INVESTIGATING DISPERSAL BEHAVIOR LEAD TO AN EXPLOSION OF ENGINEERED NANO MATERIAL USING COMPUTATIONAL FLUID DYNAMICS (CFD) APPROACH

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CHEMICAL ENGINEERING

UNIVERSITI TEKNOLOGI PETRONAS

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by

Nur Shamimi Binti Abdul Rahim
15576

Dissertation submitted in partial fulfillment of
the requirements for the
Bachelor of Engineering (Hons)
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Universiti Teknologi PETRONAS,
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CERTIFICATION OF APPROVAL

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Approved by,

____
(Dr. Risza binti Rusli)

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BANDAR SERI ISKANDAR, PERAK
September 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 references and acknowledgements, and that the original work contained herein have not been undertaken or done by unspecified sources or persons.

NUR SHAMIMI BINTI ABDUL RAHIM

ABSTRACT

A CFD model is developed with the aim of simulating the turbulent kinetics energy flow field induced by the aluminium particles with nano and micron size within the 20 L explosion chamber. The model was validated with a set of data from the pressure time histories that is available in the literature review. The turbulence and the particles streamline are established in the explosion chamber. The obtained results are relevant to the practice at which the severity of the explosion increases with the decrease in the size of the aluminium particles. Nevertheless, the awareness of the risk of Engineered Nano Material (ENM) is still very less especially when ENM can cause explosion if it is not handle appropriately. In spite of extensive advancement in exploration and growth with unique and valuable impact on nanotechnology sector, there are still hazard that being mentioned all these while that might be harmful for both people and environment that associate with the process industries as well.

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CHAPTER 1

INTRODUCTION

1.1 Background

During the second half of the previous century, the term “nano-technology” was not familiar as it is now. In nanotechnology, any particles that fall between 1nm to 100 nm are defined as nanoparticles. Nanoparticles are also known as nanomaterials, nano powder and ultra-fine particles. With the fine sizes, it tends to dictate the bulk behavior of any materials. For example, materials that would typically be conductors of electricity have a tendency to be as an insulator at nanoscale or vice versa.

Although, in general, nanoparticles are considered a discovery of modern science, they were actually has a long history. Human have been using copper and silver nanoparticles in the production of ceramic glass and pottery. Nanotechnology is all about synthesizing and manipulating the materials according to the market demand and consequently improves the quality and durability of a product (Amin & Abu el-hassan, 2015). This is also known as engineered nanoparticles as the atomic molecules need to be deployed into required nanoscale patterns. In the past ten years, nanotechnology had attracted a lot of attention and grown tremendously in different industry application such as electronic, biomedical, pharmaceutical, cosmetic, energy, environmental, catalytic and material applications (Nowack & Bucheli, 2007). Nanoparticles are under great scientific research as there are the bridge between the bulk materials and the atomic structure. According to Nowack and Bucheli (2007) ever since nanoparticles have been massively used in many sectors, great investment had been ventured through the research and development and the production of engineered nanoparticles will increase up to 58, 000 tons by 2020.

1.2 Problem Statement

The use of nanotechnologies envisaged to an extent of providing means for the production of light and durable materials, pure water, clean energy, and not to forget medical application as well. In spite of extensive advancement in exploration and growth with unique and valuable impact on nanotechnology sector, there are still hazard that being mentioned all these while that might be harmful (Savolainen et al., 2010). One of the particular areas of interest is the fire and explosion hazard which are associate with the process industries that manufacture, use and/or handle the nanoparticles materials.

There are few important parameters that contribute for a nanoparticles explosion to happen as per highlighted by Murillo et al. (2013). These are the particle shape, the particle size distribution (PSD), the agglomeration degree, the dust concentration within the cloud and the degree of turbulence suspension. But from a study, an explosion severity increase with the decreasing of the particle size.

Basically most of the manufacturing units that process the nanoparticle material are under the risk of fires and explosion. Referring to (Wu, Chang, & Hsiao, 2009), there were 11 cases that been reported in Taiwan due to dust explosion between the year of 1991 to 2003. Due to these accidents and many others, a new area arisen especially dealing with nanoparticles. Thus this study is focusing on the factors that affecting the dispersal behaviors produced by the engineered nanoparticles.

1.3 Objectives

The objectives of this project entitled of “Investigating Dispersal Behavior Lead to an Explosion of Engineered Nano Material Using CFD Approach” are as following:

- To develop a transient dispersion model for nanoparticles using Computational Fluid Dynamics (CFD) simulation software.
- To study the influence of particle size on the dust explosion.
- To investigate the combustion due to the explosion of dust particles.

1.4 Scope of Study

The scopes of study for the project entitled of “Investigating Dispersal Behavior Lead to an Explosion of Engineered Nano Material Using CFD Approach” are as following:

- Aluminium nanoparticles are used for the entire study and the reason of choosing aluminium nanoparticles is because it is one of the explosive materials and cause ignition when the particles are suspended in the air as a dust clouds. Apart from that there were many theoretical data available and plenty of studies had been conducted using aluminium particles.
- This project will be simulated using ANSYS FLUENT to simulate the transient dispersion model of engineered nanoparticles with Euler-Lagrange approach.

CHAPTER 2

LITERATURE REVIEW

2.1 Nano Particles

Nanoparticles are defined as a microscopic particle that is measured in nanometers (nm). The typical diameter of a nanoparticle is between 1-200 nm. Nanoparticles that occur naturally such as volcanic ash or soot from forest fires or as a byproduct of combustion such as welding and through diesel engine are usually physical and chemically heterogeneous are also known as ultrafine particles. On the other hand, a nanoparticle exits in various shapes such as in a spherical, tubular or irregular as shown in Figure 2.1 and can exist in fused, aggregated or agglomerated forms. Due to its size, nanoparticles have large surface area per mass and these increase its ability to behave as a great conductor, high strength besides improve in durability and quality of a product (Amin & Abu el-hassan, 2015).

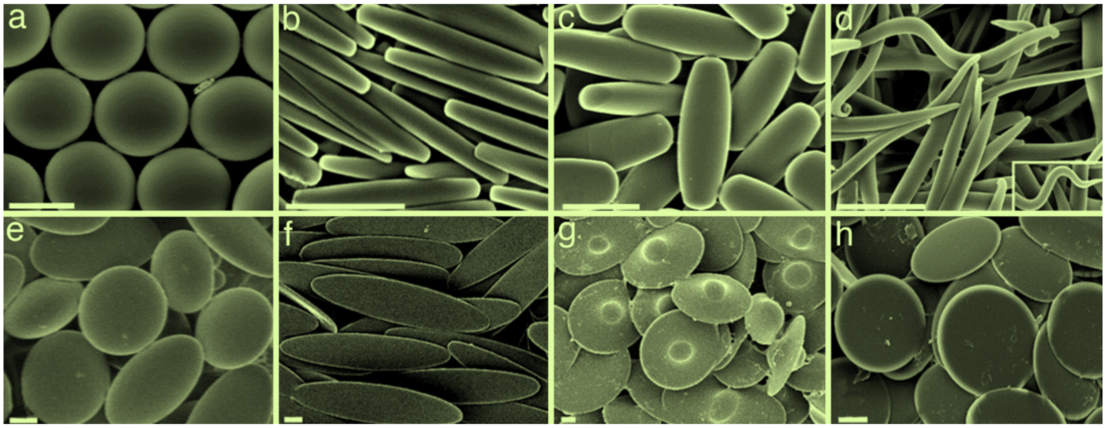

FIGURE 2.1 Various shapes of Nano-material

Engineered nanoparticles are produced and designed purposely with a very precise and specific properties associate to shape, size, surface properties and chemistry and it is reflected in aerosols, colloids or powders (Stanford, March 2009). It is synthesized by experimental procedures through research and development in the laboratory (e.g, CNTs can be produced by laser ablation, HiPCO (high pressure carbon monoxide, arc discharge, and chemical vapor deposition (CVD)). Other examples of nanoparticles are titanium dioxide, zinc oxide and carbon nanotubes and it can be used widely in many application such as from lightweight materials, drug-delivery system, and catalytic converters to be used in food, cosmetics and leisure products (Helland et al., 2008). Nanoparticles can be produced using two way approaches which are ‘top-down’ and ‘bottom-up’ method.

2.1.1 Hazard from Engineered Nanoparticles

Most of the manufacturing unit that produces or process nanoparticles is facing the risk of explosion and fires. The irreplaceable applications of nanoparticles have grabbed a lot of attention due to its technologically interesting properties. Although nanotechnology sector is promising such a great deal, but the health, safety and environment issue still questionable. Due to this, it has urged the scientist, the regulators and the industrial representative to study the structure and characteristic of nanoparticles in a way that it will be safe to be used (Savolainen et al., 2010). Exposure to nanoparticles has been linked with numbers of health issues including pulmonary inflammation, genotoxicity, and circulatory effects.

Recently, in June 2015, flammable starch-based powder exploded at Formosa Fun Coast in Taiwan, injuring about 508 people, 199 in critical condition and 15 deaths due to the explosion of colored corn starch which happened due to presence of spark. On the other hand in August 2014, an explosion occurs in an automotive parts factory located in China that killed 146 workers. A massive explosion occurred at the factory when the flames igniting the metal polishing dust. Where else, Georgia sugar refinery explosion that happened in February 2008 killed 14 people and leave 42 in injuries occurred in a sugar refinery factory. The sugar dust acts like gunpowder and cause a massive explosion.

According to Mittal (2014) the evaluation of flammability and explosion risks of a micron size particles is not valid if it is not determined using the nanoparticles via the standard apparatus and procedure for measuring the dust explosion. It is difficult to draw the boundaries between the ‘fire’ hazards, ‘deflagration’ hazard and ‘explosion’ hazard when dealing with particles that have high dispersion ability and high mobility

2.2 Determining Characteristics of Dust Explosion

2.2.1 Characteristics of Dust Experiment

The fire triangle is a simple model to understand the necessary elements for the fires. The three elements are heat, fuel and an oxidizer which is oxygen usually. Fire can occur naturally when the elements that present and combined in the right mixture. In these cases, the dust acts as a fuel. Apart from that, a dust must be dispersed with the present of ignition source for an explosion to occur. Combustion of a solid material, especially dust explosion is mainly influenced by the dispersion characteristics of the particles in the combustion air.

