Simulation of Natural Gas Dispersion and Explosion in Vented Enclosure using 3D CFD FLACS Software

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Abstract. Natural gas is used as fuel in industries, power plants, commercial installations, and households. In its application, natural gas leaks can be considered as a major hazard because of its flammable and explosive nature. In addition to fuel, heat and oxygen sources, fires and explosions can occur if the concentration of natural gas in the air is between Low Flammable Limit (LFL) and Upper Flammable Limit (UFL). If the release of natural gas is not ignited, it will immediately form a Vapor Cloud Explosion (VCE) that can cause an explosion if it meets ignition point. Therefore, a research on dispersion patterns in a particular area or space is needed to minimize hazards and to develop safety procedures and regulations. This research aims to determine the external parameters that affect the dispersion and explosion caused by natural gas by using FLACS software from PT. Gexcon Indonesia. This software can display overpressure graphs of time and 3D visuals of simulations. The external parameters consist of vent size (5.4 m² and 2.7 m²), wind direction, lighter position (center and back), day and night condition, and the presence of a obstacle (with and without obstacle). From the research results by the simulations, it is obtained that the highest overpressure value when there is an obstacle with a vent size of 2.7 m²; wind direction from the north; night condition, and back ignition point is 0.503 bars at 40,835 s which can cause most buildings to collapse and the death rate to increase.

1. Introduction

Natural gas is used as fuels, raw materials, and energy commodities for export [1], however it is a major hazard that can cause fires, explosions, and leaks [2]. It is lighter than air so it tends to be easily dispersed in the atmosphere, but if it is isolated in a closed space, then its concentration can reach explosive mixture point, which if it is ignited by fire it can cause explosion that can destroy buildings. Natural gas can be dangerous because of its flammability and explosion [3]. Fires and explosions can occur if the concentration of natural gas in the air reaches between LFL and UFL [4]. Computed Fluid Dynamics is a computer-based tool for simulating the behavior of systems involving fluid flow, heat transfer, and other related physical processes. CFD models find numerical solutions to the partial differential equations, Navier-Stokes equations with turbulence models, gas diffusion models and combustion models governing the gas explosion process, and then can model complex geometries and provide a wealth of information about flow fields. Recently, CFD has been used for simulation of gas explosions because the strength of gas explosions depends on the geometry, such as size, confinement and turbulence-generating obstructions, and on the gas mixture, such as composition, location and quantity [5].

There are several studies that consider the effects of external gas explosions, which are as follows:

- Pedersen, H. H., & Middha, P. (2012) [6] simulate experiments conducted by Bauwens, C. R.[7], Chao, J., & Dorofeev, S. B. (2010) regarding the effect of location of ignition, vent size, and obstacle on explosions of propane-air mixtures using FLACS software.
Vyazmina, E., & Jallais, S. (2016) [8] simulate experiments conducted by Bauwens, C. R., Chao, J., & Dorofeev, S. B. (2012) [9] regarding the effect of location of ignition, vent size, and obstacle on explosions of hydrogen-air mixtures using FLACS software.

Sezer, Kronz, Akkerman, & Rangwala, (2017) [10] simulate experiments conducted by Bauwens, C. R., Chaffee, J., & Dorofeev, S. (2008) [11] regarding the effect of location of ignition, vent size, and obstacle on explosions of methane-air mixtures using FLACS software.

In addition, factors that influence the increase in pressure and propagation of fire in ventilated explosions include the size of the enclosure and geometry, the size of the vent, the location of ignition, the nature of the mixture, the cloud turbulence etc [8]. Therefore, it is necessary to do research concerning simulations of natural gas dispersions and explosions to determine the radius and the impact caused by natural gas leaks in the industry as a form of prevention and control effort. One of the ways that can be done is by using FLACS software simulation that has the ability to represent detailed geometry with the concept of distributed porosity and display overpressure simulations of time.

