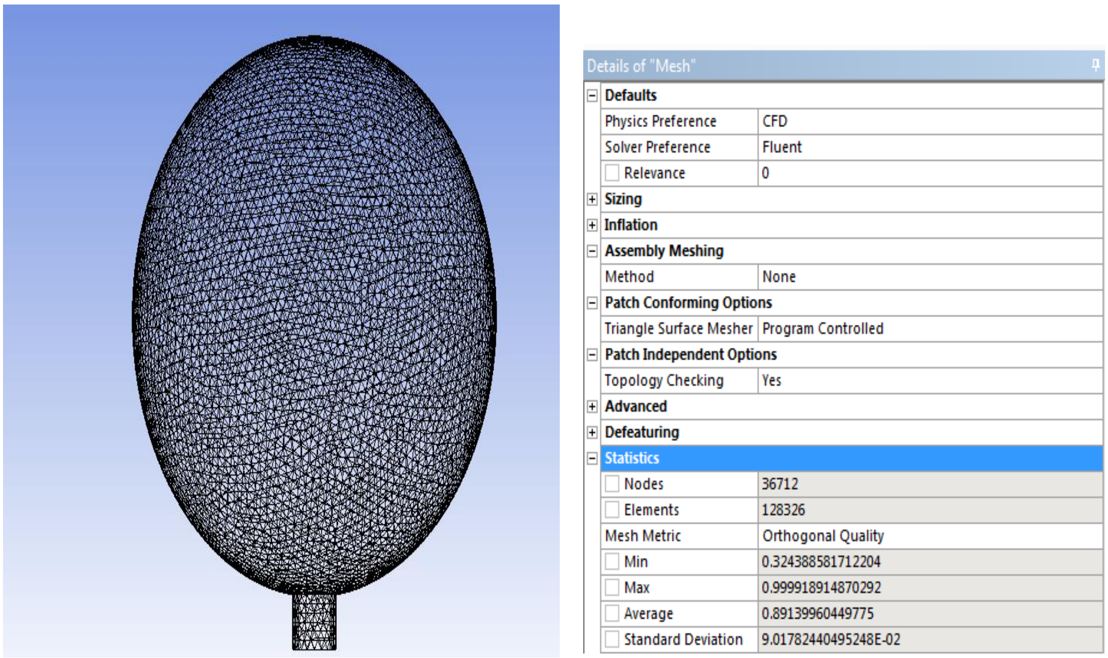
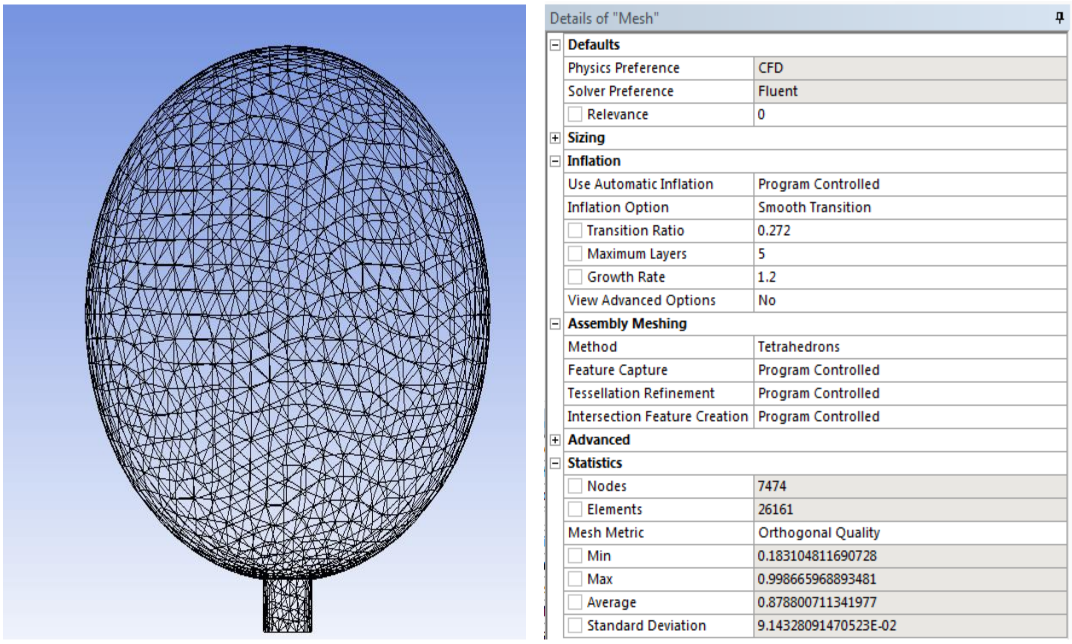
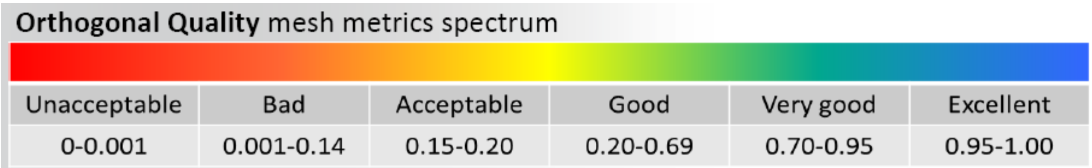