Many studies had been carried out on the aluminium explosibility parameters such as minimum ignition energy and temperature, minimum explosible concentration, maximum explosion pressure and maximum rate of pressure rise. But here, the most important parameters that been focused are minimum ignition energy (MIE) and minimum ignition temperature (MIT). Most of the nanopowders have the MIE less than 1Mj and the lowest MIE indicate that the powder is extremely combustible (Wu et al., 2009). As the particle size decreases, the minimum ignition temperature (MIT) and minimum ignition energy (MIE) decrease which indicate high potential of explosion.

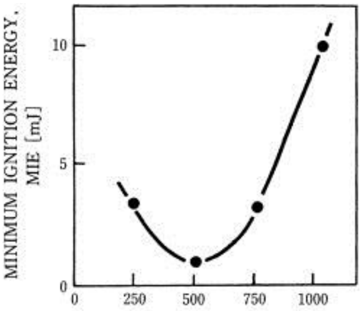

FIGURE 2.2 MIE with the respect of dust concentration (Eckhoff 2009)

Figure 2.2 illustrates the relation between the dust concentration and the minimum ignition energy (MIE). It shows that dust concentration of 500g/m3 has the lowest MIE which will ignite faster than the rest. Various particle sizes with different particles had been observed as well with the respect of the minimum ignition temperature, MIT as per Figure 2.3. For a same particle size of 50 micron meter, aluminium has the lowest ignition energy compared to polyethylene and optical brightener. Thus it is really crucial to study the impact of aluminium on the explosion since it can ignite with the less MIE.

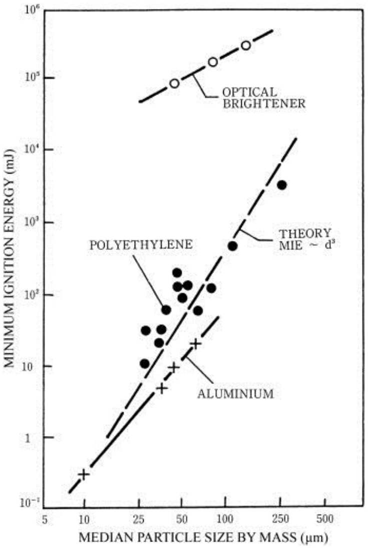

FIGURE 2.3 Ignition temperature for various type of particle (Eckhoff 2009)

2.2.2 Type of Experiment

Normally, for dust explosion researchers will conduct an experiment in order to determine all the parameters that cause the occurrence of the explosion. For the past few years, experiments on dust explosion were conducted using common calibrated equipment’s such as, Hartmann Tube and 20L Sphere

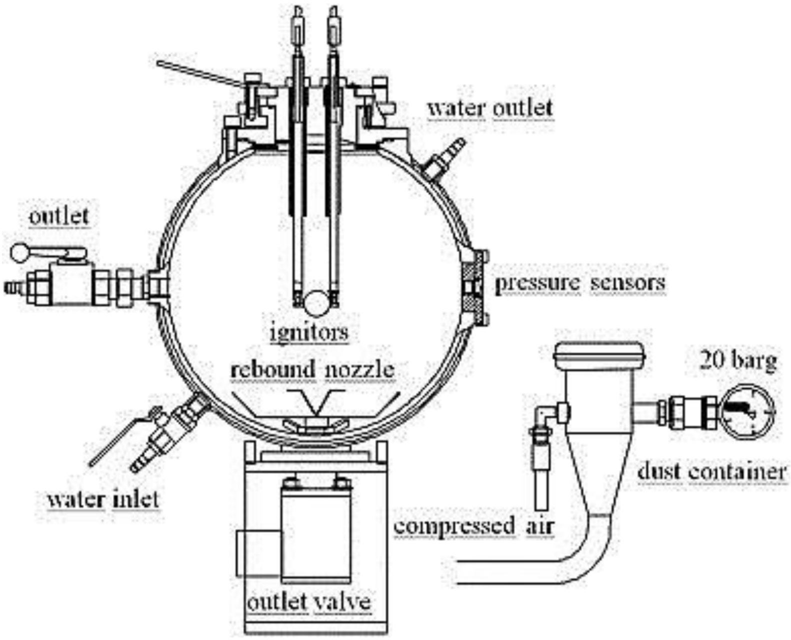

FIGURE 2.4 Parts of the explosion chamber

The 20L explosion chamber is a double-layered stainless steel vessel is referred with Figure 2.4. Water or other fluid is used to maintain initial temperature of explosion test. Normally water is used to cool the vessel to room temperature. The vessel wall consist of few connections such as the vacuum, exhaust, fuel inlet and air inlet. A glass window can be used to observe the light of ignition and explosion flames. Dust injection inside the vessel produces a turbulent fluid flow which will be decay over the time. The timing between the turbulent decay and the mixture ignition is of major relevance, since the flame propagation is significantly affected by the pre-ignition turbulence level (Cashdollar, 2000).

A sample vessel with volume by 0.6L is connected to the fast act valve. The dust sample can be dispersed to the chamber by compressed air through the dispersion nozzle. The pressure history in the chamber is recorded by the pressure sensor and data acquisition system. Explosion pressure p_m and normalized rate of pressure rise K_m can be obtained by analysis of the pressure history curve (Shengjun, 2010).

2.3 Previous Study on Dust Explosion

2.3.1 Experiment Based

With increase in the influence of nano technology, more and more materials are being generated within the nanometer range. It became to an interest of the researcher to find out the proper way during the production, handling and transportation of these materials as it can cause risk (Krietsch, Scheid, Schmidt, & Krause, 2015). Combustion of the solid materials especially dust explosion is mainly due to the influenced of the dispersion characteristics of the particles in the combustion air (Murillo et al., 2013) and ample of studies had been done on the particle sizes, particles concentration and influence of humidity on the aluminium itself.

Explosion dust clouds will be generated from the most organic and some from the non-metallic inorganic materials. Turbulence can affect the properties of the dust cloud and promote the dust explosivity and the mixing of the fuel and oxidizer have the impact of the dust concentration distribution as well (Murillo et al., 2013). As mention by (Pritchard, 2004), dust explosion involved with range of particle sizes range from a few micron to hundreds micron and the primary factor that stimulate the ignition sensitivity and explosion violence of a dust cloud is the particle size or the specific surface area. Here as per mention, the surface area increase as the particle size increase and based on a rule of thumb, explosion clouds will not be generated from dusts composed of particles with a size more than 500 micron. Dust is not homogeneously dispersed within the vessel as the multiple turbulent vortex is present as well and particles diameter greater than 100 micron meter is mainly pushed towards the wall (Murillo et al., 2013).

Another research done by (Wu, Ou, Hsiao, & Shih, 2010), discussed that, the risk of dust explosion is mainly due to the diameter of particles and it is evaluated as one of the important factors that contribute to the risk of dust explosion. Hence, there are also few parameters that ignite the explosion such as the turbulence, initial pressure and oxygen concentration. Using the 20L sphere apparatus, few experiment had been conducted that focus on the sizes of the aluminum. Table 2.1 below summarize the specification that been measured with various sizes. MEC is used to determine the smallest concentration of the material in the air that can denote flame propagation upon the ignition at a dust cloud state. From the ignition from the dispersing powders, it results in a dust cloud with an energetic ignition source whereas; the MIE is due to the lowest energy to ignite the dust.

TABLE 2.1 Properties of Aluminium particles with different sizes

Chemical Code	P_{max} (bar)	$(dP/dt)_{max}$ (bar/s)	K_{st} (bar.m/s)	MEC (g/m3)	MIE (mJ)
Al-35nm	7.3	1286	349	40	<1
Al-100nm	12.5	1090	296	50	<1
Al-40μm	5.9	282	77	35	59.7

(Wu Hong-Chun, Gau Chung-Yun, Ou Hsin-Jung , Deng-Jr Peng, & Shih, 2010)

Table 2.1 shows the smaller the particle sizes, the smaller the MIE and judging by the trend, the MIE would be smaller than 1mJ for aluminium particle that have the diameter size less than 10 μm.

2.3.2 CFD Simulation

Dust explosion is becoming one of the biggest threats to the industry. But now, from the latest technologies, there are two ways of studying the dust explosion. One is through setting up the different devices and equipment's either in small scale in laboratories or a large scale from the real equipment from the industry. The alternative way is by using the Computational Fluid Dynamics (CFD), in order simulate and also to validate the experiment from the laboratories (Di Sarli, Russo, Sanchirico, & Di Benedetto, 2014). CFD model is developed with the aim of simulating the turbulent flow in a confined, gas-solid flow induced by dispersion of the dust, with the effects on the dust concentration (Murillo et al., 2013).

CFD had been carried out to study the hydrodynamics of the flow of solid gas in a confined space. The two phase flow simulation was based on the Euler –Lagrange approach since the solid phase does not characterized with a high volume mixture. Besides, the simulation was simulated using the ANSYS FLUENT™ with a transient setup that uses DPM model to track the particles in the simulation. The result identified that the dust is dispersed accordingly to the variation in the mean diameter of the discrete phase at the ignition sources. The increase in pressure and velocity of the fluid phase cause the immediate expansion of gas in the vessels.

The concentration and the density of the aluminium is equal to 250g/m3 and 2700 kg/m3 respectively. At these condition, it is possible to assume the particle-laden flow approach in which the Eulerian method is used for the fluid phase and Lagrangian method is used for the solid phase (A. Di Benedetto, 2013). The fluid flow was simulated by resolving the time-averaged Navier-Stokes equation (Eulerian method) written in polar coordinates that shown below. The flow of the solid phase was solved using the discrete phase model (DPM) (Lagrangian approach). The interaction between the solid phase and the fluid phase is different based on the one-way, two-way and four-way coupling depending on the particle volume fraction, particle density and particle concentration.