2. Methods

The objective of this research is to find out the highest dispersion and explosion simulation results on natural gas and to find out the impact of the explosion based on the overpressure of time by using FLACS in vented enclosure. The first thing to do is verification by making a scenario modeling using FLACS Software which refer to the Bauwens research, C. R., Chaffee, J., & Dorofeev, S. (2008) which has carried out experiments using variable area holes, methane-air concentrations, and the position of the ignition point in the center and back of the vented enclosure. The next is comparing the experiment and the FLACS Software. The grid used in this research is:

a. Core domain: Minimum (0; 0; 0)
   Maximum (4.6; 4.6; 3)

b. Cell Size: 0.5 m

c. Stretch Domain: Minimum (-10; -10; -10)
   Maximum (30; 15; 30)

And for the shape of 3D experiment space is as in FIGURE 1:

![FIGURE 1. The shape of 3D experiment space a) Hole wide 5,4 m2 (b) Hole wide 2,7 m2](image)

The validation stage is followed with the research variables which were wind direction, vented enclosure hole width of 5.4 m2 and 2.7 m2, the presence and the presence of obstacle (as can be seen in FIG. 3), day and night conditions, and the position of the ignition point in the moment of back and center. The natural gas composition used is shown in TABLE 1:

| Component | % kmol |
|-----------|--------|

TABLE 1. Natural Gas Composition
Carbon Dioxide \[ \text{CO}_2 \text{(g)} \] 5
Methane \[ \text{CH}_4 \text{(g)} \] 87.43
Ethane \[ \text{C}_2\text{H}_6 \text{(g)} \] 3.73
Propane \[ \text{C}_3\text{H}_8 \text{(g)} \] 2.11
Butane \[ \text{C}_4\text{H}_{10} \text{(g)} \] 1.15
Pentane \[ \text{C}_5\text{H}_{12} \text{(g)} \] 0.386666
Hexane \[ \text{C}_6\text{H}_{14} \text{(g)} \] 0.193334

This research used FLACS to perform simulations as shown in FIGURE 2, the overall dimensions of the vented enclosure were of 4.6 m x 4.6 m x 3 m with the overall volume of 63.7 m$^3$.

FIGURE 2 - Simulation of vented enclosure geometry in FLACS software

From the simulations of natural gas dispersions and explosions obtained, the analysis of the highest and lowest yields of overpressure and the impacts that were generated could be used as a basis for alertness.

3. Result and Discussion

A vapor-air mixture is flammable only when its composition is between LFL and UFL [12]. By using the natural gas concentration with the composition specified in table 1, FLACS log files were obtained with 5% (LFL) and 14.9% (UFL). Dispersions and explosions modeling by using FLACS software were based on several external variables which were wind direction, ignition location, vent size, presence of barrier, and day and night conditions.
3.1 Based on Wind Direction

The wind direction variations used in this research were North, South, West, and East. The wind direction is written in FLACS as North (0°), South (180°), West (270°), and East (90°).

In FIGURE 4 is the geometry visualization above when z = 0.5 m and In FIGURE 5, it is shown that the highest overpressure in the north which is 0.503 bar at 40.84 s while the lowest is in the east wind direction at 0.239 bar at 41.916 s. The followings are dispersion visualizations of various wind directions in the same condition:

- **North**
- **South**
- **West**
- **East**

FIGURE 4 – Geometry Visualization on z = 0.5 m

FIGURE 5 – A Comparison based on Wind Direction with Vent Size of 2.7m², with obstacle, Night, and Back Ignition

In FIGURE 4 is the geometry visualization above when z = 0.5 m and In FIGURE 5, it is shown that the highest overpressure in the north which is 0.503 bar at 40.84 s while the lowest is in the east wind direction at 0.239 bar at 41.916 s. The followings are dispersion visualizations of various wind directions in the same condition:

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- **South**
- **West**
- **East**

FIGURE 6 – Dispersion visualizations based on wind direction with vent size of 2.7m², with obstacle, night, and back ignition (a) north; (b) south; (c) west; (d) east
Judging from the wind direction and the vented enclosure facing eastward in FIGURE 6, it showed that the distribution of air-gas concentrations varied. At the East wind direction, the concentration of air-natural gas which is high or near the UFL is characterized by maroon dominant color (i). This is due to the wind direction from the East which is in contrast to the direction of the leak from the West. It gave rise to the accumulation of natural gas in the vented enclosure. Therefore, the overpressure produced from the east is smaller than the other wind directions.