Figure 14 : Mesh Static for Method 'None'



Details of "Mesh"	
Defaults	
Physics Preference	CFD
Solver Preference	Fluent
Relevance	0
Sizing	
Inflation	
Use Automatic Inflation	Program Controlled
Inflation Option	Smooth Transition
Transition Ratio	0.272
Maximum Layers	5
Growth Rate	1.2
View Advanced Options	No
Assembly Meshing	
Method	Tetrahedrons
Feature Capture	Program Controlled
Tessellation Refinement	Program Controlled
Intersection Feature Creation	Program Controlled
Advanced	
Statistics	
Nodes	7474
Elements	26161
Mesh Metric	Orthogonal Quality
Min	0.183104811690728
Max	0.998665968893481
Average	0.878800711341977
Standard Deviation	9.14328091470523E-02

Figure 15: Mesh Static for Method ‘Tetrahedron’



Orthogonal Quality mesh metrics spectrum

Unacceptable	Bad	Acceptable	Good	Very good	Excellent
0-0.001	0.001-0.14	0.15-0.20	0.20-0.69	0.70-0.95	0.95-1.00

Figure 16: Orthogonal Quality Mesh Metric Spectrum

3.2.3 CFD Analysis

After the computational mesh for sphere and cylinder had been created, next step is to insert relevant input for the simulation process using ANSYS Fluent. There are two parameter in the CFD analysis which are Solution Setup and Solution. There are 7 components under Solution Setup which are:

No	Components
1	General
2	Models
3	Materials
4	Cell zone conditions
5	Boundary condition
6	Dynamic mesh
7	Reference values

Table 3: Component of CFD Analysis

In general tab under solver component there are three parameter need to be selected which are type, velocity formulation and time. Based on Di Sarli et al. (2013), 'pressure-based' type is most suitable since the project involved uncompressible flow.

The description of gas-solid flows has been developed by different approach based on the materials analysed in the study case. However, most of the numerical studies are based on Euler-Lagrange approach. In this project, the time-averaged Navier-Stokes equation was used since it is most reliable in order to study on the fluid flow. The flow of solid phase was solve with the Lagrangian approach using Discrete Phase Model (DPM) while the fluid flow was solved using Eulerian approach.

In the Viscous Model, for turbulence condition, k-ε model with enhanced wall treatment was selected because it is suitable for complex shear flows involving rapid strain, moderate swirl, vortices and locally transitional flows. In addition, this model commonly used for standard cases. The model constant were remained unchanged. The k-ε model solves for two variables: k; turbulence kinetic energy, and ε; the rate of dissipation energy. The k-ε model is very popular among other models due its good convergence rate and relatively low memory requirement. (Frei,2013).

The Discrete Phase Model (DPM) tracks the motion of individual particles. The particles can be a solid or a liquid. The DPM implemented in Fluent uses a Lagrangian approach, the fluid phase is treated as a continuum by solving the Navier-Stokes equation, while the dispersed phase is solved by tracking a large number of particles through the calculated flow field. The dispersed phase can be exchange momentum, mass and energy with the fluid phase (Gennaro, 2011). The trajectory is calculated by integrating the particle force balance equation (Bakker, Discrete Phase Modeling, 2006):

$$\frac{du_i^p}{dt} = F_D\left(u_i - u_i^p\right) + \frac{g_i(\rho_p - \rho)}{\rho_p} + \frac{F_i}{\rho_p}$$

Where,

$F_D\left(u_i - u_i^p\right)$ = Drag force is a function of the relative velocity

$\frac{g_i(\rho_p - \rho)}{\rho_p}$ = Gravity force

$\frac{F_i}{\rho_p}$ = Additional force (Brownian motion, Thermophoretic, Saffman lift and etc.)