Figure 2.5 is the classification proposed by (Elghobashi, 1994) It appears in these simulation that the condition of the aluminium (particle volume fraction = 0.00012, particle density, ρ_p=2719 kg/m^3 and the particle concentration, C=250 g/m^3)and the nature of the interaction between the fluid phase and the particles is two-way coupling, suggesting that the fluid flow affects the particles motion and vice versa neglecting the one-way and the four-way coupling. This assumption is also in line with the recent findings by Vreman, Geurts, Deen, Kuipers, and Kuerten (2009) who presented that, for particle volume fractions larger than 1.5%, the particle–particle interactions has a significant role in the development of the flow. The fluid flow was simulated by solving the time-averaged Navier-Stokes equation (Eulerian approach) that is written in polar coordinates that show in Equation 1:

$$\frac{1}{r^2}\frac{\partial(\bar{\rho}r^2\bar{v}r)}{\partial r}+\frac{1}{r\sin\theta}\frac{\partial(\bar{\rho}\bar{v}_\theta\sin\theta)}{\partial\theta}+\frac{1}{r\sin\theta}\frac{\partial\left(\bar{\rho}\bar{v}_\phi\right)}{\partial\phi}=0 \qquad (1)$$

Equation 2 to 4 was solved by using the k-epsilon model for the substantial derivatives velocity for the sphere.

Momentum balance equation, r co-ordinate

$$\bar{\rho}\left(\frac{\partial \bar{v}_r}{\partial t}+\bar{v}_r\frac{\partial \bar{v}_r}{\partial r}+\frac{\bar{v}_\theta}{r}\frac{\partial \bar{v}_r}{\partial \theta}+\frac{\bar{v}_\phi}{r\sin\theta}\frac{\partial \bar{v}_r}{\partial \phi}-\frac{\bar{v}_\theta^2+\bar{v}_\phi^2}{r}\right)=-\frac{\partial p}{\partial r}-\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\bar{\tau}_{rr}^{(v)}\right)+\frac{1}{r\sin\theta}\frac{\partial}{\partial\theta}\left(\bar{\tau}_{\theta r}^{(v)}\sin\theta\right)+\frac{1}{r\sin\theta}\frac{\partial}{\partial\phi}\left(\bar{\tau}_{\phi r}^{(v)}\right)-\frac{\bar{\tau}_{\theta\theta}^{(v)}+\bar{\tau}_{\phi\phi}^{(v)}}{r}\right]$$
$$-\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\bar{\tau}_{rr}^{(t)}\right)+\frac{1}{r\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\bar{\tau}_{\theta r}^{(t)}\right)+\frac{1}{r\sin\theta}\frac{\partial}{\partial\phi}\left(\bar{\tau}_{\phi r}^{(t)}\right)-\frac{\bar{\tau}_{\theta\theta}^{(t)}+\bar{\tau}_{\phi\phi}^{(t)}}{r}\right]+\bar{\rho}g_r \tag{2}$$

Momentum balance equation, θ co-ordinate

$$\bar{\rho}\left(\frac{\partial \bar{v}_\theta}{\partial t}+\bar{v}_r\frac{\partial \bar{v}_\theta}{\partial r}+\frac{\bar{v}_\theta}{r}\frac{\partial \bar{v}_\theta}{\partial \theta}+\frac{\bar{v}_\phi}{r\sin\theta}\frac{\partial \bar{v}_\theta}{\partial \phi}+\frac{\bar{v}_r\bar{v}_\theta-\bar{v}_\phi^2 cot\theta}{r}\right)=$$
$$-\frac{1}{r}\frac{\partial p}{\partial\theta}-\left[\frac{1}{r^3}\frac{\partial}{\partial r}\left(r^3\bar{\tau}_{r\theta}^{(v)}\right)+\frac{1}{r\sin\theta}\frac{\partial}{\partial\theta}\left(\bar{\tau}_{\theta\theta}^{(v)}\sin\theta\right)+\frac{1}{r\sin\theta}\frac{\partial}{\partial\phi}\left(\bar{\tau}_{\phi\theta}^{(v)}\right)+\frac{\bar{\tau}_{\theta r}^{(v)}-\bar{\tau}_{r\theta}^{(v)}-\bar{\tau}_{\phi\phi}^{(v)}cot\theta}{r}\right]-$$
$$\left[\frac{1}{r^3}\frac{\partial}{\partial r}\left(r^3\bar{\tau}_{r\theta}^{(t)}\right)+\frac{1}{r\sin\theta}\frac{\partial}{\partial\theta}\left(\bar{\tau}_{\theta\theta}^{(t)}\sin\theta\right)+\frac{1}{r\sin\theta}\frac{\partial}{\partial\phi}\left(\bar{\tau}_{\phi\theta}^{(t)}\right)+\frac{\bar{\tau}_{\theta r}^{(t)}-\bar{\tau}_{r\theta}^{(t)}-\bar{\tau}_{\phi\phi}^{(t)}cot\theta}{r}\right]+\rho g_\theta \tag{3}$$

Momentum balance equation, φ co-ordinate

$$\rho\left(\frac{\partial \bar{v}_\phi}{\partial t}+\bar{v}_r\frac{\partial \bar{v}_\phi}{\partial r}+\frac{\bar{v}_\theta}{r}\frac{\partial \bar{v}_\phi}{\partial \theta}+\frac{\bar{v}_\phi}{r\sin\theta}\frac{\partial \bar{v}_\phi}{\partial \phi}+\frac{\bar{v}_\phi\bar{v}_r-\bar{v}_\theta\bar{v}_\phi\cot\theta}{r}\right)=-\frac{1}{\sin\theta}\frac{\partial p}{\partial\phi}-\left[\frac{1}{r^3}\frac{\partial}{\partial r}\left(r^3\bar{\tau}_{r\phi}^{(v)}\right)+\frac{1}{r\sin\theta}\frac{\partial}{\partial\phi}\left(\bar{\tau}_{\phi\phi}^{(v)}\right)+\frac{\bar{\tau}_{\phi r}^{(v)}-\bar{\tau}_{r\phi}^{(v)}-\bar{\tau}_{\phi\theta}^{(v)}\cot\theta}{r}\right]$$
$$-\left[\frac{1}{r^3}\frac{\partial}{\partial r}\left(r^3\bar{\tau}_{r\phi}^{(t)}\right)+\frac{1}{r\sin\theta}\frac{\partial}{\partial\theta}\left(\bar{\tau}_{\theta\phi}^{(t)}\sin\theta\right)+\frac{1}{r\sin\theta}\frac{\partial}{\partial\phi}\left(\bar{\tau}_{\phi\phi}^{(t)}\right)+\frac{\bar{\tau}_{\phi r}^{(t)}-\bar{\tau}_{r\phi}^{(t)}-\bar{\tau}_{\phi\theta}^{(t)}cot\theta}{r}\right]+\rho g\phi \tag{4}$$

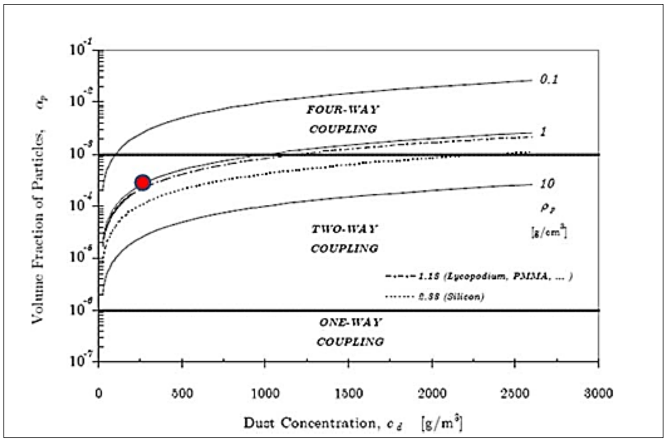

FIGURE 2.5 Classification of the interaction between fluid and particles (Elghobashi 1994)

In addition, (Laín, 2009) studied the consequence of simulation flow of two-way and four-way coupling of solid particles in a horizontal circular pipe. Particles with two different diameters 200 micron meter and 50 micron meter with a density of 1020 kg/m3 is used. The results shows that the dynamics of the larger particles (200 micron) is governed by the inertia due to particles-wall and inter-particles collisions. Whereas, the dynamics of the smaller particles (50 micron) is due to the turbulent fluid-particles interaction plays a significant role. But from this study, the particles volume fraction cannot be evaluated. The momentum balance equation for the DPM is shown as below;

$$\frac{du_p}{dt} = F_D(v - u_p) + \frac{g(\rho_p - \rho)}{\rho_p} + F \tag{5}$$

Where F is the gravitational force v and ρ are the velocity and density of the fluid phase, while u_p and ρ_p are the velocity and density of the particles. F_D $(v\text{-}u_p)$ is the drag force per unit mass of particle. F_D is the interphase momentum transfer coefficient and is a function of the Re number according to the following equation

$$F_D = \frac{18\mu}{\rho_p d_p^2} \frac{C_D Re}{24} \tag{6}$$

Where μ is the fluid viscosity and d_p is the diameter of the particles. The Re number in Eq 6. is a function of the difference between the fluid and the particle velocity

$$Re = \frac{\rho d_p |u_p - v|}{\mu} \tag{7}$$

For the fluid velocity (v) used in Eq. 5, values are not instantaneous, but rather they are constant over a certain time range.

2.4 Dust Explosion

Fire is caused due to these three factors which are fuel, oxidant and ignition which known as fire triangle. But for a dust explosion, it demands for two more factors which are mixing of dust and air and lastly the confinement of the dust cloud. Figure 2.6 is the explosion pentagrams that summarize the elements that trigger the explosion.

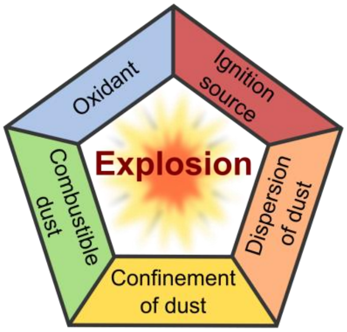

FIGURE 2.6 Explosion Pentagram

Dust explosion is produced by the rapid combustion of flammable material that suspended or dispersed in the air. Based on the various particle size of the dust, it is classified that with the decrease in particle size, the higher the rate of explosion and ignition to occur. From the studies done by Krietsch et al. (2015) these are the main properties that might either stimulate or impede the dust explosion:

- The increased specific surface area may lead to an increase in ignition sensitivity and reaction severity.
- Some powders may show pyrophoric behavior when sized down to nano-scale.
- Oxygen adsorption at reactive surfaces of individual particles may result in a passivation of the powder.
- Powders may tend to form agglomerates which are of micro-scale.