The impact that would occur due to the explosion in the North direction is that the concrete buildings were damaged and most people died. While the impact that would occur due to the explosion of the East direction is the structure of the building collapsed, serious injuries, and deaths [13]. The followings are explosion visualizations of various wind directions with the same condition:

![Explosion visualizations](image)

**FIGURE 7.** Explosion visualizations based on wind direction with vent size of 2.7m², with obstacle, night, and back ignition (a) north; (b) south; (c) west; (d) east

From the explosion visualizations above in FIGURE 7, the North direction is in the color range (i) which showed the highest overpressure at 0.5 bar. In the South and East directions were in the color range (i), which is in the range of 0.25 - 0.3 bar while the West direction is in the color range (i), which is in the range 0.3 - 0.35 bar.
3.2 Based on Ignition Point Location

The ignition point variations used in this research were the back and center in the vented enclosure. The center ignition is at coordinates of (2,3; 2,3; 0,2) and the back ignition is at coordinates of (0,2; 2,3; 0,2). The followings are the results based on ignition location with the highest explosion:

![Figure 8](image)

**FIGURE 8.** Comparisons based on ignition point location at vent size 5.4 m², east wind direction, with obstacle, day condition

**FIGURE 8.** shows the highest overpressure in the back ignition is 0.079 bar at 40.44 s while the lowest at the center ignition is 0.063 bar at 40.019 s. This is because the back ignition had a higher combination of natural gas vapor in the vented enclosure, creating a stronger external explosion [7]. Impacts that would occur due to an explosion during the back and center ignition included broken windows and minor injuries. The followings are explosion visualizations of various wind directions with the same condition:

![Explosion Visualizations](image)

(a) Center ignition  (b) Back ignition

**FIGURE 9.** Explosion visualizations based on ignition point location at vent size 5.4 m², east wind direction, with obstacle, day condition (a) center ignition; (b) back ignition

From the explosion visualizations above in **FIGURE 9**, the back ignition is in the color range ( ) which showed the highest overpressure at 0.079 bar while the center ignition is in the color ( ) and ( ) with ranges between 0.046 to 0.05.
3.2 Based on Vent Size

**FIGURE 10.** Comparisons based on vented size, north wind direction, without obstacle, night condition, and back ignition

**FIGURE 10.** shows the highest overpressure at a vent size of 2.7 m² which is 0.402 bar at 40.56 s and the lowest is at 5.4 m², which is 0.04 bar at 40.018 s. This is because the size of the vented hole is smaller than the vented hole of 5.4 m² so that the concentration contained in the vented enclosure would accumulate and take longer to spread out the vented enclosure, resulting to greater explosions. This is supported by the literature which states that the best buildings are buildings that do not have walls as open buildings can increase the dispersion area of the gas so that if an explosion occurs, it can reduce the overpressure produced [14]. The smaller the rate of dispersion of gas is, the lower the formation of explosive gas clouds. The followings are dispersion visualizations that were spread when the vented enclosures were 5.4 m² and 2.7 m²:

**FIGURE 11.** Dispersion visualizations based on vented size, north wind direction, without obstacle, night condition, and back ignition (a) 5.4 m²; (b) 2.7 m²

**FIGURE 11.** shows at the vent hole area of 5.4 m², the concentration of natural-air gas that is low or close to LFL is characterized by dominant color ( red) which is in the range 0.044 to 0.056. So, the resulting overpressure is small. Whereas in the vent hole area of 5.4 m², the air-natural gas concentration is between LFL and UFL which is marked with color ( green) and ( yellow). The followings are explosion visualizations of both vent sizes:

![Dispersion visualization](image-url-1)

![Dispersion visualization](image-url-2)
3.4 Based on the Presence of Obstacles

The variations mentioned in this research were with and without obstacle in the vented enclosure. There were 8 internal vented obstacles with two-row arrangement with a size of 0.4 x 0.4 x 4.6 m and a distance of 0.75 m each. The followings are the results based on the presence of the obstacle with the highest explosion:

**FIGURE 13.** Comparisons based on the presence of an obstacle with vent at 2.7 m²; north wind direction; night condition; back ignition

