CFD MODELING OF VAPOR CLOUD EXPLOSION, COLD BLEVE AND HOT BLEVE IN A LARGE SCALE TUNNEL

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ABSTRACT

In the present work, Computational Fluid Dynamics (CFD) explosion simulations are performed in a large scale tunnel. The length of the tunnel is approximately equal to one kilometer. Three different cases of explosion are studied: Vapor Cloud Explosion (VCE), Cold BLEVE (Boiling Liquid Expanding Vapor Explosion) and Hot BLEVE. The main purpose of this study is the calculation of the generated overpressures inside the tunnel and the comparison of the pressure dynamics among these type of explosions. Realistic scenarios are chosen for each explosion based on the traffic of the tunnel. In the Vapor Cloud Explosion case, the release and dispersion of 23100 kg propane into the atmosphere are simulated in order to calculate the concentration distribution in the tunnel. Both external wind and piston effect due to vehicles' movement was taken under account in the dispersion process. Then the mixture is ignited and the deflagration process is simulated in order to calculate the generated overpressures. In the Cold BLEVE case the total loss of confinement of a 29 m^3 high pressure (57 bar) carbon dioxide storage tank is simulated, whereas in the Hot BLEVE case the total loss of confinement of a 46 m^3 propane storage tank (at 18 bar) is considered. The total loss of confinement of the tanks lead to a violent expansion due to evaporation. As a result high overpressures are generated. The transient three dimensional Navier-Stokes equations of the multispecies mixture along with the continuity equation, the conservation equation of species and the energy equation are solved. Turbulence is modelled with the standard k-ε model. In the Vapor Cloud Explosion case a Multi-Phenomena turbulent burning velocity combustion model is used. In the Hot BLEVE case, fire is modeled using the Eddy Dissipation Concept (EDC) model. The simulation results reveal that the modeling approach that is used is capable of reproducing physical realistic results. Differences in pressure dynamics among the scenarios are revealed due to the different physics of the explosions.

INTRODUCTION

In the present work, Computational Fluid Dynamics (CFD) explosion simulations are performed in a real tunnel located in Greece. The main purpose of this study is the calculation of the generated overpressures inside the tunnel and the comparison of the pressure dynamics among these types of explosions.

The CFD code ADREA-HF [1] is used for the simulations. It is a CFD software which has been used with great success in release, dispersion and deflagration problems in complex geometries. ADREA-HF have been validated against both deflagration experiments [2][3][4] and two phase releases [5][6][7]. ADREA-HF solves the transient three dimensional Navier-Stokes equations of the multispecies mixture along with the continuity equation, the conservation equation of species and the energy equation.

Three explosion scenarios are investigated. The first one deals with the explosion of a premixed propane-air mixture. This is a Vapor Cloud Explosion (VCE) case. In this scenario, liquid propane leaks out of its storage tank and disperses into the tunnel forming a flammable mixture. This mixture is then ignited and the generated overpressures are estimated. The phenomena are simulated in two steps: First, the release and dispersion of 23100 kg propane into the atmosphere are simulated in order to calculate the concentration distribution in the tunnel. Then the mixture is ignited and the deflagration process is simulated in order to calculate the generated overpressures. The combustion model that is used is the "Multi-Phenomena turbulent burning velocity" model [8]. The model accounts for all the main physical mechanisms that appear in deflagrations such as the turbulence generated by the flame front itself, preferential diffusion and fractal structure of the flame front. This model has been extensively used in deflagration simulations.

The second explosion scenario deals with the total loss of confinement of a high pressure carbon dioxide storage tank. Carbon dioxide is stored in liquid form in a 29 m^3 tank, at 57.34 bars and at ambient temperature. The total loss of confinement of the tank leads to a violent expansion of the carbon dioxide due to its evaporation. As a result high overpressures are generated. This type of explosion is known as Cold BLEVE (Boiling liquid expanding vapor explosion).

The third explosion scenario deals with the total loss of confinement of a high pressure propane storage tank. Propane is stored in liquid form in a 46 m^3 tank, at 18 bar and at ambient temperature. Similar to the Cold BLEVE case, the total loss of confinement of the tank leads to a violent expansion of propane due to its evaporation. Propane is a flammable gas and as a result fire is also developed. Fire is modelled using the Eddy Dissipation Concept (EDC) [9] which is a widely used model in diffusion flame modeling. This type of explosion is known as Hot BLEVE.