For a confined dust explosion, the speed and heat of combustion will be supplemented by rapid increase of pressure. The flame will propagate through the dust clouds and huge amount of heat and reaction products is produced (Abbasi & Abbasi, 2007). Commonly dust explosion reaction is as shown below and nevertheless metal dust can also react with nitrogen or carbon dioxide to generate heat that cause explosion.

$$\text{Fuel} + \text{oxygen} \rightarrow \text{oxide} + \text{heat}$$

2.5 Factors Affected Dispersal Behavior

Nanoparticle is well known since it has large surface areas per unit volume which contribute for the dispersion that cause explosion. Factors that lead to the ignition, burning and propagation of the fires is when the nanoparticles suspended in the air and these factors can be characterized in order to control the explosion. Based on the previous studies by (Murillo et al., 2013), there are few elements that cause the explosion which are:

- Particle size distribution (PSD)
- Degree of agglomeration
- Particle shape
- Dust concentration within the cloud
- Degree of turbulence of the suspension

Two important factors that have high possibilities causing the dust explosions are particle size and degree of agglomeration. As mention previously, an increase in the surface per volume ratio will eventually increase the risk of explosion. It is found from a study (Bouillard, Vignes, Dufaud, Perrin, & Thomas, 2010) saying that as the particle size decreases, the minimum ignition temperature (MIT) and the minimum ignition energy (MIE), decrease. This demonstrates that, by using the nanoparticles which eventually have small size have high possibility of explosion and can cause high and enormous impact to the environment, surroundings and to the equipment.

CHAPTER 3

METHODOLOGY

3.1 Research Methodology

Computational Fluid Dynamics (CFD) is applied in this study after considering that there will be two interacting phases in a different way. To begin with, the fluid phase is described by the numerical solutions (Finite volume method) of the Navier Stoke equation as it considers air as a continuous medium. It is likely to solve the mass, momentum and energy conservation of laws for the fluid during the dispersion stage after the discretization mesh and calculating the mean value of the specific flow parameter in each and every cell.

CFD is a computational simulations tool that is used to solve, for a specified system, problems related to fluid flow, heat transfer and other physical processes. In general, CFD works by solving the governing laws of fluid dynamics numerically over a chosen domain on interest with specified boundary conditions. The fundamental basis of computational fluid dynamics is the Navier-Stoke equations which are derived from the Newton's Second Law of conservation of momentum. These equations are supplemented by equations conservation of mass (also known as continuity equations) and conservation of energy.

A Computational Fluid Dynamics (CFD) simulation is carried out to study the fluid motion and the hydrodynamics of the suspensions. The simulation was based on an Euler- Lagrange as the flow variables are characterized with two phase during the dispersion process. Apart from that Euler- Lagrange is used as the amount of the solid phase does not represent a high volume fraction in the mixture. Here Euler is used since it can be used for the fluid phase at which the fluid is in the continuous flow whereas; the Lagrange is dedicated for the solid phase which will be used for the discrete particle.

Two ways coupling is considered since the fluid flow will eventually affect the particle motion and vice versa. It is also used to solve the discrete and the continuous phase equations.

On the one hand, as this project will be conducted in the transient mode, the analysis of the process with a dynamic boundary condition needs an finer mesh during the meshing process,(Murillo et al., 2013). Transient state also affected by few characteristics of the flow and the boundary condition that will be defined at the gas injection point. This is because the momentum of the fluid flow constantly changes by the gas expansion. Besides, the micrometric size scale for the disperse phase influence greatly on the particle density which is higher than the gas density.

3.1.1 The explosion apparatus: 20 L bomb

CFD simulation was simulated using the standard 20 L sphere apparatus. The bottom line of the experiment is the spherical explosion chamber. The chamber is made up of stainless steel and can resist up to 30 bar (static pressure). Rebound nozzle is places at the bottom of the chamber pneumatically by the means of auxiliary piston. The input section of the chamber is connected to a container (V=0.0006 m^3) by means of which the dust is injected into the explosion chamber with the inlet pressure of 21 bar of compressed air. The sphere is also connected to a vacuum line that is used to prepare the aluminium-air mixture.

3.1.2 Computational domain and mesh

The computational domain and the mesh were built as tri-dimensional (3D) by the means of the software ANSYS FLUENT. The sphere is modelled with the inlet of the dust without including the rebound nozzle. Figure 3.1 is the structure of the domain that was built using Geometry Modeler and Table 3.1 is the details of the domain. Whereas Figure 3.2 is the structure of the mesh and the details is given in Table 3.2.

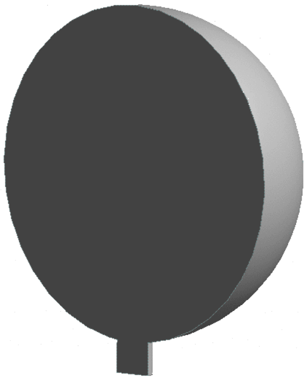

FIGURE 3.1 Structure of Domain

TABLE 3.1 Geometrical Details of the Domain

Geometry Details	Value
Sphere diameter	0.336m
Tube diameter	0.02m
Tube length	0.72m

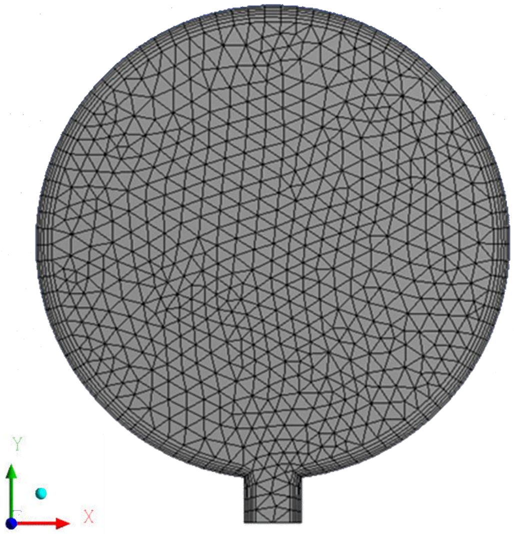

FIGURE 3.2 Structure of mesh

TABLE 3.2 Meshing Details of the Domain

Mesh Details	Values
Number of Nodes	13883
Number of Elements	43417

3.1.3 Numerics

The governing hydrodynamics fluid flow equations were discretized using the finite-volumn formulation on the three-dimensional (3D) unstructured mesh shown previously. The spatial discretization of the model equations used first-order schemes for convective terms and second order schemes for diffusion terms. First order time integration was used to discretize temporal derivatives with a time step of 1.10-4 s. Equivalent calculations were performed by means of the segregated pressure-based solver from the ANSYS Fluent. The coupled semi-implicit method for pressure linked equations (SIMPLE) was used to solve the pressure-velocity coupling. In order to achieve the convergence, all residuals were set equal to 1.10-6.

The discrete phase model was described by ordinary differential equations whereas the continuous flow described as partial differential equations. Thus, the DPM used its own numerical mechanism and discretization schemes. In situations where the particles are far from hydrodynamics equilibrium, an accurate solution can be achieved quickly with a higher order scheme. Thus, Euler integration as lower order scheme and the coupled semi implicit trapezoidal integration as higher order scheme are used. The particle tracking integration time step was taken equal to the fluid flow time step, 1.10-4 s.

3.1.4 Simulation condition

The fluid is air at constant atmospheric temperature. As initial condition, the same condition is adopted at which both air and the aluminium will be injected at the pressure of 21 bar. The mixture of the air and the aluminium is fed into the chamber for 40s with very low velocity (0.001 m/s).and the properties of the aluminium is given as below in Table 3.3.

TABLE 3.3 Aluminium particles data

Aluminium Data	Values
Density (kg/m^3)	2719
Diameter (nm)	1
Concentartion (g/m^3)	250

List of data involving the parameters for the explosion must be obtainable in order to develop the dispersion model in the CFD software. These data is obtained from the research analysis of the experiment data that been conducted from the past journals and research which will used subsequently as an input data in the simulation. All the input data for the simulation is been attached in the appendices for references.

Apparently, modelling in CFD needs some basic fundamental on how to process the software. Then, a transient model with a respect to the time will be modeled in order to study the dispersion behavior of engineered nano material that will cause the explosion. Since the input data was used from an experiment based, therefore the results from the modelling should be validated and compared with the results of the experiment before a conclusion.

CHAPTER 4

RESULTS AND DISCUSSION

4.1 Model Comparison

Dust explosion is a phenomena that a flame will be propagated in a combustible cloud particles dispersed in the air. The particle size has a significant impact on the ignition and the explosion which strongly influenced by the particle size. During the entrance of the feeding phase, the gas velocity at the entrance is at sonic condition and towards the end, the gas velocity significantly decreases. The important factor in these simulations is the pre-ignition turbulence level and the dust dispersion for nano and micron size aluminium particles. Figure 4.1 is the pressure vs. time graph as computed in the explosion sphere. From the pressure plot, the feeding phase of the mixture of air and the aluminium dust is injected form the inlet of sphere with high pressure (A. Di Benedetto, 2013). The end time of the feeding phase may vary depending on the dust concentration and the sizes. But the results shows that the final pressure profile in the sphere is compared to the experiment data that is available in the literature review. It shows that the simulation that been conducted has and error of 14% and it shows a good agreement and acceptable.

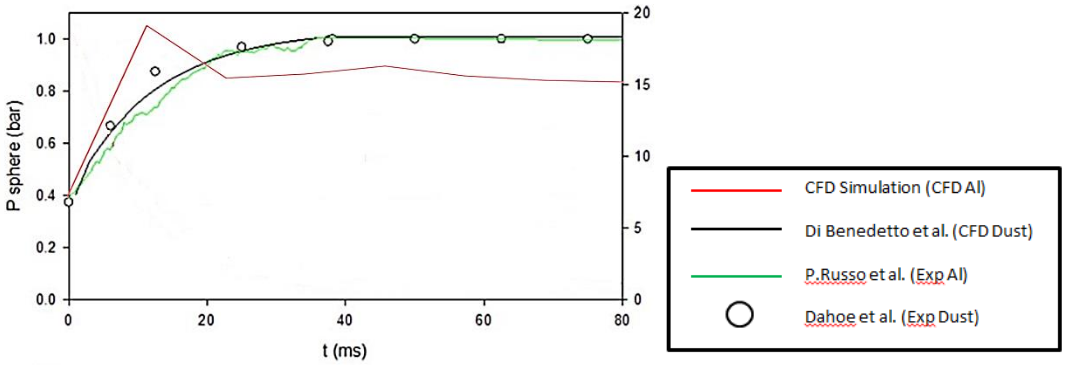

FIGURE 4.1 Pressure time histories computed in the explosion sphere

4.2 Turbulence Kinetics Energy

The pre-ignition turbulence plays an important role in the explosion behavior and as a results, turbulence kinetics energy is studied form the simulation that been simulated using ANSYS Fluent. Turbulence kinetics energy is one of the important parameter under these studies. Turbulence kinetics energy is the mean kinetics energy per unit mass associate with eddies in the turbulent flow that can be produced when there is a friction, fluid shear or external force.

