Analysis of Vapor Cloud Explosion using Computational Fluid Dynamics

Safety & Risk Engineering Project II (ENGI 915B)

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Project Report

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Abstract

The Vapor Cloud Explosion accidents are critical and caused enormous losses of personnel lives, assets, and money. The literature review of three main topics in the Vapor Cloud Explosion (VCE) is studied. These categories are the formation, where the literature proposed the nature of the VCE and the initiation of the explosions. Then the analysis using Computational Fluid Dynamics (CFD) is studied in the literature. The objective of this study is to simulate the formation of a Vapor cloud in different scenarios and then to propose different mitigation tools and evaluate the effectiveness of the tools. The mitigation techniques in literature are studied, and some useful means will be taken into consideration in the simulation and the results. The methodology involves CFD analysis of a vapor cloud explosion using FLACS software. The VCE control methods used in this study are Hyper-mist System, Water Sprinkler system & Blast Wall. The fault tree analysis is developed for the VCE to examine the causes of the VCE. Besides that, the Event tree diagram is developed to study the consequences of the VCE. The study of the vapor cloud requires initial modeling of the accident area. A crude oil section of a refinery is chosen for that purpose, and a CAD model of the crude oil section with and without fire & explosion control systems are generated in FLACS geometry module CASD. The work shows successful simulation runs of dispersion of the Vapor cloud, as found in the results section. Afterward, the work on the simulation are carried out to introduce two ignition sources with and without the control tools, and results are generated. A Design of Experiment approach has been used on some of the dispersion simulation outputs to study the impact of change in variables controlling the scenario. The results from CFD simulations show minimal impact of vapor cloud control methods used in the study. Limitations imposed by the FLACS as well as the open space scenario of the study can be considered as the reasons for such minimal impact of the vapor cloud control techniques.

Table of Contents

List of Figures:

List of Tables:

1. Introduction

Gas explosions and fire are one of the many critical and hazardous events in the oil & gas industries. The consequences of such accidents may lead to fatality, considerable losses in terms of assets, and money. Understanding the accidents through graphical simulations can provide new insight into what went wrong and what might go wrong in the future. Conducting experiments in such a disastrous situation is both expensive and dangerous. Studying such a scenario in a virtual environment reduces the risk. Literature shows how accidents related to Vapor Cloud Explosions (VCEs) are the most severe threat to the refining and petrochemical industries. Due to that, many papers discuss methodologies for this problem (Tang and Baker 1999). Others refer to a lack of knowledge in cloud formation and the hazard afterward as one of the leading causes of the problem and the developed hazardous consequences (Strehlow 1973). Mitigation of fire has been typically dealt with water spraying. New technologies such as the Hyper-mist system has gain traction in terms of efficiency to reduce fire damage. Implementation of fire control systems such as sprinkler, hyper-mist & blast wall into Computational Fluid Dynamics (CFD) analysis can provide knowledge in cloud formation and dissipation. Thus, improving the chance to understand the remaining hazard after the accident.

2. Literature Review

In this section, the literature has been studied. The VCE literature is rich, and for our project scope of work, the literature review is analyzed and categorized into three fields of studies: VC Formation & Explosion, VCE & CFD Analysis, and the mitigation techniques in the literature.

2.1 Vapor Cloud Formation & Explosion

Most of the refineries that are unconfined, semi-confined, or confined fire occurs by some form of ignition explosion. Chemical or petrochemical manufacturing plants, the vapor cloud explosions (VCE), are the leading factors of catastrophic losses. As the present tendency towards making plants to make enormous volume, higher temperature, pressure, and considerable inventory hold up, the fire has been escalating both in numbers and gravity. Usually, failure or malfunction of valves, fittings, piping, which eventually lead to vessel failures, are the common causes of the maximum number of accidents. On the other hand, transport-related accidents happen either by the derailment, which leads to fracture of the container (Dadashzadeh et al. 2013).

Epstein and Fauske (2007) imply that accidental discharge of liquid or gaseous flammable substances indoor or outside is always a safety problem and, no matter what should be considered for oil and gas industries. The discharge mostly happens in the form of negatively or positively buoyant, which mixes with the ambient of air. All possible fuel and air mixture compositions occur within the spread area and far from its source. It happens by rupturing a pipeline while transferring, overfilling of a tank, spillage from a receiving or discharging facility, uncontrolled vapor, or liquid discharge from a confined tank, etc. In most cases, liquefied hydrocarbon in various forms may lead to the formation of the vapor cloud. For a fire or explosion to happen, three essential elements are required to complete the fire triangle, which are oxygen, fuel, and heat/energy. When all these three things are present in a specific ratio, and within the flammable limits, the reaction can cause the fire or explosion, which becomes cyclic. The oil particles or gas vapor must be flammable and agitate into small particles, say up to 200 micrometers in diameter. These particles may not immediately ignite unless there is some hotspot, or the vapor falls within the specified flammability limit. In the case of oil, it must form mist, which can be immediately ignited in the presence of a hot spot.

An important matter that should be judged is fluid responsiveness to mist explosions, which can be reasoned of its likelihood to form aerosols (Krishna, Rogers, and Mannan 2004). Mist combustion and explosion require a series of occurrences: mist formation, dispersion, ignition, burning, and explosion. Again, heat transfer to aerosols depends on leak sizes, ambient conditions, thermal and fluid properties, pressure, temperature, and droplet sizes. Out of all these liquid temperature and pressure are the main factor which influences the atomization process (Krishna, Rogers, and Mannan 2004). However, more pressure causes more spray velocity and magnifies shear between liquid to the gas stage. This phenomenon, in turn, causes instability in the liquid stream and fast, productive atomization process.

Manufacturers involved in the layout phase consider for flash, fire, and auto-ignition temperature, but do not fully apprehend likely mist explosion. Minimizing leaking liquid's sensitivity to atomization by some form like masking by something will considerably reduce the mist explosion hazard (Krishna, Rogers, and Mannan 2004).

Atkinson et al. (2017) discuss the formation of a flammable vapor cloud. Various weather conditions are taken into consideration in this research. Research shows that small leaks played a vital role in vapor cloud formation. The study has shown that there is a close relationship between overpressure and the occurrence of a significant accident. One factor that is typically ignored in theories of explosion propagation is the effect of thermal radiation. Thermal radiation occurs in large turbulent flames. The flame propagation is done by large scale eddies. The results suggest that radiation effects can be studied to understand the explosion.

He et al. (2017) concentrates on the slow release of vapor in a confined space, which is unique; earlier studies considered a sudden release of flammable gas. The authors express that underground combustible storage is regarded as a safer method. However, a catastrophe resulting from a fuel vapor-air mixture can generate more harm in a confined space than in an open space. It occurs because the ventilation system is not very efficient as it is situated deep below the ground. Earlier research concentrates on the significance of the role of confined space and numerous geometries in fire or explosion accidents (Ciccarelli, Johansen, and Parravani 2010). These researches have emphasized on numerical simulation studies, identifying particular hazardous spot, chemical facilities, residential areas, velocity and density of the mixture, of leaked gas (Scargiali et al. 2005). The authors have concentrated on the phase change process of the combustible in combination with gas clouds emerge from the liquid when leaked along with slow-release gas dispersion without ventilation as it was not studied earlier (He et al. 2017). For the simulation, LES (Large Eddy Simulation) has been used, which is a numerical calculation method, simulation multiple phase flow along with a newly developed phase changed model. The evaporation phase change model in line with the two steps free surface flowing volume of fluid (VOF) model is more suitable for the CFD tool for the hazardous gas leak in volatile liquid accidents. N-butane and Decane ($C_{10}H_{22}$) are used to lessen the computational demands, which are the most and least volatile components.

2.2 VCE analysis using CFD

Many literatures talk about the modeling of fire and gas explosions using CFD. Modeling the spread of the vapor cloud using CFD can be useful to measure the overpressure created from the VCE (Qiao and Zhang 2010). Detailed computations of the consequence of explosion and fire are required to minimize the risk in oil & gas industries (Paik et al. 2010). Dispersion and explosion analysis using CFD has increased in recent years. Gavelli, Davis, and Hansen (2011) used FLACS to identify the consequences of the ignition of the flammable vapor cloud during a spillage of LNG in the offloading process. CFD produces better accuracy over integral models when analyzing concentration distribution in the dispersion field (Schleder et al. 2015). Plasmans et al. (2013) showed that significant differences might arise among simulation results when using different CFD tools with the same dispersion scenario.

Ramírez-Marengo et al. (2015) evaluated the risk of VCE using a stochastic approach. The use of stochastic is to reduce the uncertainty factor to produce better results. Using different decision variables such as the ignition source, release rate, and other conditions, as well as having many parameters for the different scenarios, the model was made with varying probabilities of occurrences. Another study of Selby and Burgan (1998) is modeled considering different parameters like congestion, ignition source location, and water mitigation. Paik et al. (2010) discussed the gas explosions and fire actions. The paper targeted the implementation of CFD simulation of gas explosions to identify the characteristics of accidents. Reframing the data to use for CFD, the paper used the test carried out by Gieras et al. (2006). While running the simulation, the authors found satisfactory results are close to the ones found in the experiments.

Flame acceleration simulator (FLACS) is a three-dimensional model used for modeling dispersion and the vapor or dust cloud explosions. Geometries are created using the pre-solver CASD6 by using simple shapes such as cylinders, cuboids, and spheres. The model can be added or subtracted from one another such that a wide variety of geometries can be constructed. Geometries can also be introduced from a CAD file using the FLACS function 'geo2flacs'. Once the geometry has been created, a computational mesh must be constructed. In FLACS, the grid is consisting of cubic or rectangular cells with grid lines arranged in vertical or horizontal directions, i.e., a single-block Cartesian grid. Most general-purpose CFD codes, such as ANSYS-CFX, Star-CCM+, and Open FOAM, use unstructured grids that can contour around complicated curved or angled walls. FLACS models turbulence using a Reynolds-Averaged Naiver-Stokes approach. FLACS decides fluid temperatures by solving a transport equation for the liquid enthalpy. Fluctuating velocities are modeled using sine and cosine waves, where the operator specifies the amplitude and frequency. For modeling multi-component flows, FLACS employs a single set of Naiver-Stokes equations to shape a homogeneous velocity field and a scalar transport equation to model the volume fraction of the different fluid components, and it is constrained to use a Cartesian grid. (As 2016)

Dadashzadeh et al. (2013) concentrate on the explosion consequences, which is unique; earlier studies considered modeling the dispersion of flammable gases. The authors did a study on the CFD model of combustible gases and analyzed the explosion using FLACS. In the current study, FLACS CFD software was used to model the dispersion and explosion of the flammable vapor cloud. Using a finite volume method in a Cartesian grid, the concentration equations of mass, momentum, and enthalpy are solved in FLACS. Mixture fraction and mass fraction equations are also addressed in FLACS, and the combustion model is used to close the set of equations. The dispersion model is then run, and based on the results, a sensitivity analysis is used to define the optimum size of grids. The time of simulation was assumed, while the first 60s were the startup period where only the ventilation points were in operation. The study shows that the release of flammable gas started after 60 s. CFLC and CFLV numbers were selected. To be flammable, the fuel cloud formed through the dispersion simulation should be in the flammable limit. The gas mixture has a Low Flammable Limit and an Upper Flammable Limit The flammable vapor was then used in explosion simulation. The time of ignition was observed after 320s. The congestion parameter is an important factor in complex geometry, which is calculated through dividing the total length (m) of all items on the main deck (cylinders and boxes) by the total volume (m3) of the area of interest. One important parameter affecting the explosion consequence is ventilation condition. By investigating different wind and ventilation conditions to reduce, the results determined an overpressure in an engine room. It also found out that lower overpressure was observed in the low congested/confined area and higher overpressure in the highly congested/confined area.