The interaction between the fluid phase and the solid phase was assumed as two-way since the fluid flow affects the particle motion and vice versa, while the particle-particle collision is neglected since it is accounted only in four-way coupling (Di Benedetto et al., 2013)

The injection tab in DPM defines the release condition for the DPM particles. The user need to specify the particle type, material and initial conditions. The injection type selected was 'surface'. The other parameter such as start and stop time, velocity magnitude, total flow rate and etc. were based on study by Di Benedetto et al.,(2013).

After input data for model is completed, next step is define the material used in the modelling. Since this project is about the dispersion of aluminium nanoparticle inside 20L explosion vessel, so the material involved are aluminium and air. The properties of the material are shown in the **Table 4.**

Initial Pressure of Sphere	0.4 bar
Aluminum density	2719 kg/m^3
Air density	Default

Table 4: Properties of material

Next step is specifying the cell zone condition and boundary condition. The mesh consists of large number of finite cells and it is grouped into one or more cell zones. Each cell is bounded by a number of faces then grouped into a number of face zones. Some of these faces are located on the boundaries of the model. The zones to which such faces belong are known as boundary zones.

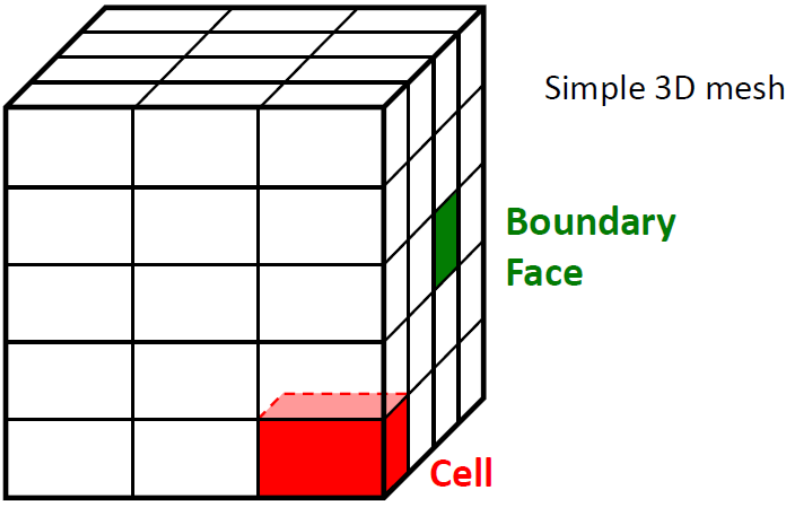


Figure 17: Cell Zone

It is crucial to setup appropriate initial condition and boundary condition as poorly defined both conditions can have significant impact on the solution. Boundaries are required components of the mathematical model since it directs the motion of flow.

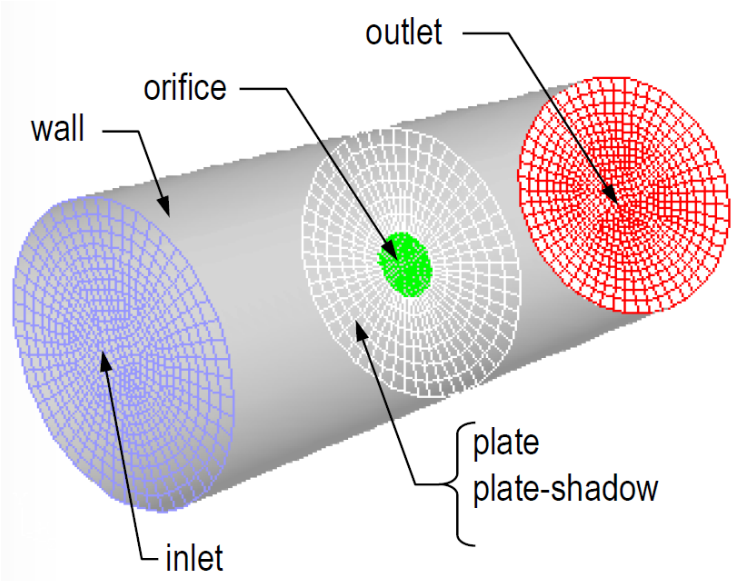


Figure 18 : Example of Boundary Condition

In this study, the boundary condition as shown in **Figure 19** below:

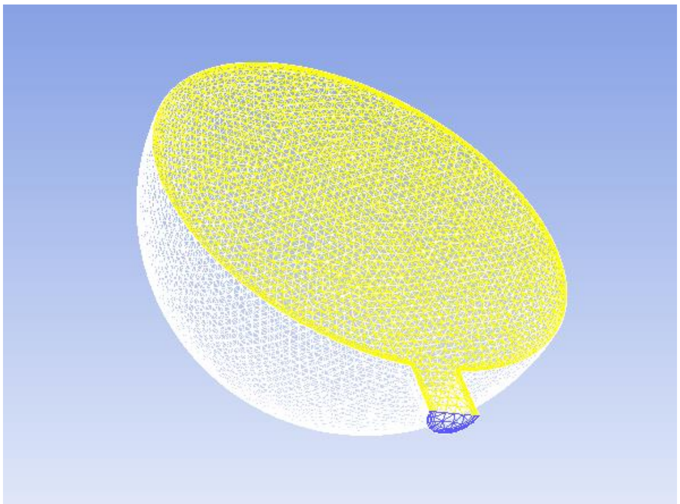


Figure 19: Boundary Conditions of the Computational Domain

Velocity inlet (blue mesh)

Symmetry (yellow mesh)

Wall Fluid (White Mesh)

There are two boundary condition that need to be further specified which are velocity-inlet and wall. **Figure 20** and **Figure 21** show the parameter of the boundary condition. The direction of particle is upward (+ y-axis) so the velocity magnitude was inserted at the corresponding plane (y-axis). For wall boundary condition, 'stationary wall' was selected since the sphere is static.