**FIGURE 13.** shows the highest overpressure on the ground with an obstacle that is 0.503 bar at 40.835 s while the lowest without an obstacle is 0.402 bar at 40.565 s. The followings are dispersion visualizations that were spread with and without obstacle:
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FIGURE 14. Dispersion visualizations based on the presence of an obstacle with vent at 2.7 m²; north wind direction; night condition; back ignition (a) With an obstacle; (b) Without an obstacle

From FIGURE 14, it can be seen that the spread pattern with an obstacle is more concentrated than without an obstacle. It is in accordance with a literature which explains that air flow has an influence on dispersion which can increase atmospheric turbulence so that buildings that become an obstacle will cause concentrations to accumulate behind the building obstacle when compared to dispersion in free space [15]. The followings are explosion visualizations with and without obstacle:

FIGURE 15. Explosion visualizations based on the presence of an obstacle with vent at 2.7 m²; north wind direction; night condition; back ignition (a) With an obstacle; (b) Without an obstacle

From FIGURE 15, the impacts caused by an explosion with an obstacle and without an obstacle were that parts of the building were damaged and increased death rate.

3.5 Based on Day and Night Conditions

The variables of day and night conditions are based on temperature, wind speed and atmospheric stability. Daytime condition has a temperature of 33.2 °C, wind speed of 4 m/s, and atmospheric stability of class B, while nighttime condition has a temperature of 23.2 °C, wind speed of 2 m/s, and atmospheric stability of class F. Atmospheric stability is defined by Pasquill and Gifford, which are generally from class A-F [16][17]. The followings are the results based on the presence of the obstacle with the highest explosion:
FIGURE 16. Comparisons based on day and night conditions with vent at 2.7 m²; north wind direction; with an obstacle; back ignition

FIGURE 16. shows the highest overpressure at night which is 0.49 bar at 40.823 s while the lowest during the day is 0.178 bar at 41.78 s. The followings are dispersion visualizations that were spread during day and night:

(a) Day  (b) Night

FIGURE 17. Dispersion visualizations based on day and night conditions with vent at 2.7 m²; north wind direction; with an obstacle; back ignition (a) Day; (b) Night

The more stable atmospheric stability (approaching class D) can reduce the mixing of fuel gas and air [18]. The simulations above show that night condition had a more stable atmospheric stability (class F) than day condition (class B). Therefore, in FIGURE 17 (a) daylight has a higher concentration or nears UFL when compared to night condition.
FIGURE 18. Explosion visualizations based on day and night conditions with vent at 2.7 m²; north wind direction; with an obstacle; back ignition (a) Day; (b) Night

From FIGURE 18. The impacts caused by the explosion at night were some buildings were damaged and the death rate increased, while the explosion at day resulted in moderate damage to buildings and lightly injured workers.

5. Conclusion

1. The highest dispersion and explosion simulation results on natural gas according to variables divided by:
   a. Wind direction: the highest simulation in North wind direction with an overpressure of 0.503 bars at 40.84 s will give impacts of damaged concrete buildings and deaths of many people.
   b. Ignition point location: the highest simulation with back ignition point with an overpressure of 0.079 bars at 40.44 s will give impacts of damaged concrete buildings and deaths of many people.
   c. Vented enclosure hole width: highest simulation on vented hole size of 2.7 m² with overpressure of 0.402 bar at 40.56 s will give impacts of collapsed buildings, occurrence of serious injuries and deaths.
   d. The presence of an obstacle: the highest simulation when using a obstacle with overpressure which reaches 0.503 bars at 40.835 s will have impacts of some damaged buildings and increased death rate.
   e. Day and night conditions: the highest simulation at night condition with an overpressure of 0.49 bars at 40.823 s will have moderate impacts on building.

2. Safety recommendations
   a. The initial structure of building development is recommended in the form of open building. If a leak occurs, such structure can increase the gas dispersion area so that when an explosion occurs, it can reduce the overpressure produced.
   b. In a building, it should be avoided to place adjacent tools in order not to cause accumulation of natural gas when released into the air.
   c. Do not place stuffs do work that causes fire sparks around natural gas.
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