2.3 VCE Mitigation and Control Methods

Different vapor cloud control methods such as ventilation and water spray by sprinkler systems are used in the industry to control the vapor cloud (Rana, Guo, and Mannan 2010). The influence of obstacles presents within the vapor cloud can also contribute to the severity of the explosion (Li et al. 2016). The water spray from such a system can help absorb or dilute the vapor cloud, thus reducing the magnitude of the explosion (Rana, Guo, and Mannan 2010). Besides that, another recent technique that will be studied is the water hyper mist system. The hydrogen presence in air 4% to 74% in a confined space can create an explosion unless it is adequately controlled. If hydrogen and oxygen can be converted to water by using a catalyst, explosion severity can be reduced (IAEA 2001). Another method is to add nitrogen to reduce the oxygen content, which also can minimize the rate of reaction and effects of an explosion by introducing an additional thermal ballast (Aung, Hassan, and Faeth 1998). Water or Hyper mist can also mitigate by extracting heat, minimizing the rate of reaction and burning velocity, and displacing the oxygen (Yang and Kee 2002). A test had been carried out at London South Bank University (LSBU) to find out the mitigation of hydrogen deflagrations by a test rig apparatus. When the test was carried out in the presence of water mist, the FLACS CFD gas explosion code produces significantly reduced pressure rise and delay blowout of the event (Holborn et al. 2012). The test experiment revealed that nitrogen dilution and finer percentage of water mist (say 6 to 8 micrometers) are more effective than the cloud or nitrogen alone. Another study by (K. van Wingerden 2012) evaluated the risk and the possible consequences of a VCE targeting to mitigate the VCE using flame inhibitors, conducting an experiment to study the effect of having flame inhibitors in the presence of VCE, and the required number of the flame inhibitors as well as their properties. Although the result varies with different mixtures of hydrocarbons substances, and different mixture and number of flame inhibitor, it shows that flame inhibitors would significantly reduce the VCE magnitude and consequence.

Nozu et al. (2005), in their paper, used a CFD simulation for hydrogen explosion maximum pressure test together with a barrier wall, and structural integrity was considered. The test was confirmed by comparison with true explosion examinations. In the end, by observing the result, an effective shape of the barrier wall is predicted to mitigate the consequences (Nozu et al. 2005). In this case study, the type of wall (cross-section), which would mitigate the blast pressure effectively, had also analyzed. It was found that wall height = 3 m, and T-shape found the most effective and can mitigate explosion pressure effectively. The paper had tested numerous cases by different types of blast wall, for instance, I-shaped, Y-shaped, and T-shaped, and it was found that the Y shape blast wall can mitigate 26%, and T shape can do 42% at a point 2 meters behind the wall.

3. Objectives

The goal of this project is to investigate the effectiveness of Sprinkler System, Hyper-mist system, and blast wall in preventing and/ or reducing damages caused by Vapor Cloud Explosion (VCE). To reach this objective, below steps show the approach will be followed.

- Simulate release and formation of flammable vapor clouds using FLACS - Dispersion Single Phase (Natural Gas - Methane, Ethane & Propane mixture)
- Simulate ignition of well-mixed cloud & explosion using FLACS - Gas Explosions
- Record vapor cloud fuel mole fraction, equivalence ratio, explosion overpressure & combustion product mass fraction from the simulations
    1. Using the geometry of simple refinery crude oil distillation unit
    2. Introduce Hyper-mist system, Sprinkler system & Blast wall in the geometry
- Use CFD simulations compare and evaluate the effectiveness of sprinkler & hyper-mist systems to reduce damages from the vapor cloud fire & explosion
- Qualitative analysis of causes of vapor cloud explosion using Fault Tree & Event Tree
- Use design of experiment (DOE) to analyze the factors and evaluate their significance on the outcomes.

4. Methodology

In the Methodology section, the work plan for the project scope is outlined, and the below figure shows the design of the project methodology approach. The work plan for the development of the methodology can be summarized in the below steps:

1. A generic CAD model of a refinery is developed using the FLACS software geometry creating tool. A screenshot of a refinery from google maps is used to create the layout in the model.
2. Hydrocarbon Properties and initial conditions for the simulation need to be inserted into FLACS. Hydrocarbon properties can be changed to simulate different types and phases of the vapor cloud.
3. The process of detection of vapor cloud is out of the study scope. However, the concentration of the flammable cloud in the entire vapor cloud has a significant impact on the overall result.

Hence, the concentration of the flammable vapor cloud is monitored. A set of monitoring point is created within the CAD model, where overpressure after the explosion is observed.

4. Damage from the explosion or fire can vary depending on the ignition time of the vapor cloud. Two scenarios are chosen for this study- early ignition & delayed ignition.
5. The leak is generated using the Jet functionality within the FLACS software. It calculated the area, mass flow rate, and velocity of the leak depending on the duration of leakage & quantity of fuel in the reservoir.
6. The Wind Wizard tool inside FLACS is used to create wind boundaries and wind directions in the simulation model.
7. Simulation outputs such as Fuel mole fraction, equivalence ratio, velocity vectors, pressure & combustion product mass fraction are recorded for analysis.
8. Qualitative analysis of the vapor cloud explosion is done using Fault Tree Analysis (FTA) & Event Tree Analysis (ETA).
9. A statistical analysis of input variables is conducted to determine the significance of individual variables such as atmospheric temperature & wind speed.

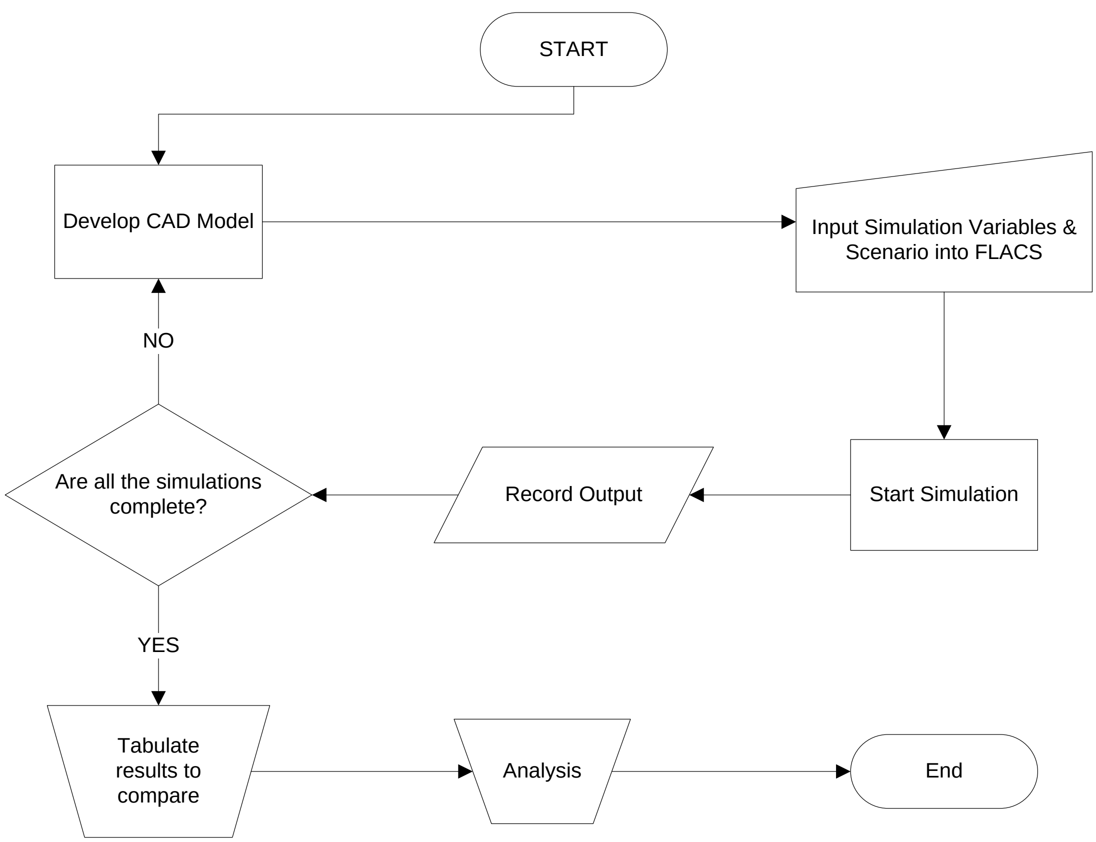

Figure 1: Flowchart of Methodology

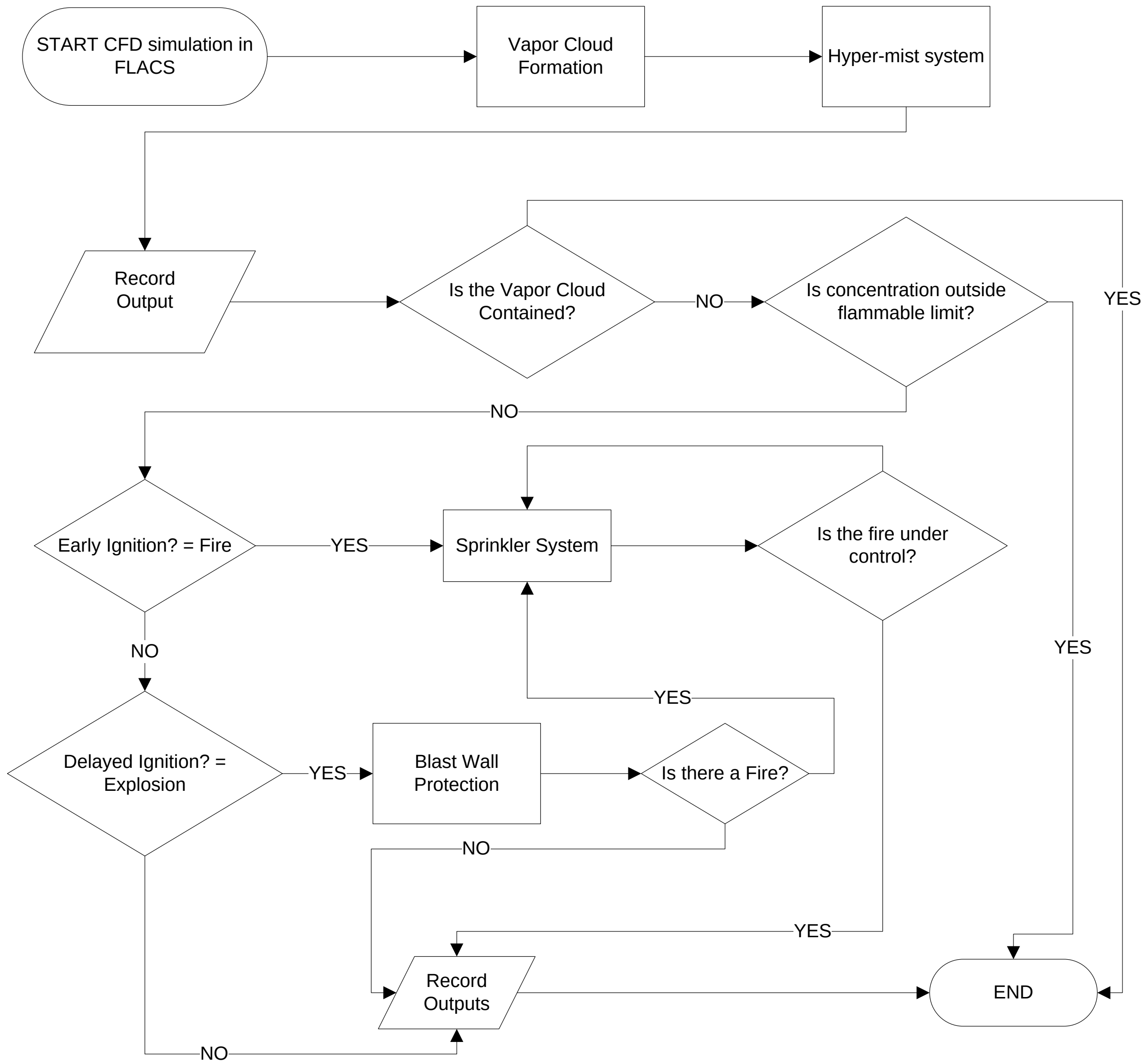

Figure 2: Flow chart of VCE mitigation/control methodology

5. VCE Risk Assessment

The on-hand problem is studied to find the reasons and the consequences of the VCE. Two main tools are used to identify the risk and the consequences, as well as the mitigation methods.

The two methods used are the Fault Tree Analysis (FTA) and the Event Tree Diagram (ETD). The following figure describes the process of the risk assessment.

