Advanced Numerical Simulation of Gas Explosion for Assessing the Safety of Oil and Gas Plant

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1. Introduction

The authors have deeply been interested in concerns about health, safety & environment (HSE) in recent years. HSE demands in engineering, particularly at the design and construction stages, are becoming stricter and stricter. In oil and gas plants, many pieces of equipment, and much of the piping, treat highly flammable gases, such as natural gas, methane, propane and hydrogen, which if released, can cause vapour cloud explosions. Therefore, gas explosions are major risks in oil and gas plants. In particular, safety evaluations in connection with gas leaks and explosions are becoming more important as a part of measures to reduce risks for plants at the design stage. A gas explosion simulation system had been developed in order to respond to the safety demands of society and for the purposes of efficient plant design within an appropriate level of investment. This paper presents a mechanism of a gas explosion, methods for numerical simulations of gas explosions and case studies. To aid such simulations and calculations, advanced numerical simulations, integration of 3D Computer Aided Design (3D-CAD), Computational Fluid Dynamics (CFD) and Finite Element Analysis (FEA) are used. The integrated gas explosion simulation is utilized to predict gas dispersions, gas explosions, blast pressures and structural responses. Understanding the explosion phenomenon can help to avoid risks in oil and gas plants, and the integrated gas explosion simulation can be used to assess the safety of oil and gas plants.

2. Theory and numerical method

2.1 Mechanism of gas explosion

A gas explosion is the sudden generation and expansion of gases associated with increases in temperature and pressure which can cause structural damage. Blast pressures propagating away from the cloud center can cause extensive damage over a wide area. If combustion occurs in a medium of low initial turbulence without obstacles, the overpressure becomes very low. If obstacles are present, the flow will generate turbulence through the obstacles. The turbulence intensity will enhance combustion rates due to increase burning velocities, and then higher combustion rates will produce stronger expansion flows and the higher turbulence intensity. This cycle continues, generating higher burning velocities and increasing overpressures (Figure 1).
A deflagration is subsonic combustion. The burning velocity is subsonic and is much lower than the speed of sound in the unburnt gas. A detonation is a self-driven shock wave where the reaction zone and the shock zone are coincident. The burning velocity is supersonic and is much higher than the speed of sound in the unburnt gas. In a detonation, propagation velocities of the combustion waves can grow up to 2000 m/s with a pressure ratio across the detonation front up to 20.

**Fig. 1. Basic mechanism of gas explosion**

### 2.2 Conventional method
Conventional methods for analysing a gas explosion are simple, are easy to use and give rough predictions of blast pressures in the field. In the conventional methods, such as the TNT equivalency model and the Multi-Energy model, the blast source strength is obtained after determining the obstacle density based solely on the total volume of the equipment, piping and structures. Therefore, the blast overpressure does not precisely reflect the complex geometries of actual plant equipment.

### 2.3 Computational Fluid Dynamics (CFD)

**Fig. 2. Representation of gas explosion simulation**
CFD 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. CFD can provide information on maximum overpressure anywhere, overpressure at given points, average pressure on walls. Therefore CFD generates more realistic and more accurate information than conventional methods (Figure 2). However CFD generally includes numerical models of deflagrations, but does not include models of detonations.

2.4 Finite Element Analysis (FEA)

FEA is a numerical technique for finding approximate solutions of partial differential equations as well as of integral equations. By use of FEA, structural analysis comprises the set of physical laws and mathematics required to compute deformations, internal forces and stresses in mechanical, civil engineering, etc. This powerful design tool has significantly improved both the standard of engineering designs and the methodology of the design process in many industrial applications.

3. Integrated gas explosion simulation

Integrated explosion simulation comprises the series of four types of simulation (Figure 3), and can provide detailed information necessary for blast resistant design and risk assessment.

Fig. 3. Workflow of integrated gas explosion simulation
Blast resistant design is used to design buildings and civil engineering infrastructure to withstand explosions. Risk assessment is a step in a risk management, and is carried out by determining quantitative and qualitative values of risks. Quantitative risk assessment (QRA) represents the risks of accidents and suggests appropriate means of minimizing the risks. Frequency analysis in QRA estimates how likely accidents will occur, and frequency is usually obtained from analysis of the previous accident experience. For such cases, the frequency data are mostly derived from trusted statistical databases such as "UK HSE Offshore Hydrocarbon Release Statistics". The probability of a gas explosion is obtained by frequency analysis from gas leak scenarios. As a criterion for explosion risk, the probability of $10^{-4}$ per year is generally considered reasonable as explosion design loads. Consequent analysis evaluates the resulting effects when accidents occur. These effects could be on the human body and plant facilities like equipment, piping and structures. The consequent data are usually overpressures obtained by gas explosion analysis or gas blast analysis, and are deformations and stresses obtained by structural analysis. Risk values can be obtained only by multiplying the magnitude of the consequences and their individual occurrence frequency. The phenomena of explosion can vary enormously depending upon conditions that contribute explosion. Therefore, determining the tendency of the phenomenon through simulations requires considerable numbers of runs with broad combination of each parameters.