Figure 4.2 shows the time sequence of maps of the turbulent kinetic energy over the symmetry plane of the chamber in the case of nano size of aluminium. It is crucial to note that the contour for turbulent kinetics energy for nano material is higher compared to the micron size (Figure 4.3) that is located at the center of the chamber, at which the particles will agglomerates and form the dust cloud. The maximum value for the turbulence kinetics energy for nano size is 4.317e-5 m^2/s^2 whereas for micron size aluminium it is quite low 3.858e-5 m^2/s^2. Based on studies by (Murillo et al., 2013) when the particles dispersed into the air, the particles tend to agglomerates each other and this is where the turbulence kinetics energy is high The reason behind this is that the nano size of aluminium has higher surface area per volume ratio compare to micron thus allowing the turbulent eddies inside the chamber for nano size is higher than micron. Apart from that, higher surface area also plays an important role where it increases the tendency of catching fire at fast rate that cause explosion. Subsequently, the MIT, of the particular particles decreases and chances for the explosion to occur is high.

Even though the contour for nano and micron size of aluminium shows a similarity but the turbulence kinetics energy for nano size has higher value. The turbulent kinetic energy is higher at 20 sec and the energy grows bigger at the middle of the chamber. The reaction between the air and the aluminium is fast at which even at the 5 sec the dust cloud is formed near to the feeding phase of the inlet.

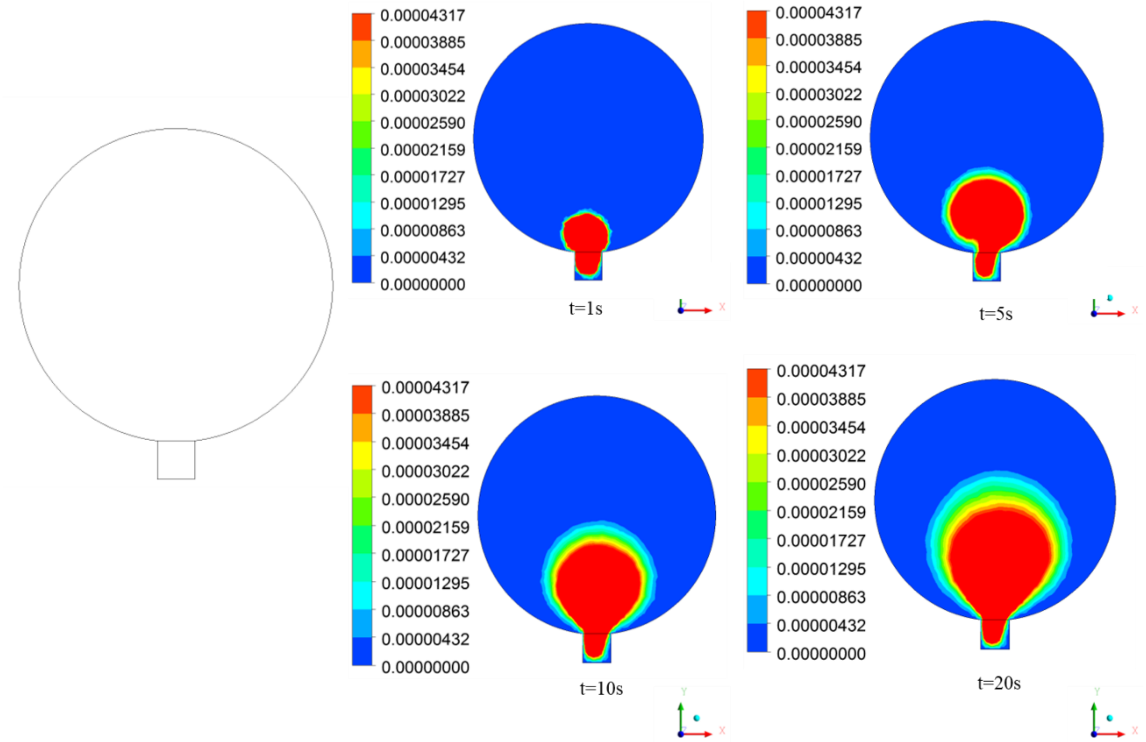

FIGURE 4.2 Time sequence of the maps of turbulent kinetic energy (m2/s2) frontal view for nano size particles

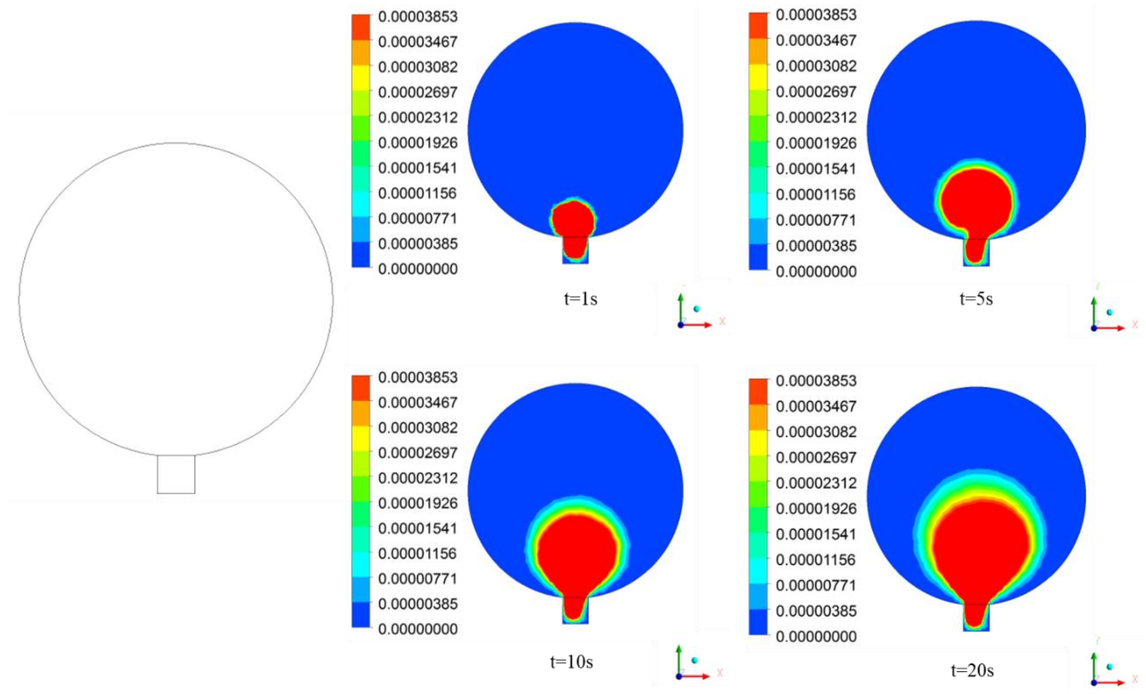

FIGURE 4.3 Time sequence of the maps of turbulent kinetic energy (m2/s2) frontal view for micro size particles

4.3 Velocity Vector

The velocity streamlines with respect to the velocity vector for the nano and micron size aluminium forms non-symmetric fields' contours as shown in Figure 4.4 and Figure 4.5. Even though the turbulence kinetic energy contour shows it is symmetrical but at the same time step, the streamline that symbolize by the velocity shows that it is non-symetric field. This behaviour has been previously found by (Kartushinsky, Michaelides, Rudi, Tisler, & Shcheglov, 2011). In specific it is pointed that the distribution is asymmetric because of the gravitational effects on the particles. The research that been done developed a 3D model of a gas-solid particle flow in a horizontal pipe showing that the presence of particles in the flow has a significant effect on all flow variables and highlighted that all the distribution become asymmetric due to gravitational effect on the particles and physical effect related to the different in the densities of two phases (A. Di Benedetto, 2013).

The velocity streamline as in Figure 4.4 and 4.5 illustrate the dispersion of the mixture of air and aluminium which the turbulence can be found at the inlet of the feeding phase itself. The turbulence can be seen more clearly from the streamline both sizes where the particles seem to be bias at one side of the chamber but it start to develop evenly after the 20 sec. The velocity of the mixture for nano size of aluminium shows a higher compare to the micron size. The reason behind these is that, a nano particle is smaller and lighter and will travel in the chamber more faster compare to the mocron size. Thus, due to its lightest weight nano particles has a velocity of 0.1356 m/s slightly higher compare to micron which is 0.1303 m/s.