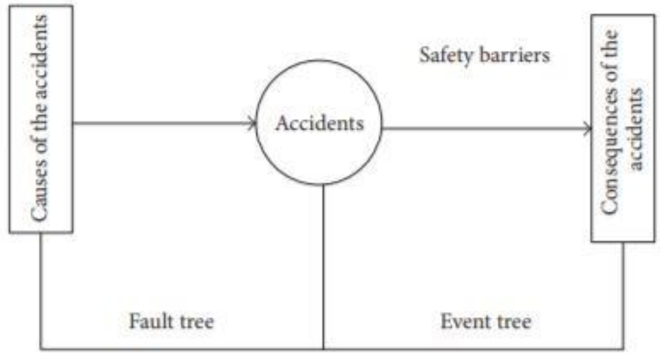

Figure 3: Risk Assessment Process

5.1 FTA

To identify the possible root cause of the VCE, a qualitative Fault Tree is developed. With further study of the topic, as well as further considerations into the development of the model, a quantitative Fault Tree will be prepared.

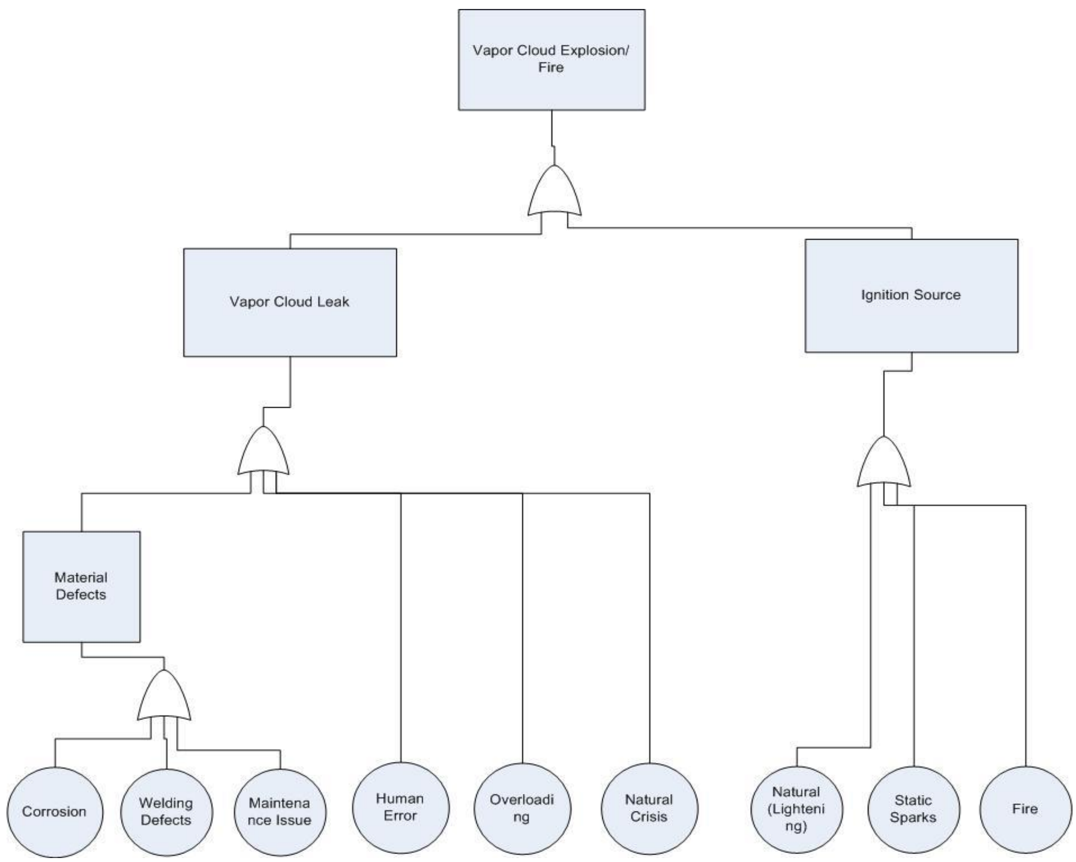

Figure 4: Fault Tree Analysis of Vapor Cloud Explosion

5.2 ETA

The Event Tree Analysis is developed to evaluate the risk and the consequences of the problem on hand. Ranging from a contained leakage to a catastrophic consequence, the qualitative ETA developed as in the figure below.

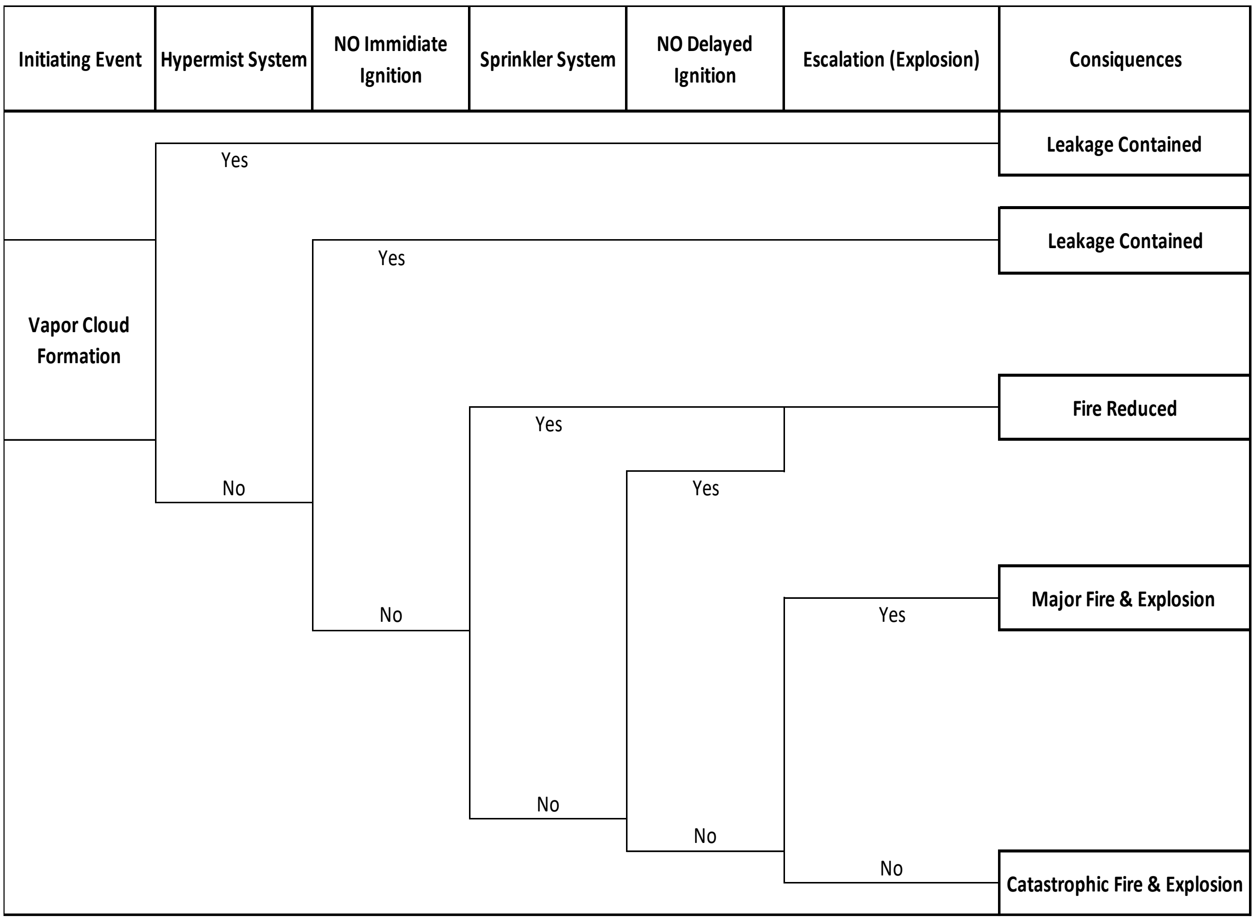

Figure 5: Event Tree Analysis of Vapor Cloud Explosion

6. Results & Discussion

To study the vapor cloud explosion and its consequences, the model of accident area is necessary. A crude oil section of a refinery in St. John's, Newfoundland and Labrador is chosen to be modeled as the accident area. The CAD model of a section of the refinery which was taken from Google Maps is developed inside the FLACS geometry module shown in Figure (6). Following the FLACS standards and to have better results, two simulations were considered, the dispersion model and the explosion model. The properties of the dispersion grid give more effective control of having parameters such as wind speed, wind boundaries, and temperature. Many parameters were considered to generate the model, such as the wind speed, temperature, pressure, reservoir volume, production flow rate, wind speed, and others, as can be found in Table (2).

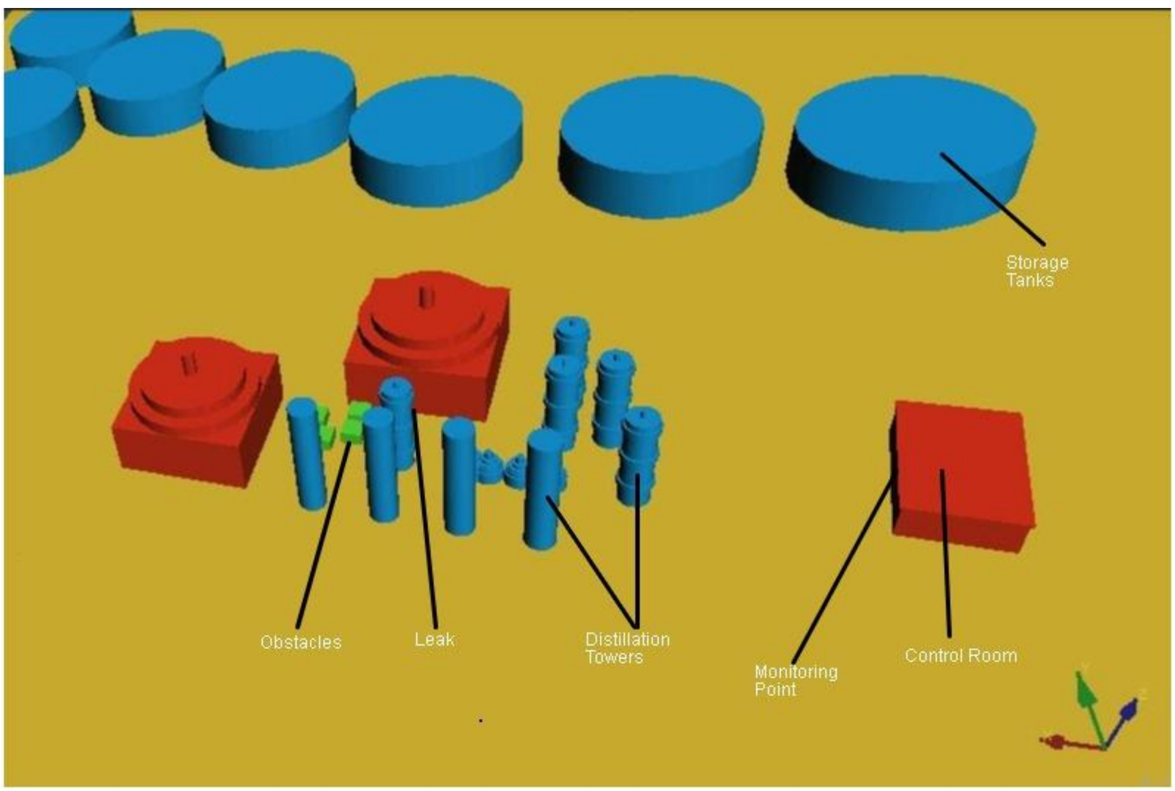

Figure 6: Layout of the Model

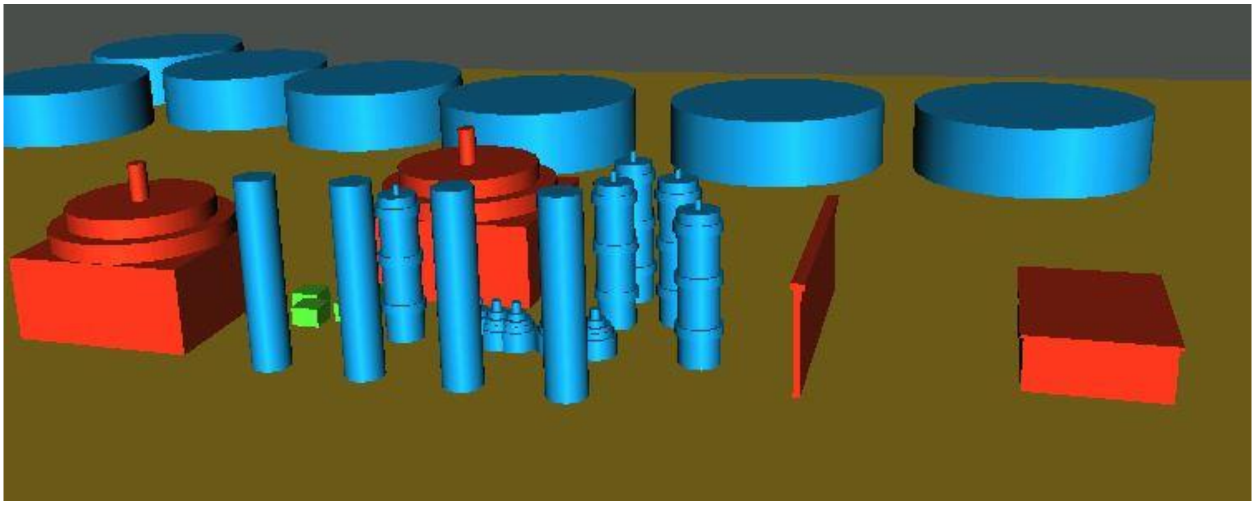

Figure 7: Model of the refinery with blast wall

Table 1: Explosion Grid

Explosion Grid	
min	0,0.5,0
max	65,15,38
cell size	1.5
stretch min	-35,0.5,-35
stretch max	100,26,73
max factor	1.2