3.1 Gas dispersion analysis
Gas dispersion analysis is performed using CFX from ANSYS Inc., which is one of the most popular and advanced CFD tools. The gas dispersion analysis employs Navier-Stokes equations with turbulence models, gas diffusion models by the finite volume method. A gas leakage scenario in which such initial conditions as the kind of leaked gas, leak rate, leak direction, temperature, and wind direction and velocity, etc. are specified. Then, gas concentrations can be provided for a scenario.

3.2 Gas explosion analysis and gas blast analysis
Gas explosion analysis and gas blast analysis are performed using AutoReaGas from TNO Prins Maurits Laboratory and Century Dynamic Inc., which is one of the special explosion CFD tools. The gas explosion analysis employs Navier-Stokes equations with turbulence models, gas diffusion models and combustion models by the finite volume method. In order to accurately represent steep gradients in shock waves, the gas blast analysis employs Euler equations without turbulence models, gas diffusion models and combustion models by Flux Corrected Transport (FCT) technique. FCT is widely used in the numerical simulation of gas dynamic phenomena. The reason is that FCT makes optimised use of numerical diffusion, then offers great accuracy and efficiency. The geometry of objects such as equipment, piping and structures can be translated from 3D-CAD data by use of the translator program developed by us. The initial conditions for the gas explosion analysis are used as the gas concentrations obtained from the gas dispersion prediction, and the initial conditions for the gas blast analysis are used as the overpressures obtained from the gas explosion prediction. These analyses can be used to simulate burning velocities and overpressures in deflagrations.
3.3 Structural response analysis
Structural response analysis is performed using Abaqus, which is one of the most advanced and powerful tools for this kind of analysis. The results of the gas blast analysis, such as time histories of the overpressures on the surfaces of the control building, are used as the loading conditions for the structural response analysis.

4. Case study
The geometry model for case studies is shown in Figure 4. This is a typical LNG plant, comprising a large number of objects, such as equipment, structures and piping, modeled in 3D-CAD, and the plot area is about 300 m x 200 m. The location of the gas leak is in the northeast area, and the control building is in the southwest area. This case study does not consider an internal explosion, like an explosion that takes place inside a reactor or a furnace. The leaked gas is assumed to be propane because methane and natural gas tend to cause a fire, rather than an explosion, because these gases are lighter than air and quickly rise and dissipate in the open air.

Fig. 4. Geometry model of typical LNG plant

4.1 Gas dispersion analysis
In this case study, it is assumed that a gas leak occurs in the northeast area (circled in Figure 4), and the conditions are those presented in Table 1. The gas dispersion prediction shows the gas cloud on the ground (Figure 5).
Numerical Simulations - Examples and Applications in Computational Fluid Dynamics

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Table 1. Gas leakage scenario

Fig. 5. Gas concentrations at 30 s after gas release

4.2 Gas explosion analysis and gas blast analysis

The gas explosion prediction shows overpressures (Figure 6). The high overpressures indicate a strong explosion on the south side, while the low overpressures indicate a weak explosion on the north side. The overpressures are very important in determining the blast strengths.

The gas blast prediction shows overpressure time histories realistically (Figure 7). The blast waves of minimum overpressure appear after the blast waves of maximum overpressure, and the pressure gradient is very high in these areas, making it very dangerous in these areas. The maximum blast overpressure reached on the control building at 1 s after ignition. Figure 7 shows a characteristic of the gas blast phenomenon.
The shape of the blast waves is shown in Figure 8(a) and the time histories of the blast overpressures on the control building are shown in Figure 8(b). In this case study, the maximum blast overpressure on the control building is only 15 kPa, while the maximum explosion overpressure is over 100 kPa (Figure 6). Furthermore, it can be seen that the maximum overpressure on the side of the control building facing the explosion (gauge point X1) is two times higher than that on the roof (gauge point X2). Thus, this information is useful for the design of plant facilities.
Fig. 8. Overpressures at 0.65 s after ignition (a) and overpressure time histories at gauge points X 1-4 on control building (b)

4.3 Structural response analysis
The structural response prediction shows a deformation of the control building (Figure 9).

Fig. 9. Deformation of control building at 1.3 s after ignition
The control building is made of reinforced concrete and has two rooms, a floor area of 42 m x 25 m and a height of 5 m. In this case study, the maximum displacement on the roof is only about 100 mm, and is relatively small. Therefore, the structural integrity is sound.

5. Key conditions in gas explosion

The following case studies show the key conditions in gas explosions at a typical LNG plant. The geometry model is shown in Figure 4, and the ignition point is shown in Table 1 and Figure 5.