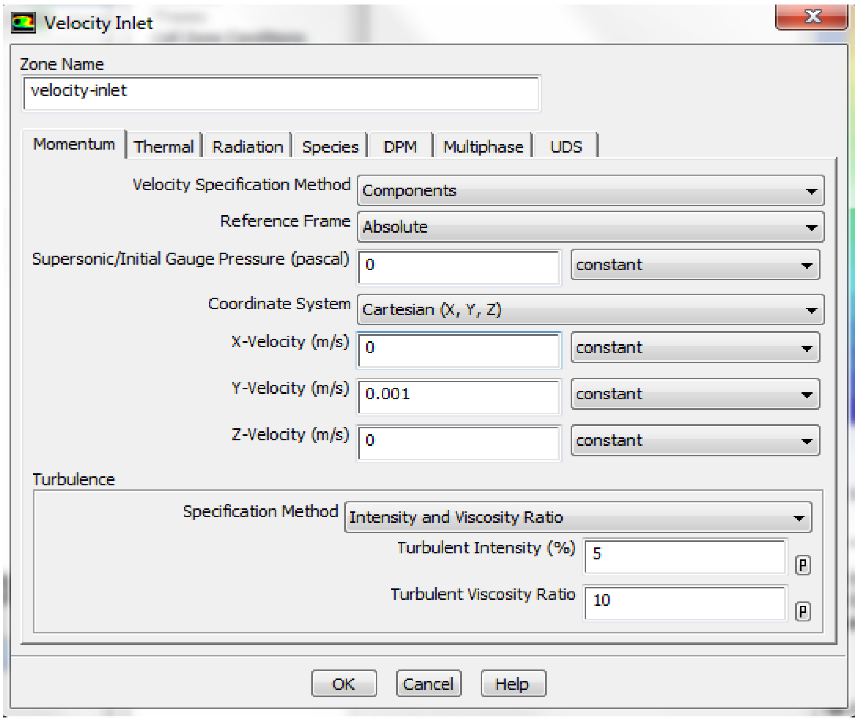


Figure 20: Velocity Inlet

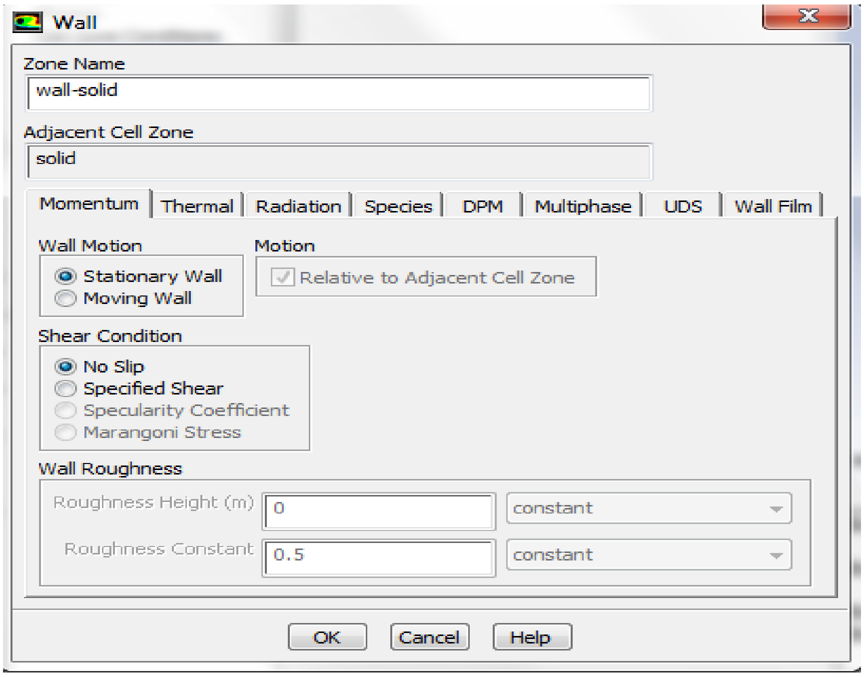


Figure 21: Wall-Fluid

The final step in this CFD FLUENT simulation is to compute the solution. In the Solution tab, there are six parameters available which are:

No	Parameter
1	Solution Method
2	Solution Control
3	Monitors
4	Solution Initialization
5	Calculation Activites
6	Run Calculation

Table 5: Parameter of Solution

Under Solution Methods, the Pressure Velocity Coupling selected was SIMPLE (Semi-Implicit Method for Pressure–Linked Equations) algorithm as it is widely used and good for incompressible flow applications. Parameters listed under Spatial Discretization and Transient Formulation was remained unchanged.

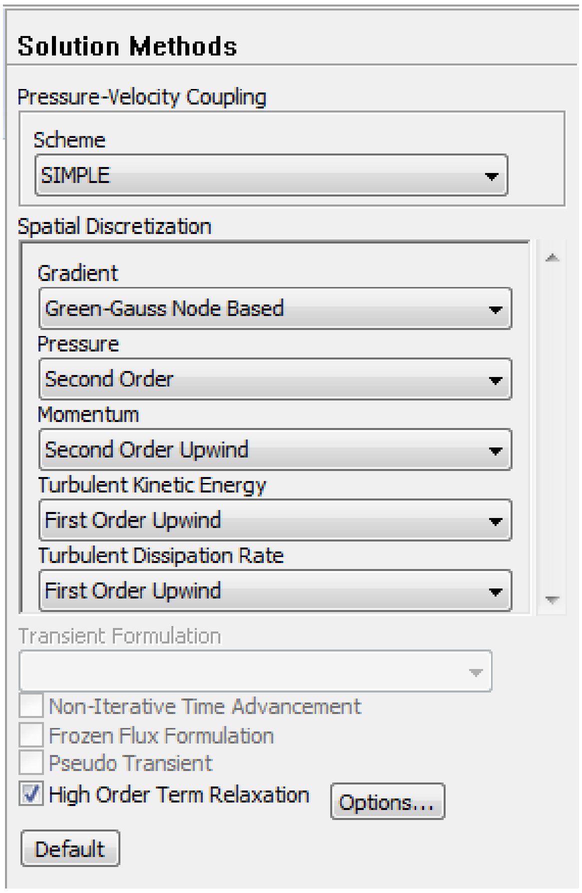


Figure 22: Solution Methods

For other parameter such as Solution Control, Monitors, Calculation Activities were kept constant. Fluent requires that all solution variables be initialized before starting iterations. Basically this means that in every individual cell in the mesh a value must be assigned for every solution variable to serve as an initial guess for the solution. Hybrid Initialization was selected under Initialization Methods as it is uses for most cases.

It is important for the user to check the case before proceed with the simulation because there might be errors or recommendation in the solution, so that the simulation can be run and converge easily.