The simulation runs were conducted on two main stages. The first is without having the proposed control method to study the aftermath of the explosions. Second is to run the simulation again with the control methods that are sprinkler system only, hyper-mist system only, sprinkler system and hyper-mist system, and blast wall. The simulation algorithm followed was to develop 4 groups of simulation runs based on the time set ups of dispersion model loading time and the ignition starting time noting that leak formation for all of sets is at 10 second. The first simulation set leak formation time at the 10th second of dispersion phase, and then load or dumb the generated values to the explosion grid at second 20. After 5 seconds of loading the dispersion onto the explosion grid; at 25th second of the simulation clock, the ignition is set. Second is to load the dispersion at 20, ignite at 70 and take the results. Third is to load at 70 and ignite at 70.1 seconds. Last is to load at 20 and ignite at 70 seconds. The reason why this algorithm is followed is to examine the scenarios at different situations. However, some of these sets showed redundant outcomes so we choose to show two of these four sets. The two sets chosen are first, the leak at 10, loading at 20, ignition at 25. Second is leak at 10, loading at 20 and ignition at 70 (seconds). Each of the two sets were conducted with and without the control methods.

There are four output measures taken into consideration in studying the dispersion and the explosion. These outputs are measured by deploying a monitoring point at specific point in simulation to read and study the outputs with the control method applied and without. These outputs are:

- FMOLE, which is related to the dispersion simulation.
- FUEL: which is the fuel fraction in the explosion simulation.
- P: Resultant pressure generated in explosion simulation.
- PROD: The explosion mass resulting in explosion simulation.

The output of the two simulation sets will be presented in next section.

In FLACS, the volume fraction of water is defined by the volume of liquid water in litre divided by total volume in a cubic meter, inside the water spray region. The FLACS code has a relatively simple water spray model implemented, where a number of areas containing water spray are defined. Thus, if the volume fraction is 0, there is no liquid water, and if the volume fraction is 1000, there is only liquid water. As each nozzle requires 80 to 120 litres of water, 800 value (near Max) has been considered from the manual. Within each region, a water droplet size (D) and a water volume fraction are determined based on the water pressure, region, droplet velocity and specific parameters characteristic for the chosen nozzle type. We have taken 1 for the Sprinkler. In the case of hyper mist, the volume fraction is considered as 0.1.

The diameter of the water droplets before breakup due to the acceleration is defined by the following Formula:

$$Dmm=10^{3} X P\text{-}0.333.$$

P= pressure of water for sprinklers (bar)

The input in the FLACS scenario file for the water spray contains the following aspects:

- Position: The position of the lower-left corner of a water spray region: Xmin, Ymin, Zmin
- Size: The size of the water spray region is given as: Xlen, Ylen, Zlen
- Droplet diameter: The mean diameter in mm of water droplets before the breakup, defined by the Sauter diameter.

P is 10 for Sprinkler as the distillation tower requires a huge amount of water flow (fire explosion manual). And for hyper mist, it is 120(fire explosion manual). For Sprinkler, using the formula, the diameter is calculated as 464. For hyper-mist, the diameter is calculated as 203.

The parameter NOZZLE_TYPE should be set equal to the text string "FACTORS: F1 F2", where F1 and F2 are the numerical values of the two factors. The F1, F2 is modelled by using the formula:

$$F1=14Uzwater$$

$$F2=14Uzwater$$

$$Uz = \text{The average droplet velocity vertically downward}=2.5(Dmm)\times 0.94$$

The Water volume fraction must still be calculated because it is needed to find the factors F1 and F2. The water volume-fraction of rectangular water spray region, estimated by:

$$\beta water=\frac{n\times\frac{Q}{60}}{Xlength\times Ylength\times Uz}$$

$$Nhypermist= 25$$

$$Nsprinkler= 6$$

$$Xlength\ Sprinkler = 4.40$$

$$Xlength\ hypermist= 3.130$$

$$Ylength\ Sprinkler =0.165$$

$$Ylength\ hyper\ mist =0.242.$$

The water flow rate depends on the operating water pressure. Q is the water flowrate [litre/min] for a single nozzle. It is assumed that the flow rate is related to the water pressure p by Q=K√P. Where k is the k-factor in l/m for Sprinkler, it is taken as 400 and hyper mist it is 20.

Thus, for sprinkler F1 and F2 are calculated as 4.4012 and 0.165, respectively. Similarly, for hyper-mist it is calculated as 3.150 and 0.242, respectively.

Inputs used in the FLACS simulations are tabulated in Table (2) and the inputs used to differentiate between sprinkler and hyper-mist are tabulated in Table (3).

Table 2: CFD Simulations' Inputs

Boundary Condition (Wind Wizard) values	
Wind Direction (deg)	180
Wind Speed (m/s)	1
Reference Height (m)	2
Wind Buildup Time (s)	0
Temperature (deg C)	20
Pasquill Class	D
Ground Roughness (m)	0.25
Boundary Condition	Nozzle
Initial Condition	
Characteristic Velocity (m/s)	1
Relative Turbulence Intensity	0.01
Turbulence Length Scale	0.01
Temperature (deg C)	20
Ambient Pressure (Pa)	100,000
Ground Height (m)	0.5
Ground Roughness (m)	0.25
Reference Height (m)	2
Canopy Height (m)	0
Pasquill Class	D
Ground Roughness Condition	Urban
Leak (Leak Wizard)	
Position (x,y,z)	39 , 4, 15
Direction	-X
Reservoir Volume (m3)	1.00E+09
Reservoir Pressure (barg)	1.5
Reservoir Temperature (deg C)	350
Atmospheric Temperature (deg C)	20
Nozzle Diameter (m)	0.6
Discharge Coefficient	0.85

Start Time (s)	10	
Heat Coefficient	0	
Atmospheric Pressure (barg)	1	
Wall Temperature (deg C)	40	
Relative Turbulence Intensity	0.01	
Turbulence Length Scale + Function	0.01*D	
Duration (s)	-1	
Gas Composition & Volume		
Equivalence Ratio	1.00E+30	
Volume Fraction	Methane	0.91
	Ethane	0.07
	propane	0.02

Table 3: Inputs used to differentiate between Sprinkler & Hyper-mist

Sprinkler		**Hyper-mist**	
Size (x,y,z) (m)	6 , 12 , 16	Size (x,y,z) (m)	6 , 12 , 16
Volume fraction	1	Volume fraction	0.1
Mean droplet diameter (mm)	464	Mean droplet diameter (mm)	203
Nozzle type (F1 , F2)	4.40 , 0.165	Nozzle type (F1 , F2)	3.15 , 0.242

6.1 Results of first scenario (Load at 20s, Ignition at 25s)

Many simulations were done for the scenario to study the explosion. The simulation result of the dispersion and explosion. First, for the FMOLE output, which shows the mixture of flammable hydrocarbon from leak with air as an output of the dispersion simulation. The ignition source is located using the Figure (8) below.

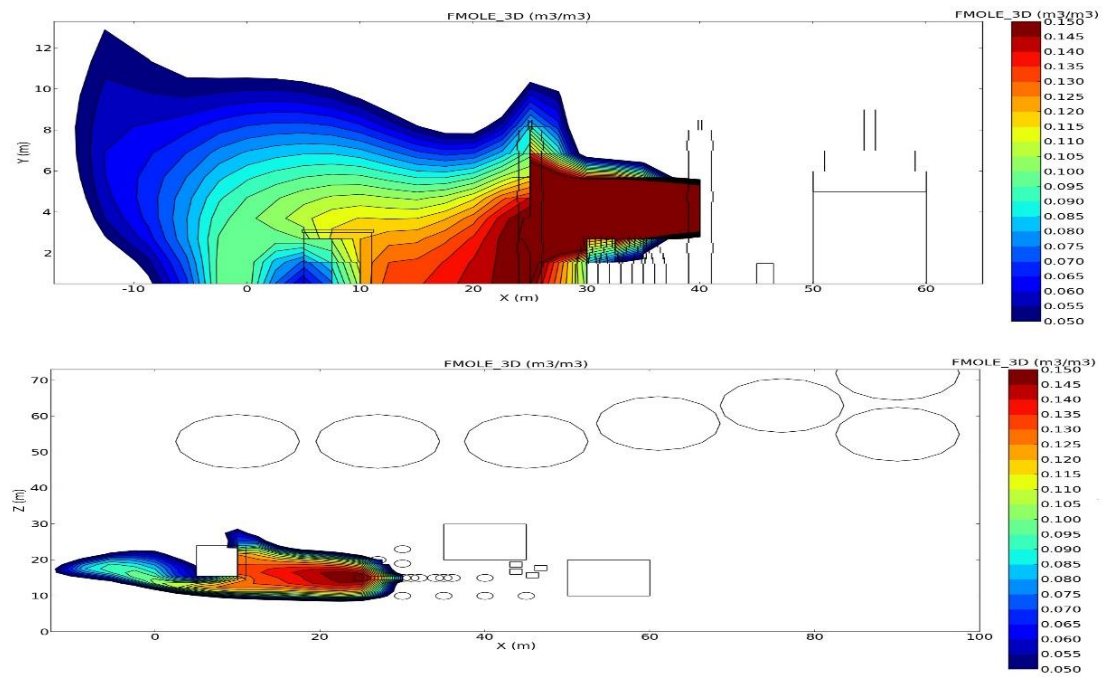

Figure 8: FMOLE Output

Fuel is second one of the outputs studied in the simulation and reducing the value of the fuel is desired. From Figure (9), we can see that the fuel is high as the dispersion simulation is loaded at 20s and that is when the control methods starts to act. Right after the ignition time at 25s, the fuel spikes again and we can see that there is a remarkable impact of applying control methods right at 27s where the difference can be seen clearly. The sprinkler comes in top to reduce the fuel, both hyper-mist and sprinkler comes second, and hyper-mist system comes of least effect. The legends description for the graphs can be found in appendix.