5.1 Gas cloud volume

In order to examine the relationship between gas cloud volumes and overpressures, the initial gas cloud of propane is distributed throughout a cylindrical volume at a theoretical fuel/air ratio of 1 (i.e., 4.0 vol.% propane in air) as shown in Figure 10.

![Initial gas cloud of cylindrical shape (propane)](image)

Fig. 10. Initial gas cloud of cylindrical shape (propane)

![Maximum overpressure vs. gas cloud diameter (propane)](image)

Fig. 11. Maximum overpressure vs. gas cloud diameter (propane)
Figure 11 shows that, at a height of 7 m or more, a diameter of 40 m or greater (volume >10,000 m³) results in a high overpressure, while at a height of 5 m or below, a low overpressure results at any diameter (i.e., volume). Thus, a gas explosion requires a gas cloud with both a height of at least 7 m and a diameter of at least 40 m, to sustain the expansion flow. Therefore, the gas cloud volume alone is not sufficient information to accurately predict an explosion, and more information is required to predict an explosion.

5.2 Gas concentration
In order to examine the relationship between gas concentrations and overpressures, the gas cloud is initially distributed throughout the area at a uniform concentration. As shown in Figure 12, there is only narrow range to burn easily within the flammable limits, i.e., 3.5-5.0 % for propane and 9.0-9.5 % for methane, and results in high overpressure over 1500 kPa. On the other hand, it is unlikely that such a narrow gas concentration range exists in real plant situations. In a realistic situation involving leaked gas, sharp gradients of local concentrations exist.

Fig. 12. Maximum overpressure vs. molar fraction (propane & methane)

5.3 Obstacle size
In order to examine the relationship between obstacle sizes and overpressures, obstacles are insufficiently imported from the 3D-CAD data. Figure 13 shows that overpressures are much lower, under 1 kPa, when only large obstacles, i.e., objects greater than 1 m in any one dimension, are imported from the 3D-CAD data. But Figure 6 shows high overpressures over 100 kPa. When gas is initially distributed throughout the area at the theoretical fuel/air ratio of 1 (i.e., 4.0 vol.% propane in air), Figure 14 shows the relationship between obstacle sizes and overpressures. Maximum overpressures generate over 1000 kPa when small objects, i.e., 0.2 m or less in all three dimensions are also imported from 3D-CAD data. Because the combination of both small and large obstacles creates strong turbulence, high flame velocities, high overpressures and finally explosions will occur, as explained above in Para. 2.1, Mechanism of gas explosion.
The case studies presented here demonstrate that the following conditions are necessary for gas explosions in typical oil and gas plants:

- Sufficient gas cloud diameter and height to sustain the gas expansion flow
- Gas concentrations close to the theoretical fuel/air ratio of 1 (i.e., 4.0 vol.% propane in air, or 9.5 vol.% methane in air)
- Both small and large obstacles to create strong turbulence

6. Conclusion

The gas explosion simulation system comprises high-level simulation technology using 3D-CAD, CFD and FEA. This system carries out computer simulations based on various conditions such as:

- Three-dimensional information including layouts for equipment, piping, and structures,
- Weather conditions such as wind direction, wind velocity, temperature, and atmospheric pressure,
- Gas conditions such as the type of gas leak and leak rate,
and predicts the behavior of gas leaks and their dispersions, fires, explosions, the spread of blast waves, and strength/deformation of structures. By designing blast resistance that reflects the simulation results and takes into account the impact on plant equipment and control building, and by conducting highly credible risk evaluation, the safety of the entire plant can be ensured.

This sort of simulation technology can be used in a wide range, such as gas processing plants, LNG plants, oil refining/petrochemical plants, as well as LPG Floating Production, Storage and Offloading (FPSO) plants. This system can provide detailed information that can be used to assess safety during the design stage. Understanding the explosion phenomenon can help to avoid risks in oil and gas plants. Therefore, this gas explosion simulation system can be used to assess the safety of oil and gas plants.

7. References

Mercx, W.P.M. (1994). Modelling and Experimental Research into Gas Explosions, Overall Final report of the MERGE project CEC contract STEP-CT-0111


Dorofeev S.B. et al. (1997). Large scale combustion tests in the RUT facility: Experimental study, numerical simulations and analysis on turbulent deflagrations and DDT, Transactions of the 14th International Conference on Structural Mechanics in Reactor Technology, Lyon, France, August 17-22


Nata belle Technology Ltd. (2000). Explosion Pressures Evaluation in Early Project Phase, Health & Safety Executive


This book will interest researchers, scientists, engineers and graduate students in many disciplines, who make use of mathematical modeling and computer simulation. Although it represents only a small sample of the research activity on numerical simulations, the book will certainly serve as a valuable tool for researchers interested in getting involved in this multidisciplinary field. It will be useful to encourage further experimental and theoretical researches in the above mentioned areas of numerical simulation.

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