3.3 Gantt Chart & Milestone

	Milestone		FYP 2													
	Process															
No	**Activties / Tasks**	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**	**12**	**13**	**14**	**15**
1	**Submission of Interim Report**															
2	**Project Work Continues**															
	Progress Report Preparation															
3	**Progress Report Submission**															
4	**Project Work Continues**															
5	**Pre-SEDEX**															
	Preparation for final report															
	Submission of draft final report															
6	**Submission of Dissertation (Soft Bound)**															
7	**Submission of Technical Paper**															
	Viva Preparation															
8	**Viva**															
9	**Submission of Dissertation (Hard Bound)**															

CHAPTER 4

RESULT AND DISCUSSION

In this project, the parameter that wanted to be monitored from the simulation is velocity vectors coloured by turbulent kinetic energy.

5.1 Result

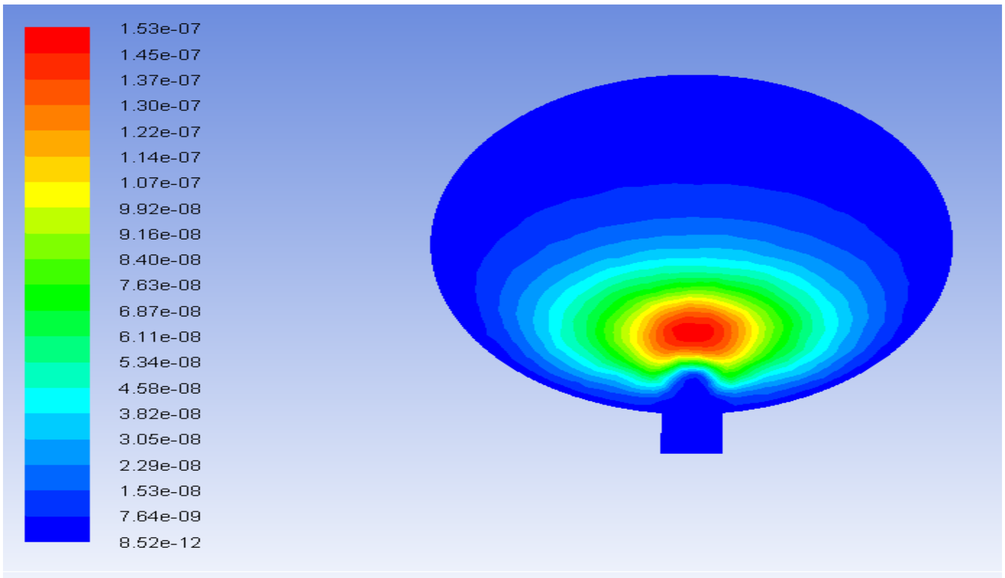


Figure 23:Turbulent Kinetic Energy (m2/s2) for micro particle: frontal view (x-y plane)