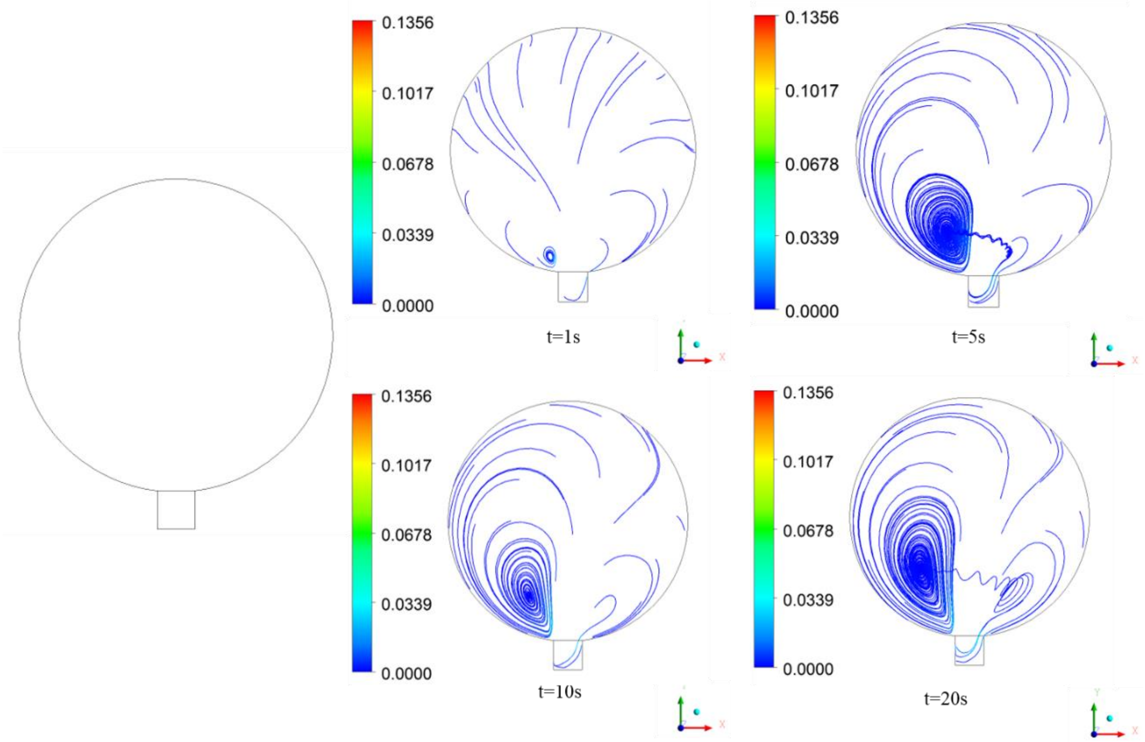

FIGURE 4.4 Time sequence of the maps of particles streamlines in velocity (m/s) frontal view for nano size particles

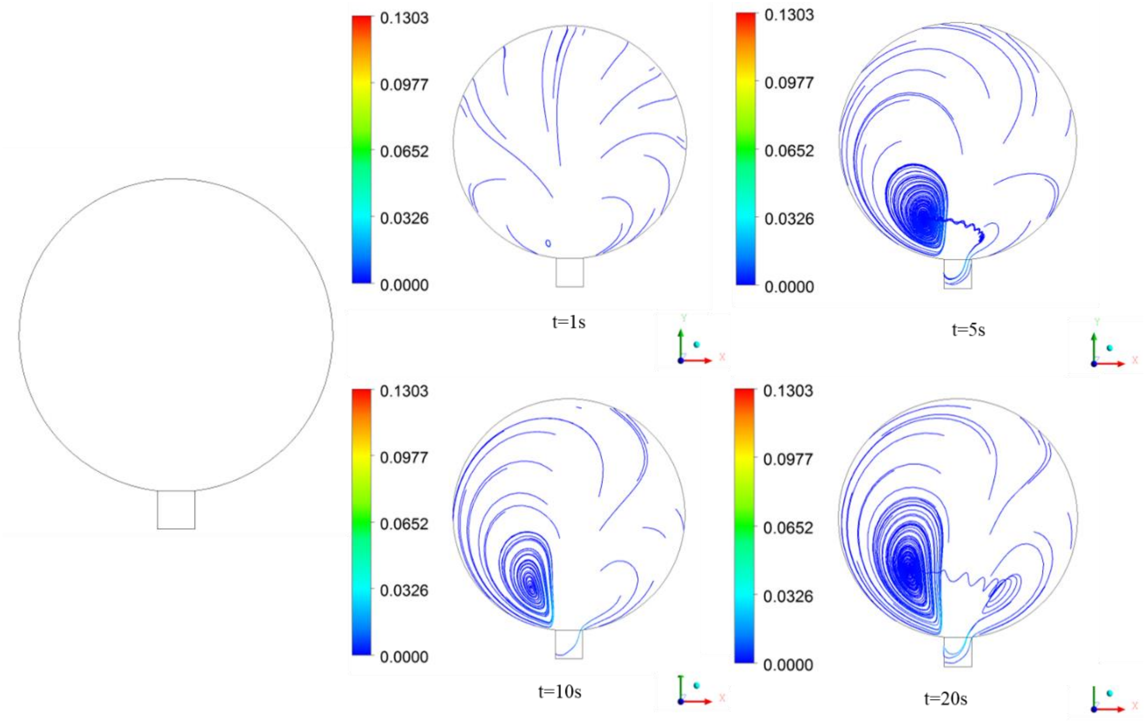

FIGURE 4.5 Time sequence of the maps of particles streamlines (m/s) frontal view for micro size particles

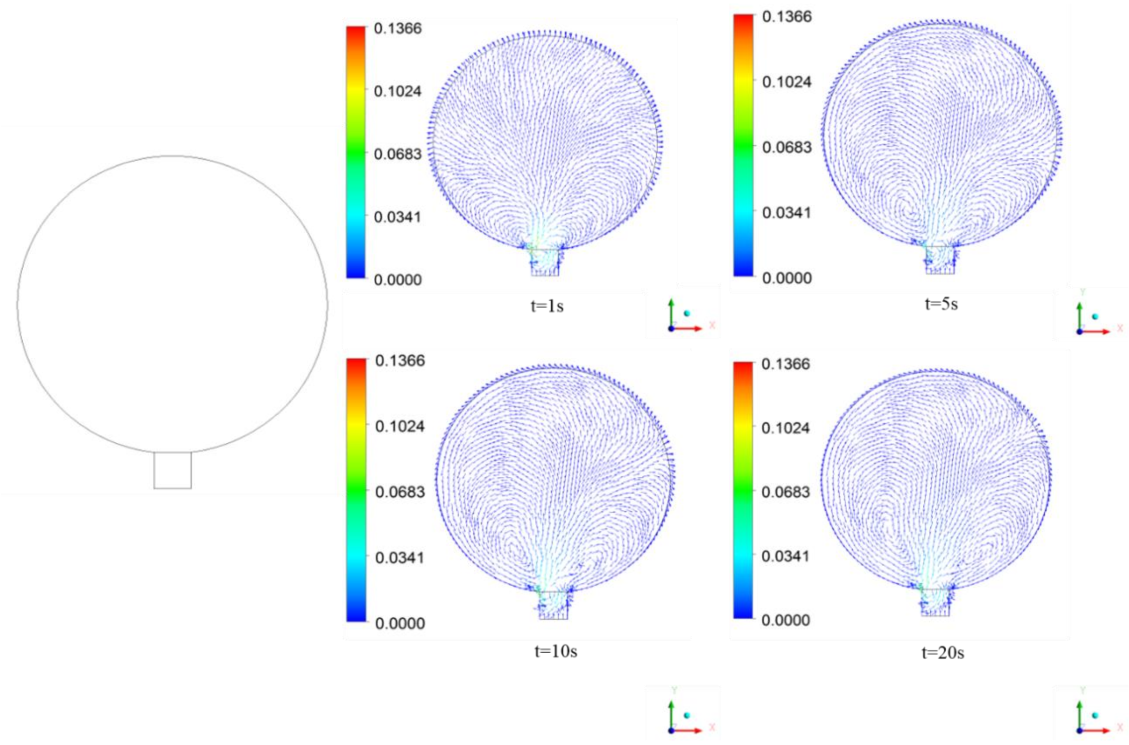

FIGURE 4.6 Time sequence of the maps of velocity vector (m/s) frontal view for nano size particles

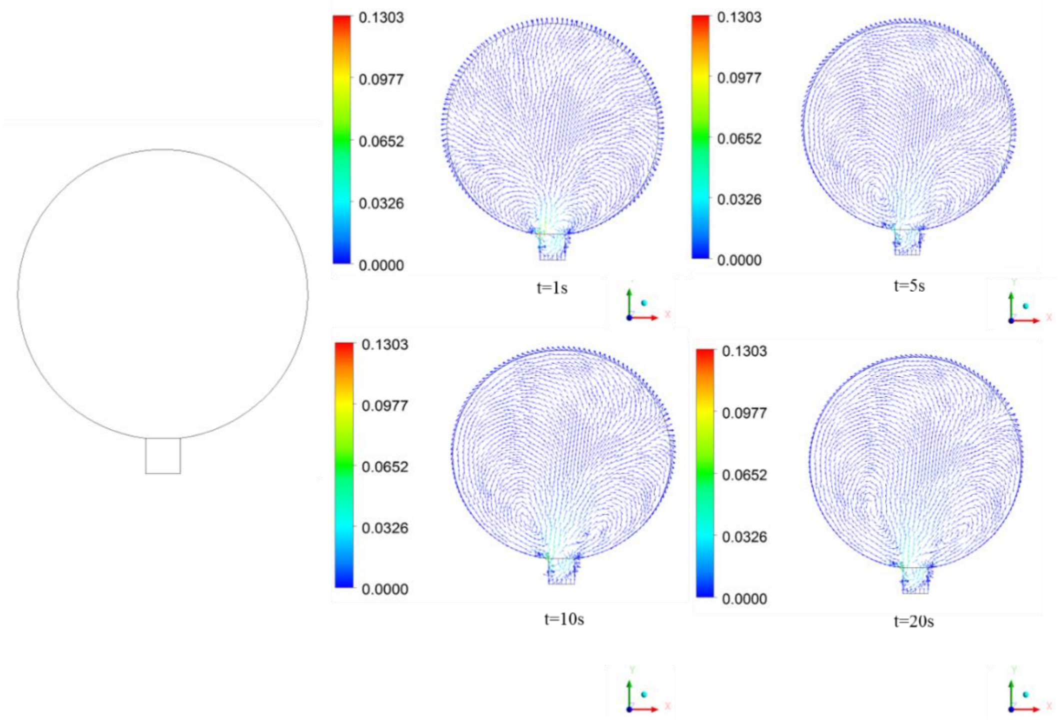

FIGURE 4.7 Time sequence of the maps of velocity vector (m/s) frontal view for micro size particles

4.4 Impact

Velocity and turbulence kinetics energy is interrelated to each other. By achieving higher turbulence kinetics and velocity vector for nano size of aluminium it illustrate that when the mixture is dispersing at fastest rate it will eventually lead to higher turbulence in the chamber that associate with the kinetic energy. The agglomeration of the particles take place rapidly once both air and the aluminium particles is injected at the inlet of the feeding phase. The dispersion of the mixture will form a dust cloud that disperse in the explosion chamber and eventually will cause the explosion to happen once it reach it’s the minimum ignition energy.

As of the application of this project, CFD simulation can simulate to understand the parameters of the dispersion that will lead to the explosion to occur in the real industries and understand how the dust cloud is generating that lead to agglomeration and explode once it reach its maximum point.