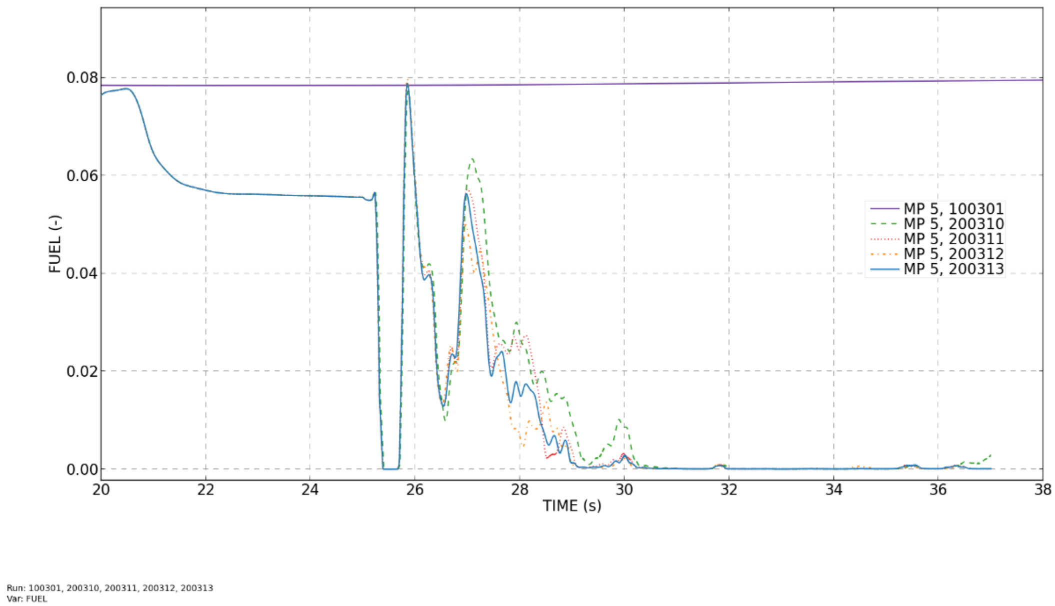

Figure 9: Fuel at 20 Loading, 25 Ignition

Third output studied is the PROD output. We see from figures (10-13) there is no significant difference in using control methods. In fact, using control methods show slightly higher PROD results than not using any.

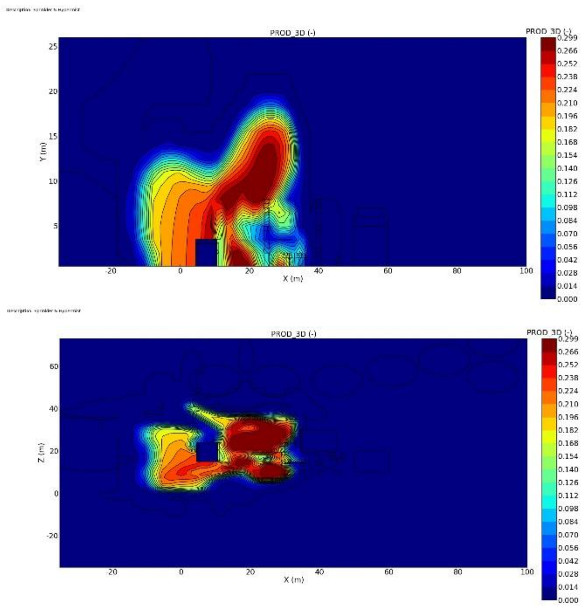

Figure 11: PROD with Hyper-mist

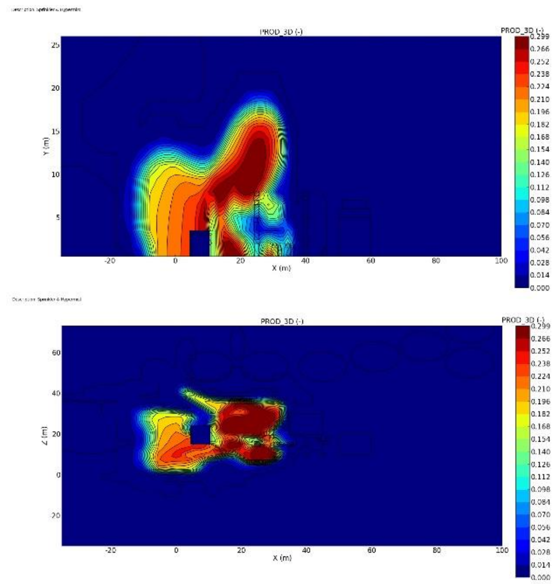

Figure 10: PROD with Hyper-mist and Sprinkler

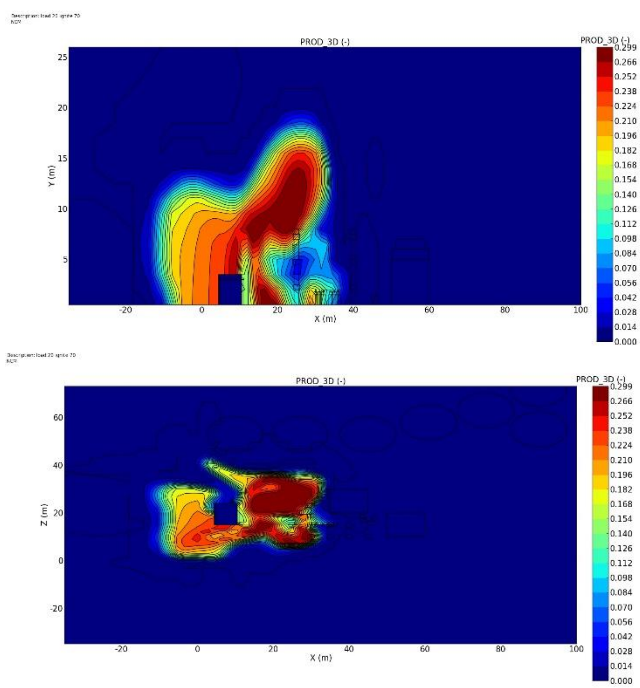

Figure 13: PROD with NO Control Methods

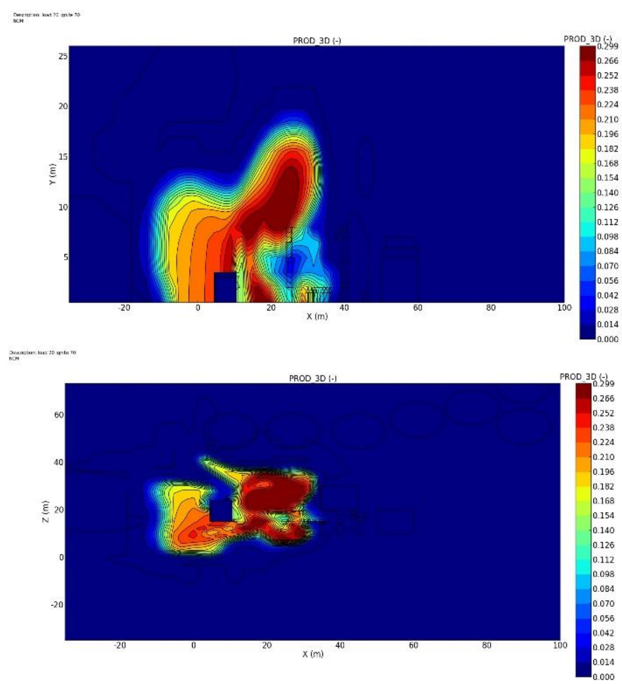

Figure 12: PROD with Sprinkler System

For the pressure output (barg), the pressure will spike once the ignition occurs reaching 0.08 barg and it took about 4 seconds to stabilize. Control methods does not show any significant impact on the pressure generated as seen in below Figure (14).

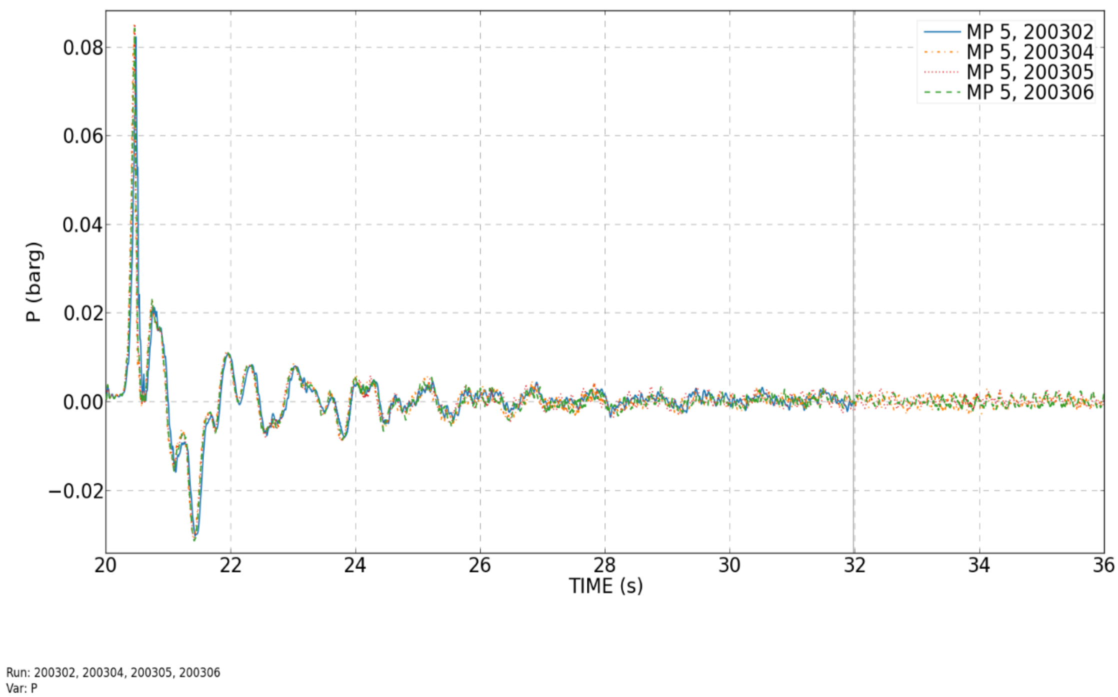

Figure 14: Pressure Comparison (barg)

6.2 Results of second scenario (Load at 20s, Ignition at 70s)

The same outputs are studied for a delayed ignition scenario. For the FMOLE, the same figure of loaded at 20s is used. Studying the fuel output and the effect of using the control methods, we see no significant impact of using control methods as can be noted from below Figure (15).

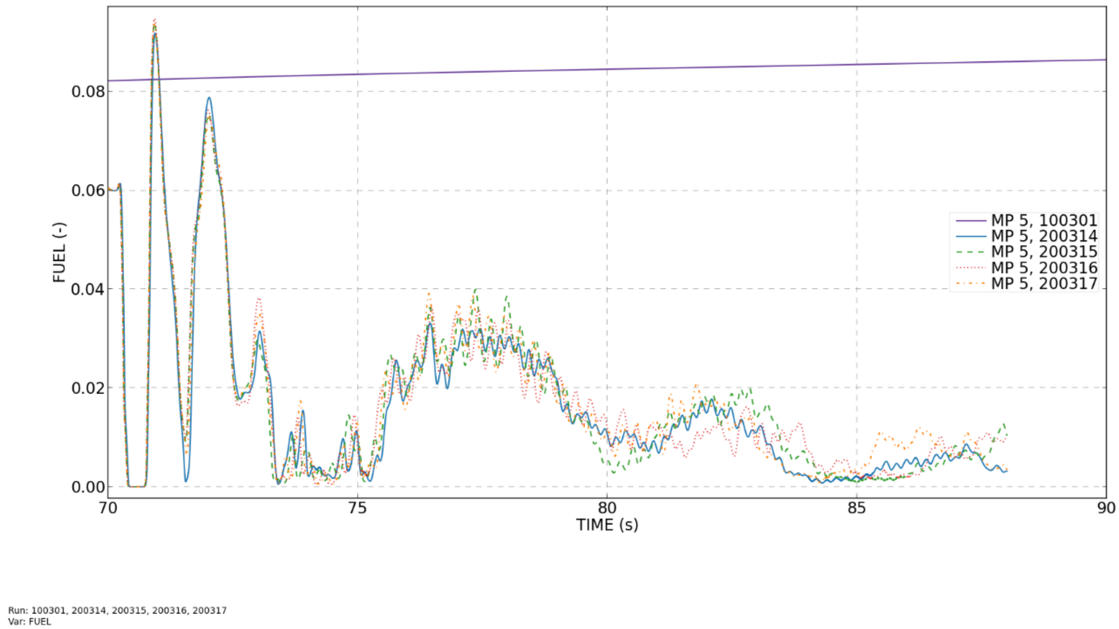

Figure 15: Fuel at 20 Loading, 70 Ignition

The PROD results for the late ignition show higher PROD levels 0.309 compared to 0.299 as in early ignition. Although the magnitude of PROD is slightly reduced (as can be seen from the color difference), the control methods did not show significant improvement on PROD levels as can be seen in Figures (16-19).