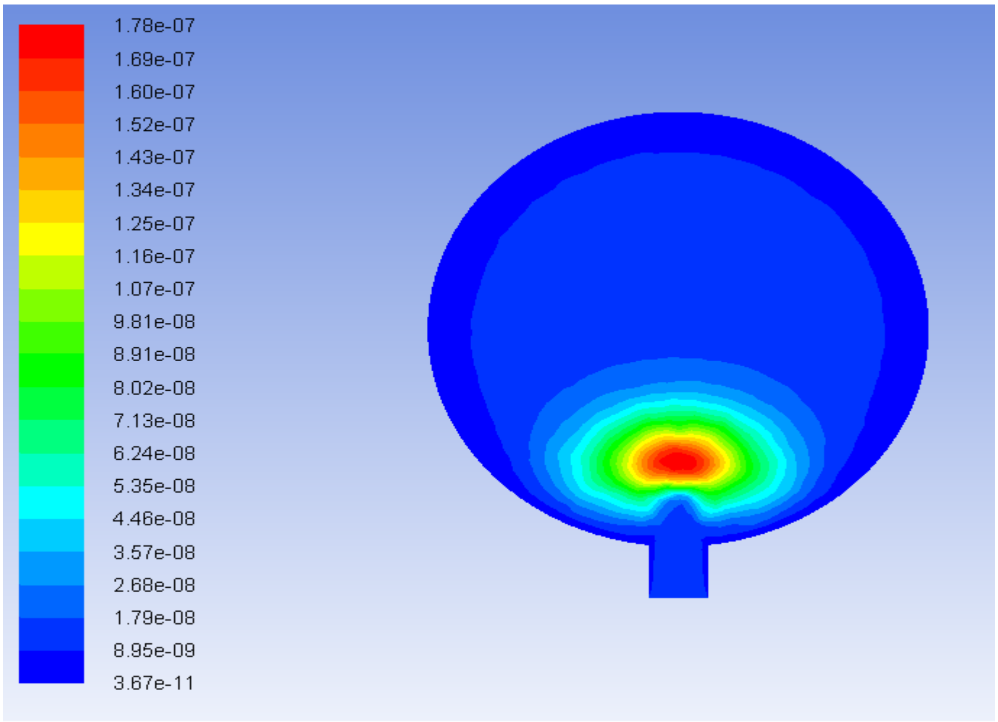


Figure 24:Turbulent Kinetic Energy (m2/s2) for nano particle: frontal view (x-y plane)

The indicator on the left hand side of the picture shows the value for the kinetic energy in which red colour indicates the region with high kinetic energy while blue region has the lowest kinetic energy.

Dust explosion is a phenomenon that a flame is propagating in combustible particle cloud dispersed.in the air. The particle size has significant effect on the ignitability and explosion violence because the gasification strongly depends on the particle size. Therefore, the parameters of nanoparticles might be much different from those of the particles of micron scale.

Based on the figure shown as computed over frontal (x-y) plane, the highest kinetic energy is at the centre (red colour) where the particles are agglomerate. According to research by Dufaud et al., (2011), when particles disperse into the air, the particles tend to agglomerate among each other. This will affect the total surface area where the total surface area increases making it more easily to catch fire. This will cause the MIT of the particle decrease and the risk of flammability and explosion become higher.

Based on study by Di Sarli et al., (2013) it has also been found that the dust dispersion is affected by the dust size: as the dust diameter is increased, the dust concentration distribution becomes less uniform. The kinetic turbulent energy in **Figure 24** is higher than **Figure 23** and it shows that as the size of material injected into the vessel is smaller, the turbulent kinetic energy of the material when dispersed in the spherical vessel is increase.

In order for an explosion to occur, there are five factors as shown in the figure below need to be fulfilled:

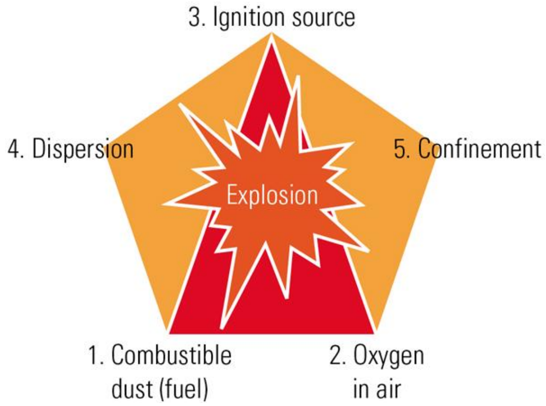


Figure 25: Factors of explosion

For this project, all the elements required are available such as the combustible dust refers to the aluminium particles, oxidant refers to air which is injected inside the explosion vessel together with aluminium particles, dust dispersion refers to movement of aluminium-air mixture inside the vessel. In the experiment of dust dispersion to study the explosion properties solid particles of using 20L explosion vessel, the igniter is located at the center of the sphere.

CHAPTER 5

CONCLUSION AND RECOMMENDATION

The popularity of ENMs among researchers and scientists has exceptional benefits however, due to the fact of ENMs having lower MIE, the risk of it to catch into fire and explosion easily serve a great threat towards the safety aspect of the industry. In order to minimize the risks of dust explosion of nanomaterial, the potential hazard of dust explosion must be understood appropriately. However, the potential hazard of dust explosion especially nanoparticle are not clear because there are only few reported data. With the aid from CFD simulation software, it is hoped that the mechanism of ENM explosion can be understood so that the risk assessment of ENM explosion will be implemented to ensure the use of ENM. Based on the velocity vectors coloured by turbulent kinetic energy, it shows that for nanoparticle has higher turbulent kinetic energy compared to microparticle.

For future recommendation, conduct the simulation of dust dispersion for different concentration of particle. Different concentration will affect the movement of the particle when it is disperse into the air. Therefore, by having this study, it will improve the understanding on the flow of particles for heavier particles.

Besides that, it is recommended to study the dust dispersion with varies discharge flow in transient mode. So that, it will further help to understand the behaviour of the particle which time the taken for particle to become uniform and agglomerate.

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