CHAPTER 5

CONCLUSION & RECOMMENDATION

From this project entitled “Investigating Dispersal Behaviour Lead to an Explosion of Engineered Nano Material using Computational Fluid Dynamics (CFD) a 3D model was developed to describe the turbulent flow field induced by the dust feeding and the dispersion with the 20L explosion bomb. The developed CFD model has been successfully validated against the measurement of the time histories of the pressure that is available in the literature with 14% error.

By simulating the entire project through a transient mode, more accuracy is expected due to the time marching solutions. It is crucial to analyze the dust explosion using the transient mode since the time scale factor can be used to understand more precisely on the particle sizes and the degree of agglomeration that cause the dispersion of the dust within the chamber .

Aluminium with nano size particles has a higher surface area that will eventually cause explosion due to its tendency of catching the fire at a fast rate. The turbulence kinetic energy is tremendous higher at the center of the chamber for nano size aluminium. It is pointed that the distribution of all parameter is asymmetric because of the gravitational effects on the nano size particles. Nano size particles will have lower ignition energy that will allow the ignition due to electric/electrostatic sparks, collision, or mechanical friction/impact during various chemical operation such as mixing, grinding, drilling, sanding, cleaning (Mittal, 2014). Careful precaution need to be taken to prevent ignition of the dust clouds from the particles in the air by the ignition sources.

As for recommendation, it is recommended to study the dust dispersion with various types of particle with different concentration as per available in the literature to observe how does different particle react with the air with different concentration that will cause dust dispersion in the confined chamber that lead to explosion.

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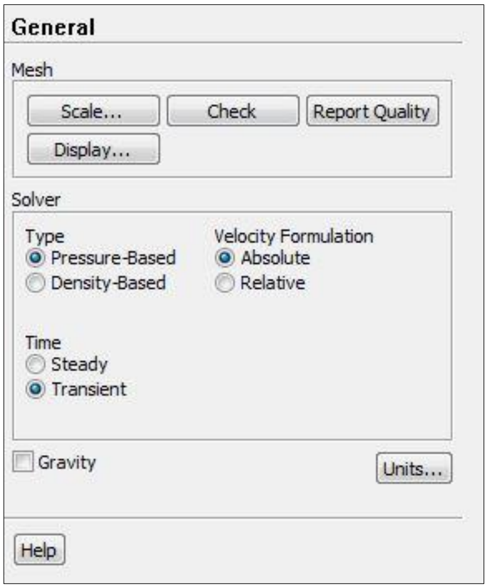
APPENDICES

The attached figures is the raw data that been used in the ANSYS FLUENT software version 14.0.



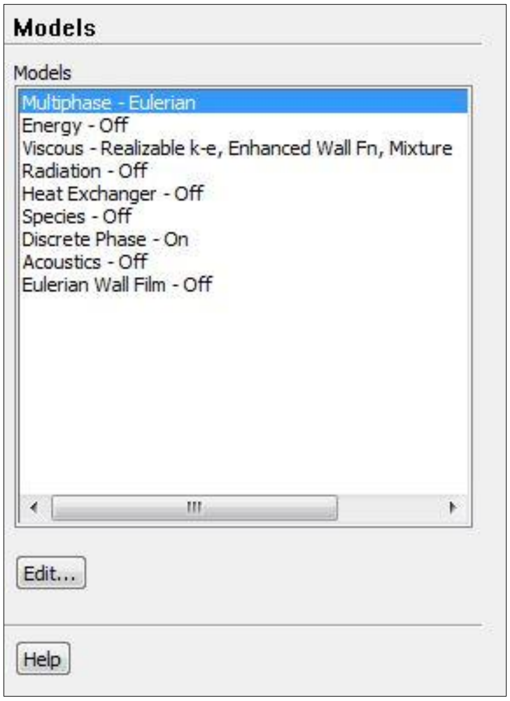
Solver

Type
● Pressure-Based
○ Density-Based

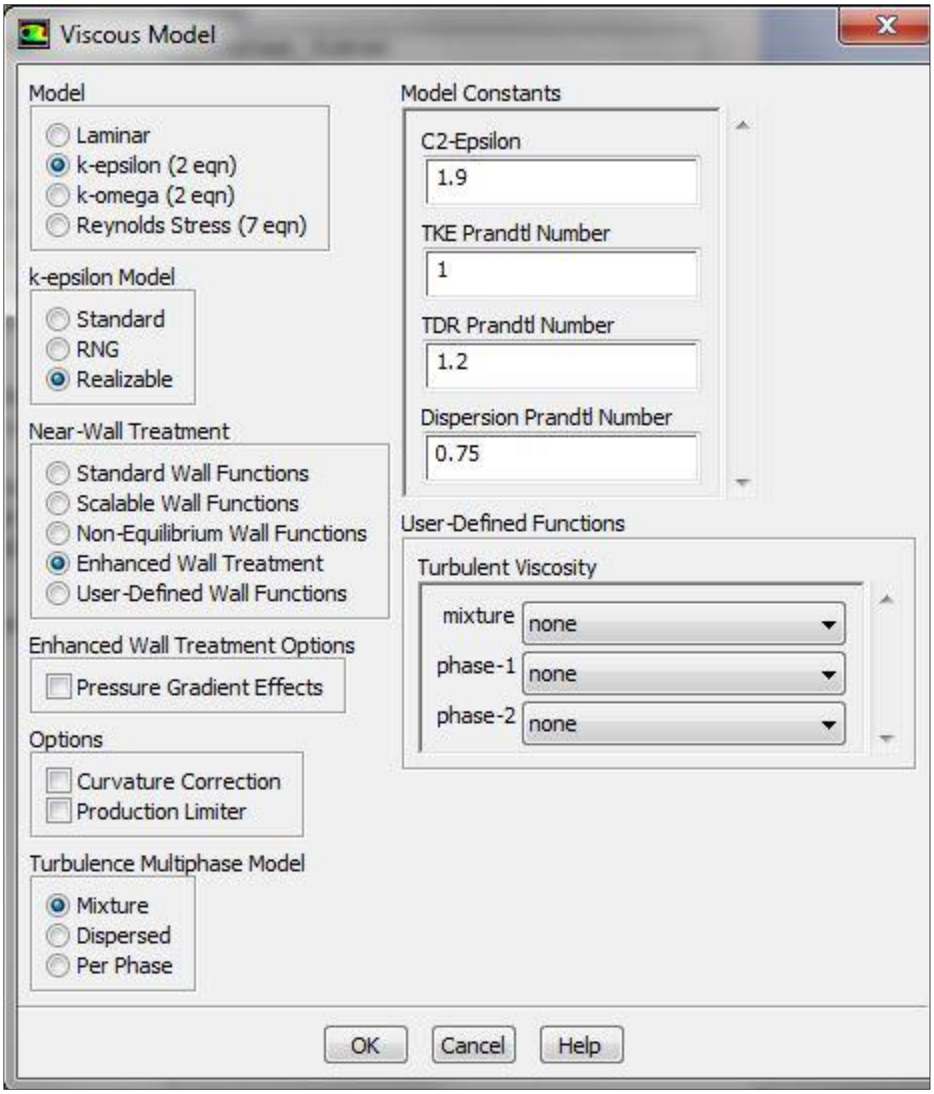
Velocity Formulation
● Absolute
○ Relative

Time
○ Steady
● Transient

☐ Gravity



Models
Multiphase - Eulerian
Energy - Off
Viscous - Realizable k-e, Enhanced Wall Fn, Mixture
Radiation - Off
Heat Exchanger - Off
Species - Off
Discrete Phase - On
Acoustics - Off
Eulerian Wall Film - Off



Viscous Model

Model
- ○ Laminar
- ● k-epsilon (2 eqn)
- ○ k-omega (2 eqn)
- ○ Reynolds Stress (7 eqn)

k-epsilon Model
- ○ Standard
- ○ RNG
- ● Realizable

Near-Wall Treatment
- ○ Standard Wall Functions
- ○ Scalable Wall Functions
- ○ Non-Equilibrium Wall Functions
- ● Enhanced Wall Treatment
- ○ User-Defined Wall Functions

Enhanced Wall Treatment Options
- ☐ Pressure Gradient Effects

Options
- ☐ Curvature Correction
- ☐ Production Limiter

Turbulence Multiphase Model
- ● Mixture
- ○ Dispersed
- ○ Per Phase

Model Constants

C2-Epsilon: 1.9

TKE Prandtl Number: 1

TDR Prandtl Number: 1.2

Dispersion Prandtl Number: 0.75

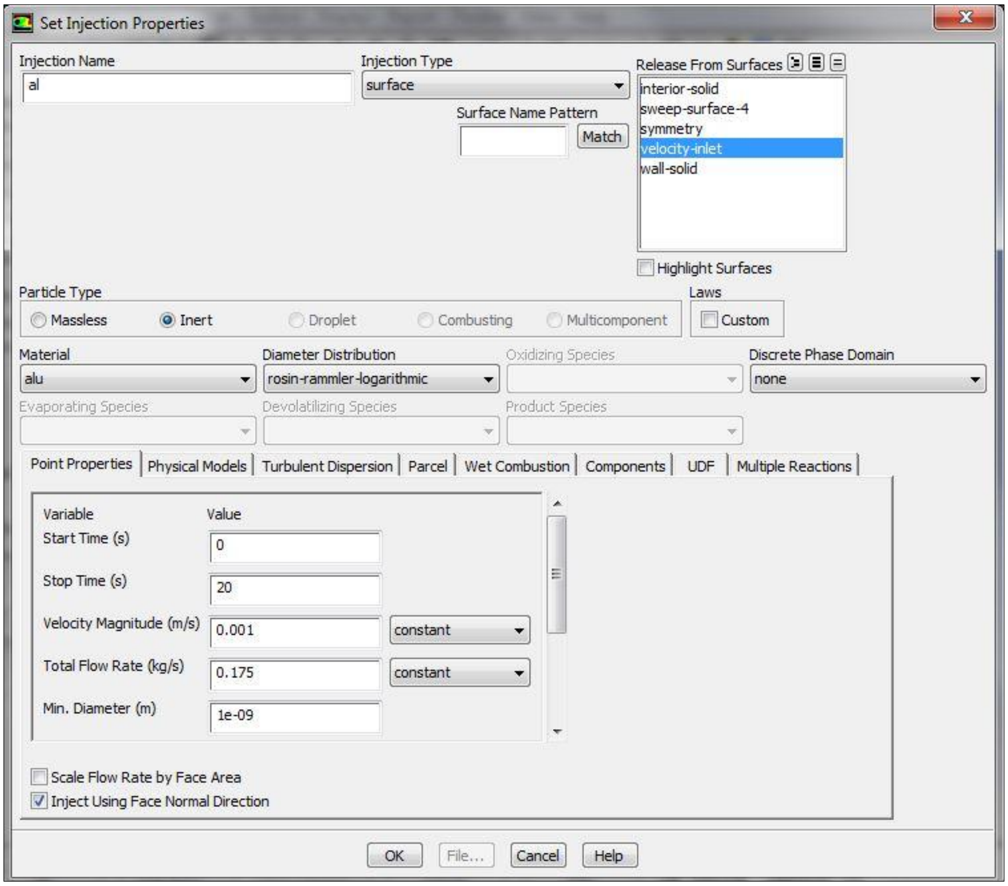
User-Defined Functions

Turbulent Viscosity

mixture: none

phase-1: none

phase-2: none



Set Injection Properties

Injection Name: al

Injection Type: surface

Surface Name Pattern: Match

Release From Surfaces:
- interior-solid
- sweep-surface-4
- symmetry
- velocity-inlet (selected)
- wall-solid