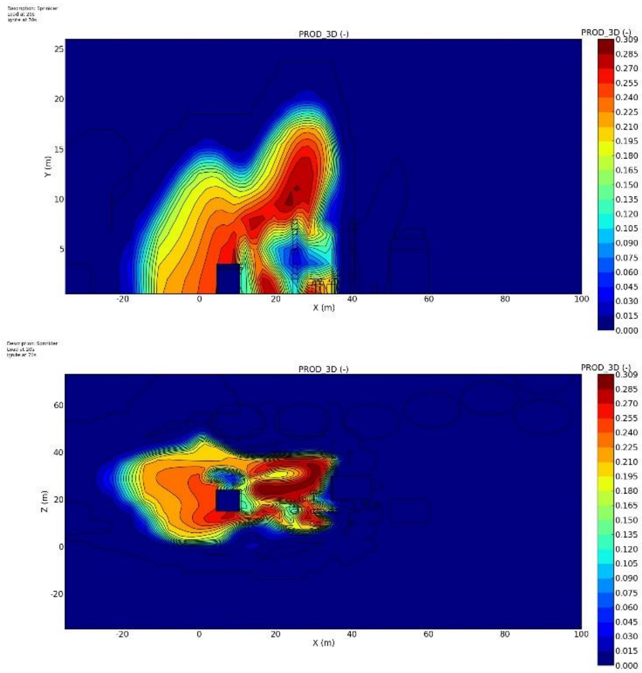

Figure 17: PROD with Sprinkler System

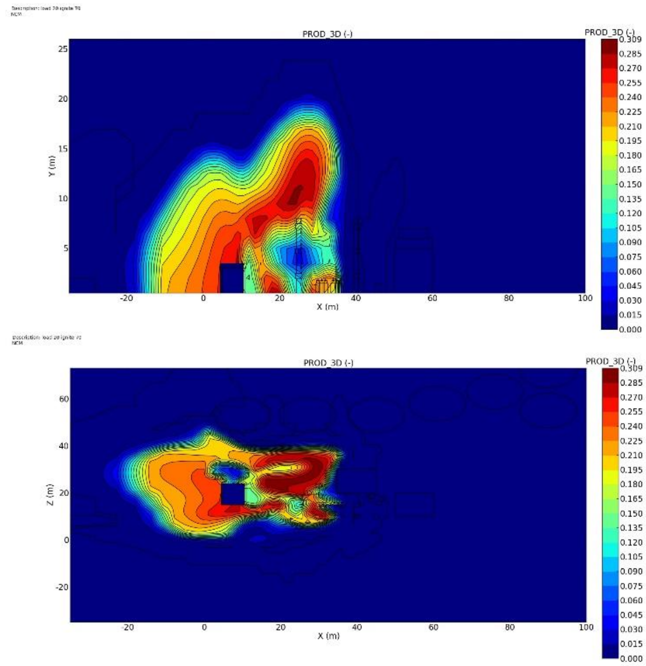

Figure 16: PROD without Control Methods

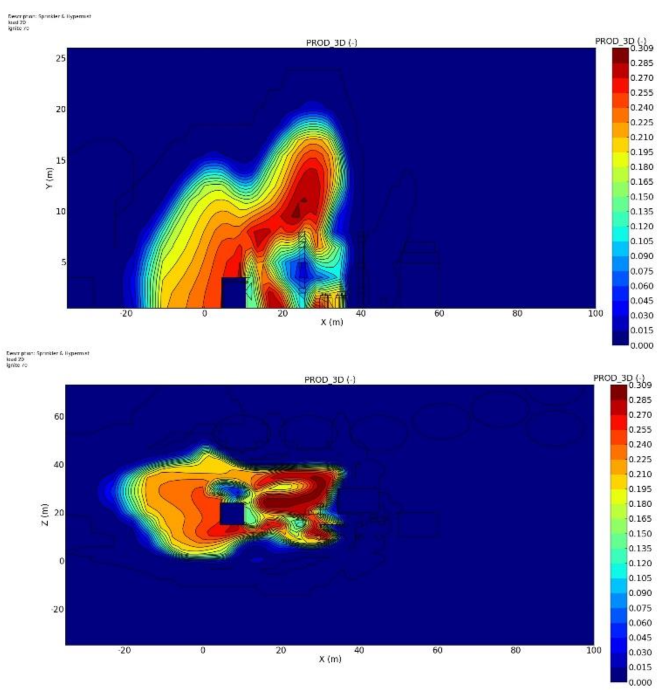

Figure 19: PROD with Hyper-mist

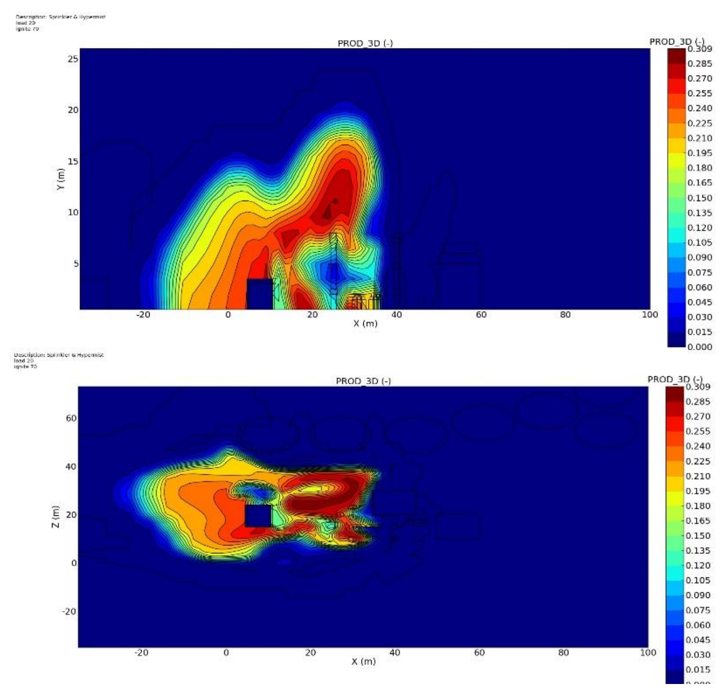

Figure 18: PROD with Hyper-mist and Sprinkler

The pressure reaches the maximum of approximately 0.08 barg at the ignition time, shown in Figure (20). It took around three seconds to stabilize. Utilizing control methods does not show a significant difference on the pressure.

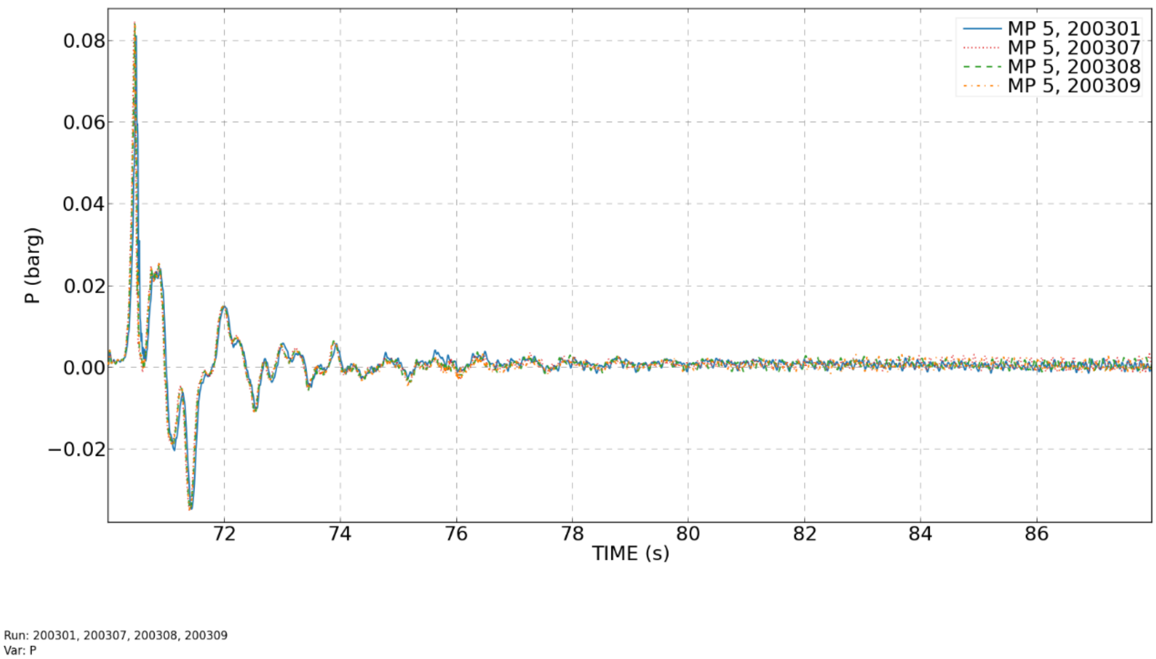

Figure 20: Pressure at Late ignition

6.3 Blast Wall effect on PROD and Pressure

The blast wall is introduced to the geometry of the simulation as a barrier. It was tested to see the effectiveness on limiting the explosion PROD and Pressure. The readings were taken after the explosion and there is a significant impact of using the blast wall as can be seen below.

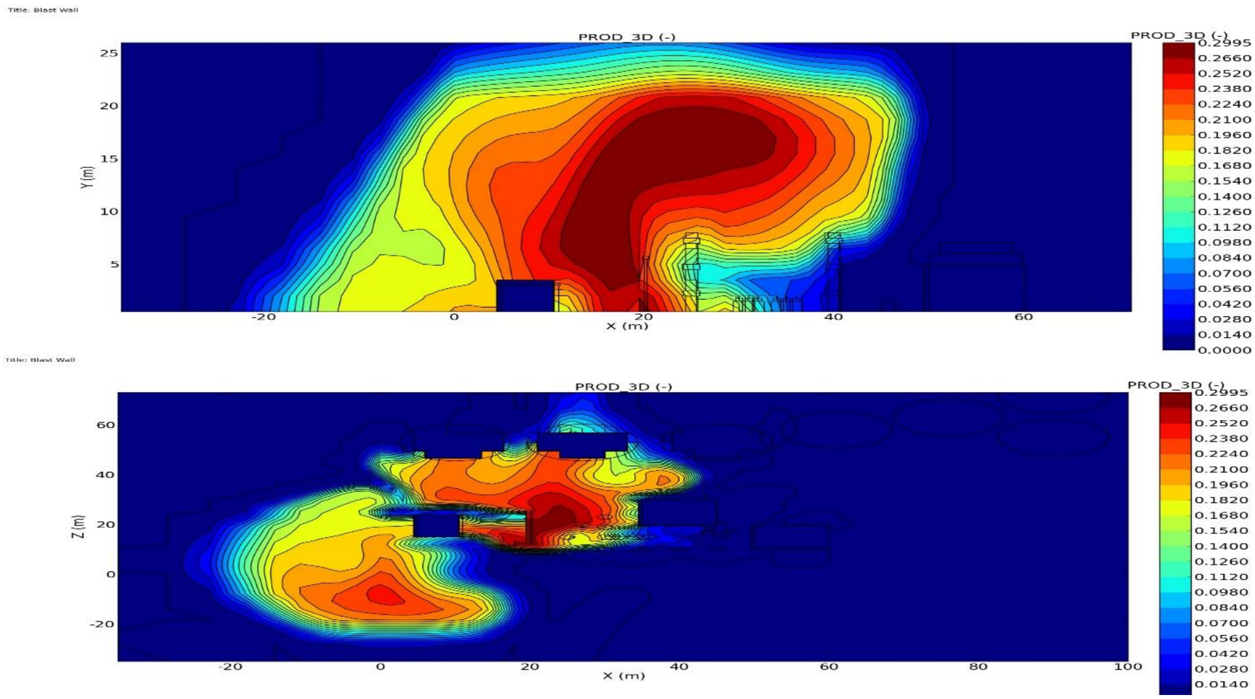

Figure 21: Blast Wall Effect on PROD

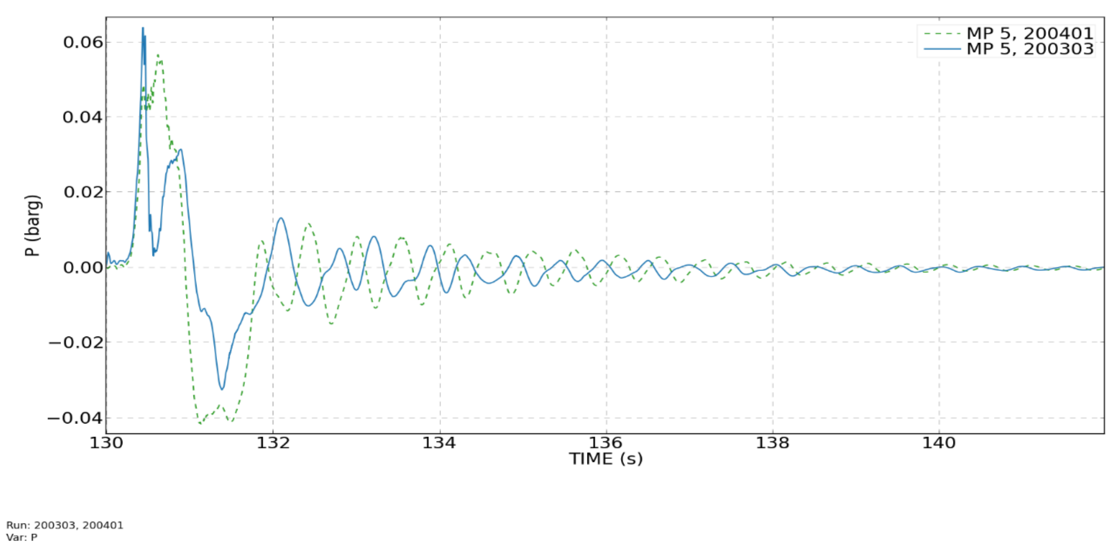

Figure 22: Blast Wall Effect on Pressure

6.4 Design of Experiment

Design of Experiment is one of the techniques used to examine the factors and see their impact of outputs. In this project, we have chosen to test which factors or inputs are significantly affecting the outputs or the responses. We wanted to test 5 factors using half fraction factorial design. There are 16 runs made using FLACS and the output was recorded. The data was then tested using Design Experts (11^{th} edition) with the following set of data:

Inputs:

Each one of the inputs was tested on two different levels (Low and High) as part of the factorial design as below Table (4).

Table 4: Input Factors

Inputs/ Degree	Low	High
Wind Speed (m/s)	1	2
Reference Height (m)	2	6
Reservoir Pressure (barg)	1.5	5
Reservoir Temperature (deg C)	350	600
Nozzle Diameter (m)	0.6	1

The outputs that we want to study are the following:

- ER
- Pressure (barg)
- Fuel (Kg)
- FMOLE
- FDOSE($\frac{m^3}{m^3 * s}$)

Equivalence Ratio (ER) is the measure of concentration of fuel compared to stoichiometric concentration. If the vapor cloud contains no fuel the ER value is zero. The ER value reaches infinity for pure fuel in the vapor cloud. Monitoring the ER value provides valuable information about the mixture of the vapor cloud. ER value is dependent on the amount of fuel leaked which in turn is dependent on the nozzle diameter of the leak. Monitoring pressure difference in a certain area can identify any abnormal situation. In the case of this study, a sudden spike in pressure represents the leak scenario. This Pressure difference is dependent on the reservoir pressure and temperature. The reference height and windspeed work hand in hand to determine what the Volume fraction of gas air mixture (FMOLE) and accumulated FMOLE (FDOSE) of the vapor cloud would be. Monitoring FMOLE can identify potential ignition scenario of vapor cloud. FDOSE can be very useful to pinpoint certain areas where the risk of fire is high.

Running the simulation for each combination (16 runs) for the inputs is conducted and the results for each one of the outputs was obtained.

INPUTS					OUTPUTS				
Wind Speed (m/s)	Reference Height (m)	Reservoir Pressure (barg)	Reservoir Temperature (deg C)	Nozzle Diameter (m)	ER	Pressure (barg)	Fuel (Kg)	FMOLE	FDOSE (m3/m3*s)
1.00	2.00	1.50	600.00	0.60	1.41	0.04	3,030.00	0.12	6.59
2.00	6.00	5.00	600.00	1.00	2.26	0.02	4,090.00	0.18	10.34
1.00	6.00	1.50	600.00	1.00	2.71	0.34	6,250.00	0.21	10.90
1.00	2.00	1.50	350.00	1.00	2.67	0.04	5,530.00	0.21	11.02
2.00	2.00	1.50	600.00	1.00	2.30	0.02	2,890.00	0.18	10.18
2.00	2.00	1.50	350.00	0.60	1.45	0.02	1,800.00	0.12	7.22
2.00	6.00	1.50	600.00	0.60	1.35	0.03	2,450.00	0.12	6.52
2.00	2.00	5.00	350.00	1.00	2.60	0.02	3,160.00	0.20	11.55
2.00	2.00	5.00	600.00	0.60	2.16	0.02	2,620.00	0.17	9.26
2.00	6.00	1.50	350.00	1.00	2.81	0.03	5,150.00	0.21	12.09
2.00	6.00	5.00	350.00	0.60	2.77	0.02	4,830.00	0.21	11.99
1.00	2.00	5.00	350.00	0.60	2.91	0.03	6,050.00	0.22	12.16
1.00	6.00	5.00	350.00	1.00	2.96	0.02	6,930.00	0.22	12.10
1.00	6.00	5.00	600.00	0.60	2.61	0.03	5,840.00	0.20	10.37
1.00	2.00	5.00	600.00	1.00	2.50	0.03	5,130.00	0.19	10.48
1.00	6.00	1.50	350.00	0.60	1.57	0.02	4,020.00	0.13	7.35

Figure 23: Simulation Output Data

Analysis of Variance (ANOVA) is conducted for the data gathered and the outcome of each output is as follows:

- ER Output:

From Pareto chart, we see the main contributing factor/s and the interaction between factors on ER output. After that we test whether these factors are significantly affecting the ER output or not using ANOVA as in table below.

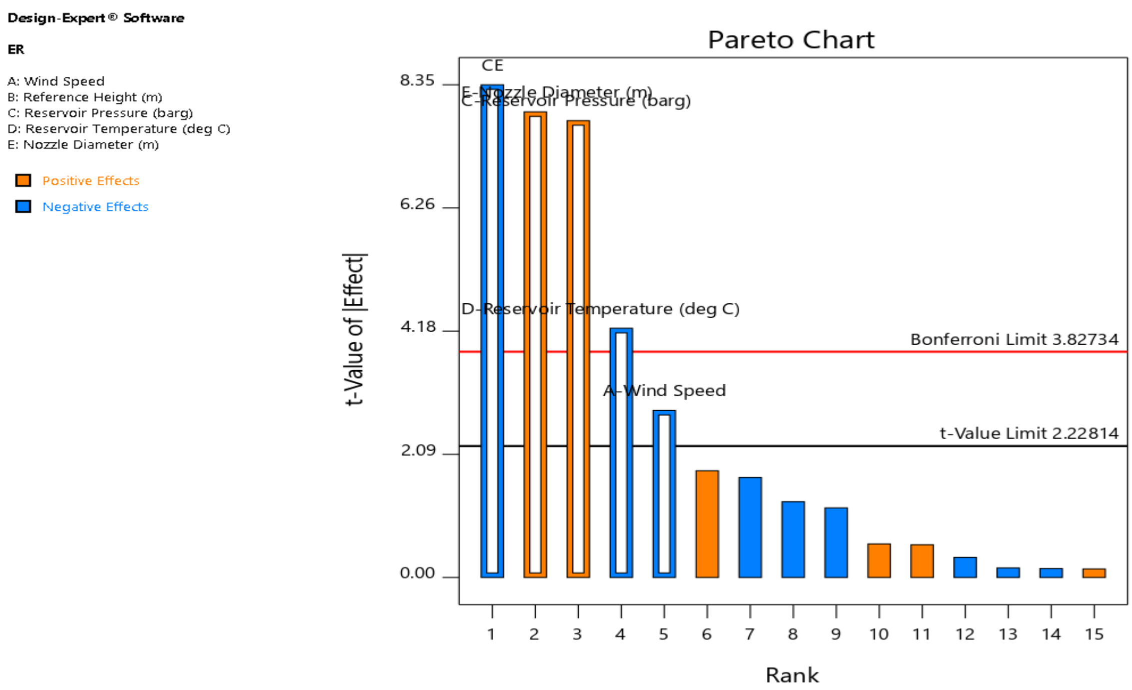

Figure 24: Pareto Chart for ER

The Table (5) below implies that Wind speed, Reservoir Pressure, Reservoir Temperature, Nozzle diameter, and the interaction between (pressure and nozzle diameter) is significantly affecting ER value.

Table 5: ANOVA for ER

Source	**Sum of Squares**	**df**	**Mean Square**	**F-value**	**p-value**	
Model	4.56	5	0.913	43.6	< 0.0001	significant
A-Wind Speed	0.168	1	0.168	8.02	0.0178	
C-Reservoir Pressure (barg)	1.26	1	1.26	60	< 0.0001	
D-Reservoir Temperature (deg C)	0.374	1	0.374	17.8	0.0018	
E-Nozzle Diameter (m)	1.30	1	1.30	62.3	< 0.0001	
CE	1.46	1	1.46	69.8	< 0.0001	
Residual	0.209	10	0.021			
Cor Total	4.77	15				

There are three assumptions that needs to be checked when conducting factorial design and ANOVA. One is Normality, second is data independence and third is randomness. The three assumptions were checked and verified for the all the outputs.

Pressure:

For the second output, we see that non of the factors are significantly affecting the pressure.

Table 6: Pressure ANOVA Results

Source	Sum of Squares	df	Mean Square	F-value	p-value	
Model	0.062	9	0.007	1.29	0.391	not significant
A-Wind Speed	0.009	1	0.009	1.69	0.242	
B-Reference Height (m)	0.005	1	0.005	1.01	0.355	
C-Reservoir Pressure (barg)	0.008	1	0.008	1.49	0.268	
D-Reservoir Temperature (deg C)	0.006	1	0.006	1.19	0.316	
E-Nozzle Diameter (m)	0.006	1	0.006	1.17	0.320	
AC	0.007	1	0.007	1.22	0.311	
AD	0.006	1	0.006	1.19	0.316	
BD	0.006	1	0.006	1.21	0.314	
CE	0.008	1	0.008	1.43	0.276	
Residual	0.032	6	0.005			
Cor Total	0.094	15				

Fuel:

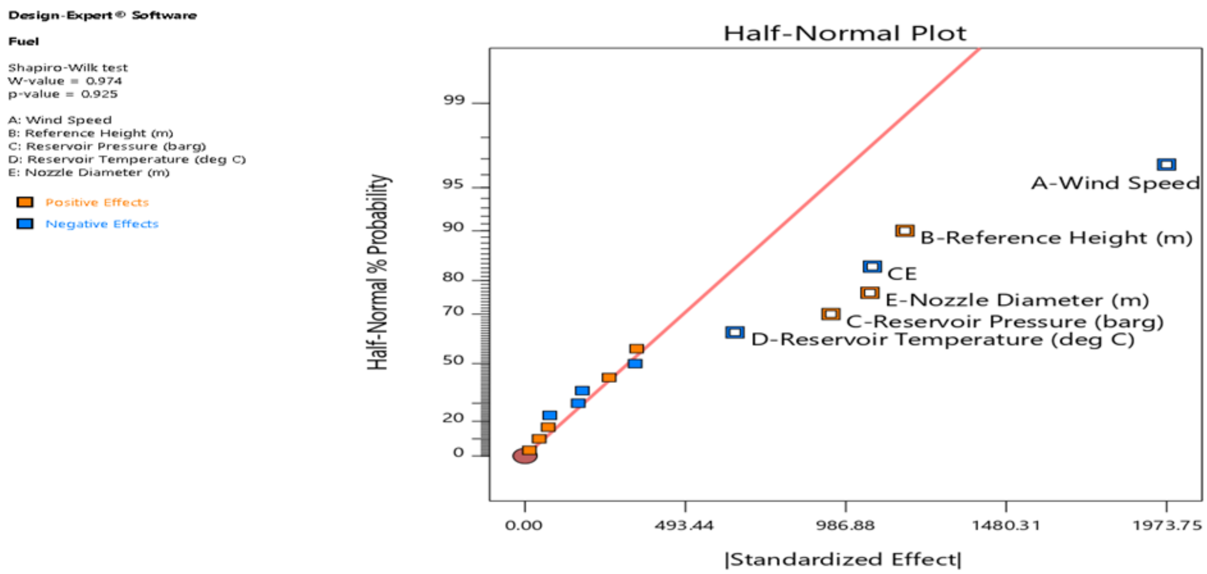

Figure 25: Fuel Affecting Factors

Using the half normal plot, we see that factors (A, C, D, E and CE) are affecting the Fuel results. Conducting the ANOVA, we find that the factors are significant.