☐ Highlight Surfaces

Particle Type: ○ Massless ● Inert ○ Droplet ○ Combusting ○ Multicomponent

Laws: ☐ Custom

Material: alu

Diameter Distribution: rosin-rammler-logarithmic

Oxidizing Species:

Discrete Phase Domain: none

Evaporating Species:

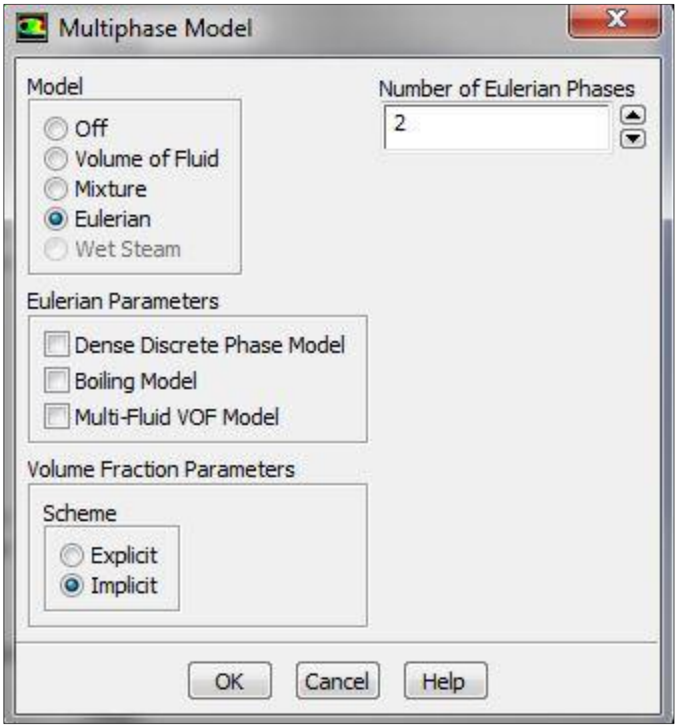
Devolatilizing Species:

Product Species:

Variable	Value	
Start Time (s)	0	
Stop Time (s)	20	
Velocity Magnitude (m/s)	0.001	constant
Total Flow Rate (kg/s)	0.175	constant
Min. Diameter (m)	1e-09	

☐ Scale Flow Rate by Face Area

☑ Inject Using Face Normal Direction



Multiphase Model

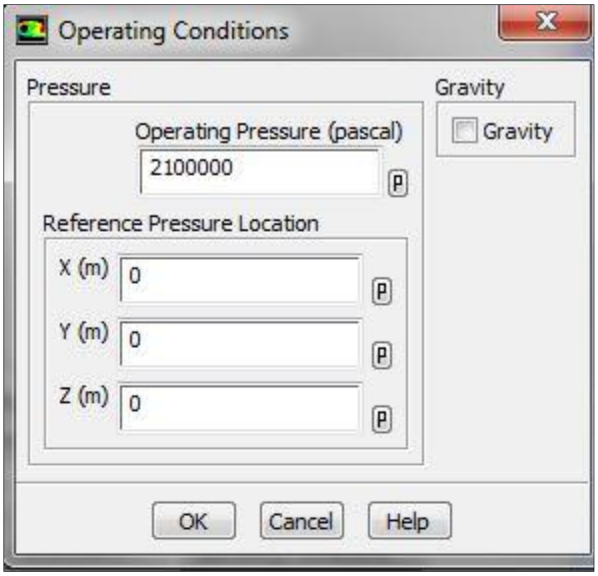
Model:
- ○ Off
- ○ Volume of Fluid
- ○ Mixture
- ● Eulerian
- ○ Wet Steam

Number of Eulerian Phases: 2

Eulerian Parameters:
- ☐ Dense Discrete Phase Model
- ☐ Boiling Model
- ☐ Multi-Fluid VOF Model

Volume Fraction Parameters

Scheme:
- ○ Explicit
- ● Implicit



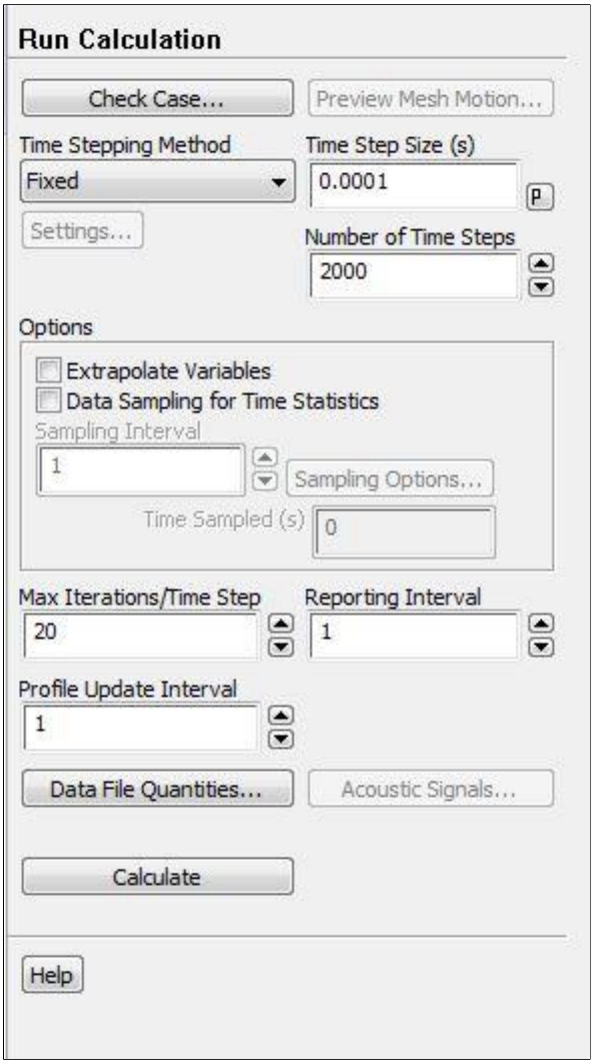
Operating Pressure (pascal): 2100000

☐ Gravity

X (m): 0

Y (m): 0

Z (m): 0



Time Stepping Method: Fixed

Time Step Size (s): 0.0001

Number of Time Steps: 2000

☐ Extrapolate Variables

☐ Data Sampling for Time Statistics

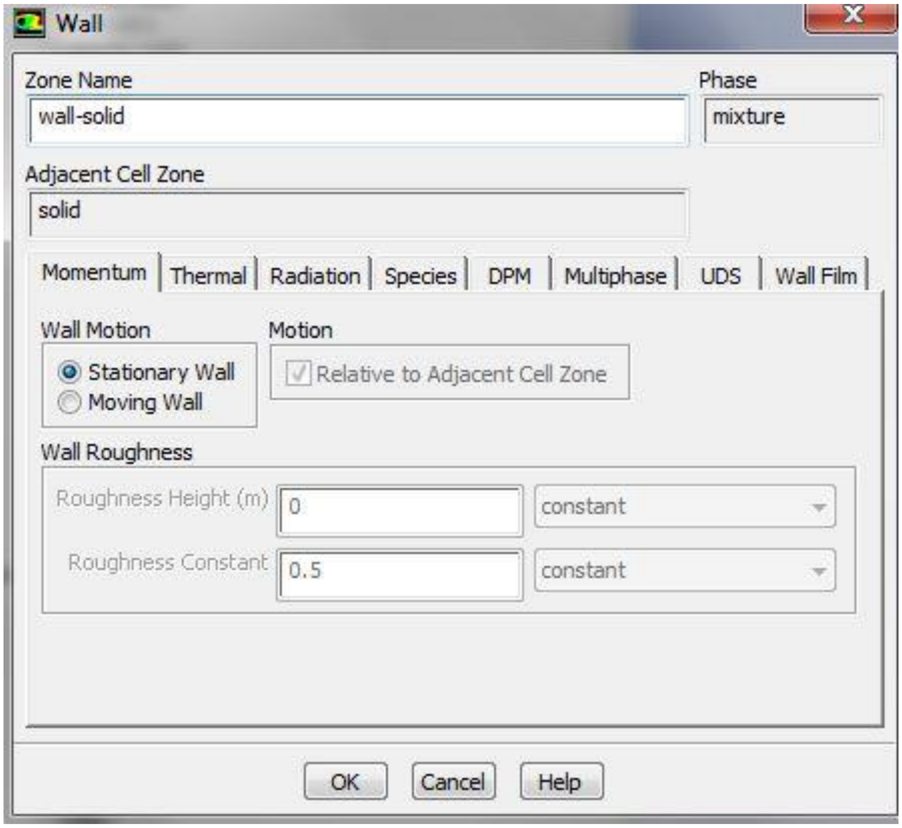
Sampling Interval: 1

Time Sampled (s): 0

Max Iterations/Time Step: 20

Reporting Interval: 1

Profile Update Interval: 1



Zone Name: wall-solid

Phase: mixture

Adjacent Cell Zone: solid

Wall Motion
● Stationary Wall
○ Moving Wall

Motion
☑ Relative to Adjacent Cell Zone

Wall Roughness

Roughness Height (m)	0	constant
Roughness Constant	0.5	constant