FDOSE:

From the chart below, we see that factors C, D and E affecting the output the most and were found significant testing them in ANOVA.

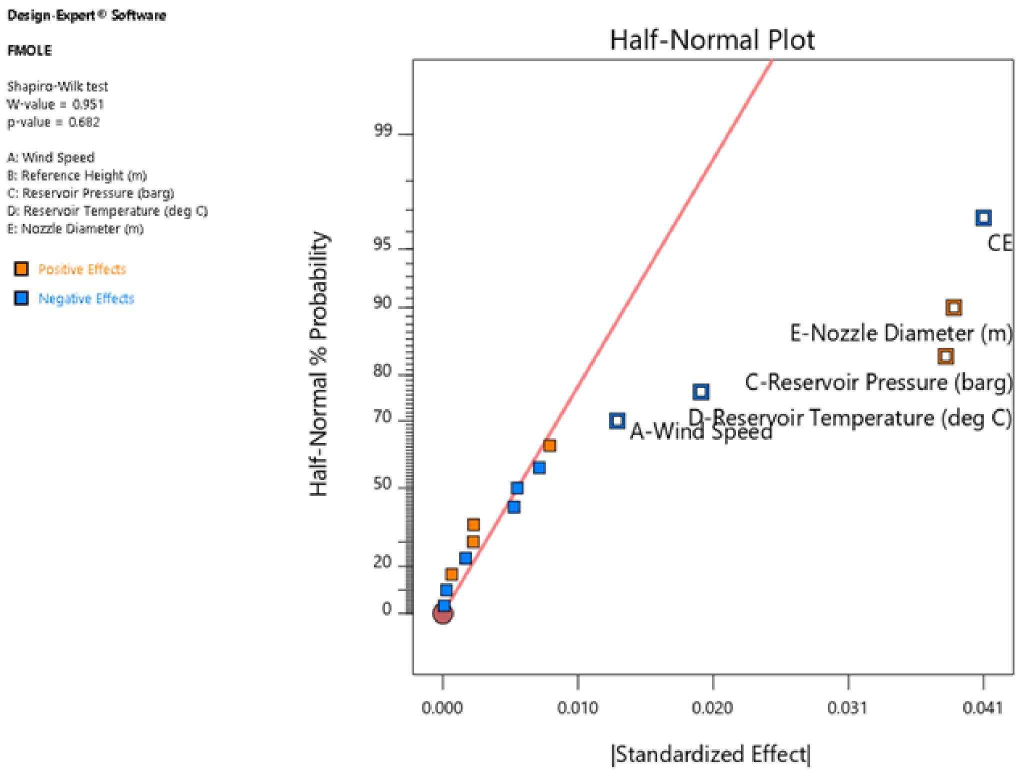

Figure 26: FMOLE Half Normal Plot

Using DOE tools, we can conclude that factor B (reference Height) is not affecting any of the outputs. The Effect of the interaction between nozzle diameter and reservoir pressure (C&E) is important and relatively affecting most of the outputs significantly. We notice that Pressure output was not affected by changing the inputs, nor their interactions.

6.5 Discussion

The dispersion of vapor cloud depends on the leak rate & wind condition. A higher leak rate with low wind condition is used in the study to simulate reasonable explosion scenario. With a north-east wind direction, the cloud is pushed towards the monitoring point. Since the simulation is carried out in an open space, the wind direction dictates the accumulation of vapor cloud in given area. The results will vary if the wind direction or the wind speed is changed. The Fuel Mole Fraction (FMOLE) plots are used to identify the spread of flammable gas inside the vapor cloud. The FMOLE range, which represents flammable gas, is between 5% to 15%. From the results it is observed that for the given conditions, sufficient amount of FMOLE within the flammable range is present near the monitoring point and it increases with time. Ignition might occur at any point within this region if an ignition source is reached. For the simulation to continue, specific times haven been chosen to differentiate the results of explosions. With a delayed ignition, there is more flammable fuel to increase the magnitude of the explosion.

The overpressure resulting from the explosion shown by Pressure plots does not show any significant difference depending on any control methods. One explanation for such scenario could be the lack of necessary amount of water or mist required to bring the vapor cloud out of the flammable range. The length of time the control methods are active before and after the explosion also contribute heavily. On the other hand, using a blast wall in front of the monitoring point reduce the pressure measured. A simple explanation for this condition is the presence of obstacle in front of the monitoring point which is breaking the flow of shockwave from the explosion.

The amounts of FUEL are seen to reduce with control methods which can be interpreted as faster burning of the flammable cloud in the presence of sprinkler or hyper-mist system. As the hydrocarbons mix with water and mist from the control methods and break down into hydrogen, carbon dioxide and carbon monoxide the plots of FUEL spikes at later stage of the simulation. One explanation of such occurrence can be explained through the definition of the FUEL output produced by FLACS. The FUEL output is the mixture of hydrocarbon and hydrogen. So, as the hydrocarbon break down into more hydrogen, the amount of FUEL is observed to increase which might not represent the actual flammable fuel mixture.

The PROD plots are useful to see the difference between the burning condition of the vapor cloud in the presence of control methods. There are slight differences between the PROD results while using control methods for a longer period. Initially the image of combustion mass fraction with no control method are like that with using control methods. The difference created for the prior is due to the extended period of exposure to running sprinkler or hyper-mist system. The water and/or mist present in the cloud alters the burning scenario of the vapor cloud. The magnitude of PROD near the monitoring point is significantly lower in presence of a blast wall. It is due to the barrier created by the wall that stops the explosion mass to reach the monitoring point. The difference in PROD observed for the scenario with blast wall emphasizes the importance of a blast wall in front of any significant establishments which houses living beings.

To keep the simulation realistic, use of control methods in vast area is avoided. The goal of this study is to identify the vapor cloud formation from a leak in an open space of a refinery and to investigate the effect of sprinkler and hyper-mist system. However, it is observed that a vast area poses significant challenge for such control methods to work efficiently. It is not financially feasible to install sprinklers and/or hyper-mist systems throughout a refinery. With limited number of nozzles and area covered, the results obtained show mediocre improvements.

The thesis paper by (Gandhi et al. 2019) studied the vapor mitigation. The thesis showed no noticeable impact on the evaporation process of the propane droplets using sprinkler system, which we can relate to the results obtained in our study by not observing significant improvement on the cloud formed. In terms of area constraint, the thesis stated that there is not significant change in the vapor concentration in an open area. In addition to that, the response of the flammable cloud did not improve with the sprinkler water system. These results can be related to the results obtained in our work as we find no major improvement in using sprinkler water system. Another study by (Wingerden 1995) stated that the mitigation methods do not significantly reduce the explosion aftermath in an open area.

The study can be further expanded with better geometry model and more accurate sprinkler & hyper-mist system configurations. Collaborating machine learning to identify areas most important for a control method along with this study can provide significant results. This study can be utilized to setup experiment in real time before designing and building a new refinery plant. Safety zones, and high-risk zones needing maximum fire control techniques can be identified through experimental results developed on this study.

7. Limitations

The results obtained from the CFD simulation heavily depends on the accuracy of the mesh grid created by the software. The grids make up the control volumes of the model at which the individual data points such as fuel mole fraction, equivalence ratio, pressure & velocities are calculated. It is recommended in the FLACS manual to use a uniform mesh grid of size 0.5m or less for accurate results of explosion simulation. However, they also recommend starting with a coarser grid size to reduce computation time. The geometry model in our work is vast in size, and it is very time-consuming to run a simulation with a finer grid size.

8. Conclusion & Recommendation

The project focuses on the study of the vapor cloud explosion using the computational fluid dynamics approach. Considering previous work that is found in literature, the methodology and steps to be followed are determined.

Simulation of many fire and explosion scenarios are made considering early and late ignition. The mitigation and/or control techniques using the Hyper-mist system, Water Sprinkler System & Blast Walls, are introduced to the simulation model to capture their effect in mitigating the explosion. There are four outputs of the simulations that are FMOLE, PROD, Pressure (P) and Fuel that are studied. The simulations runs are conducted successfully, and the outputs of the different proposed scenarios are discussed. The control methods are tested in the simulation runs for early and late ignition for the outputs. The results did not show significant impact in utilizing the hyper-mist, sprinkler water nor both in explosions unlike the blast-wall that showed better outcomes in mitigating the pressure and the PROD.

A design of experiment approach is used to study the impact of changing factors on the outputs of dispersion. A 2-level factorial design is used, and the results showed the factors significantly affecting the outputs. Using DOE, we validated some of the assumption such as the effect of wind speed on the dispersion simulations. This study could be expanded to see the effect on the explosion simulation as well as improving the time constraint of the simulations knowing what factors to focus on. Based on the simulations results, unlike the blast wall, using sprinkler system and hyper-mist in an open area may not provide a significant improvement on explosion mitigation.

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Appendix

- N- No control method.
- H- Hyper mist
- S- Sprinkler
- H, S- Hyper mist and sprinkler.
- CFLC- This is a Courant-Friedrich-Levy number based on sound velocity. The value of CFLC connects simulation time step length to control volume dimension through signal propagation velocity (in this case the velocity of sound)
- CFLV- This is a Courant-Friedrich-Levy number based on fluid flow velocity. The value of CFLV connects simulation time step length to control volume dimension through signal propagation velocity (in this case the fluid flow velocity)
- MODD-This is a parameter that may be used to determine how often data for scalar-time plots are written to the results file during a simulation: data are namely stored every MODD time steps.
- NPLOT- This is a parameter that may be used to determine how often data for field plots are written to file during a simulation: data are namely stored at given fuel levels where NPLOT is the number of fuel levels equally spaced between zero and a maximum.
- DTPLOT- This is the time interval (in seconds) for field output. This is useful in gas dispersion simulations and also in gas explosion simulations when frequent output is required. The field output file will become very large if DTPLOT is set small. This variable does not influence simulation results, only the amount of data which is stored.
- NLOAD- Set load identification and load data at simulation start
- FSTOP- Stop simulation at given fuel level
- XLO, XHI, YLO, YHI, ZLO, ZHI- The lower boundaries in X-, Y-, and Z-direction are denoted by XLO, YLO and ZLO respectively, and the upper boundaries likewise by XHI, YHI, ZHI.
- MP5, 200305-Hyper mist activated after 20s and fuel concentration decreased up to 26s then fluctuating till 37s.
- MP5, 200306- Hyper mist and Sprinkler together, it started after 20s

Table 7: Name of simulation & description

Name of Simulation Run	**Description**
200302-N	Ignition at 20s, Load control methods at 20s
200305-H	
200304-S	
200306-H,S	
200310-N	Ignition at 25s, Load control methods at 20s
200311-H	
200312-S	
200313-H,S	
200301-N	Ignition 70s, Load control methods at 70s
200308-H	
200307-S	
200309-H,S	
200314-N	Ignition at 70s, Load control methods at 20s
200315-H	
200216-S	
200317-H,S	
200303-N	Explosion with Blast Wall Ignition at 130s, Load control methods at 130s
200401	
100301	Dispersion with no control method
100401	Dispersion with Blast Wall

Table 8: Inputs used to create dispersion & explosion simulation's grids

Dispersion Grid		Explosion Grid	
min	0,0.5,0	min	0,0.5,0
max	65,15,38	max	65,15,38
cell size	2.5	cell size	1.5
stretch min	-35,0.5,-35	stretch min	-35,0.5,-35
stretch max	100,26,73	stretch max	100,26,73
max factor	1.2	max factor	1.2
refined cell size	1		

Table 9: Inputs for Simulation output control

Dispersion Simulation Output Control		**Explosion Simulation Output Control**	
Maximum Time (s)	131	Maximum Time (s)	-1
CFLC	20	CFLC	5
CFLV	2	CFLV	0.5
MODD	1	MODD	1
NPLOT	-1	NPLOT	100
DTPLOT	0.5	DTPLOT	0.5
		Minimum time	35
		Time step ode	KEEP_LOW