NOMENCLATURE

t	[s]	Time
x	[m]	Distance
u	[m/s]	Velocity
p	[Pa]	Pressure
g	[m/s^2]	Gravity
Pr	[-]	Prandtl number
Sc	[-]	Schmidt number
H	[J]	Static enthalpy
q	[-]	Mass fraction
$\bar{R}$	[kg/m^3/s]	Mean reaction rate
N_{subs}	[-]	Number of species
S_t	[m/s]	Turbulent burning velocity
S_u	[m/s]	Laminar flame speed
u'	[m/s]	Fluctuating velocity component (m/s)
MW	[gr/mole]	Molecular weight

Greek letters

ρ	[kg/m^3]	Mixture density
μ	[kg/m/s]	Viscosity
Ξ	[-]	Correction factor
ε	[m^2/s^3]	Turbulence energy dissipation rate
k	[J/kg]	Turbulence kinetic energy
v	[-]	Stoichiometric coefficient

Subscripts superscripts and bars

i	Index of spatial direction (i=1, 2, 3)
t	Turbulent
eff	Effective
f	Fuel
u	Unburned
o_2	Oxygen
v	Vapor
$\bar{\ }$	Time-averaged quantity
$\tilde{\ }$	Mass-weighted average quantity

MATHEMATICAL METHODOLOGY

ADREA-HF models the transient three dimensional turbulent flow field and the dispersion of a multispecies mixture. The mixture is assumed to be ideal and in thermodynamic equilibrium (i.e. all parts of the mixture have the same pressure and temperature). Every species can be in vapor, liquid or solid state. Discretization of the conservation equations is performed using the control volume approach on Cartesian grids. Intersection of geometry with the grid is treated with the porosity formulation. Resulting grid cells can be fully active, fully blocked by solid parts or partially active.

The Navier-Stokes equations, the continuity equation and the energy equation of the mixture are solved along with the conservation equation of species. The Favre-averaged equations are (Einstein summation convention is used):

$$\frac{\partial \bar{\rho}}{\partial t}+\frac{\partial \bar{\rho}\tilde{u}_i}{\partial x_i}=0 \tag{1}$$

$$\frac{\partial \bar{\rho}\tilde{u}_i}{\partial t}+\frac{\partial \bar{\rho}\tilde{u}_j\tilde{u}_i}{\partial x_j}=-\frac{\partial \bar{p}}{\partial x_i}+\frac{\partial}{\partial x_j}\left(\mu_{eff}\left(\frac{\partial \tilde{u}_i}{\partial x_j}+\frac{\partial \tilde{u}_j}{\partial x_i}\right)\right)+\bar{\rho}g_i \tag{2}$$

$$\frac{\partial \bar{\rho}\tilde{H}}{\partial t}+\frac{\partial \bar{\rho}\tilde{u}_j\tilde{H}}{\partial x_j}=\frac{\partial}{\partial x_j}\left(\frac{\mu_t}{\mathrm{Pr}_t}\frac{\partial \tilde{H}}{\partial x_j}\right)+\frac{D\bar{p}}{Dt} \tag{3}$$

$$\frac{\partial \bar{\rho}\tilde{q}_k}{\partial t}+\frac{\partial \bar{\rho}\tilde{u}_j\tilde{q}_k}{\partial x_j}=\frac{\partial}{\partial x_j}\left(\frac{\mu_t}{Sc_t}\frac{\partial \tilde{q}_k}{\partial x_j}\right)+\bar{R}_k,\quad k=1,\ldots,N_{subs} \tag{4}$$

Turbulence is modelled using the standard k-ε model with wall functions. The temperature of the mixture and the phase distribution of the species are calculated using the Raoult's law for ideal mixtures, given the pressure, the mixture enthalpy and the species mass fractions. Non-vapor phase exists only if the temperature of the mixture is lower than its dew temperature. In that case, if the temperature is higher than the triple point, liquid phase is consider otherwise solid phase. ADREA-HF code contains an extensive thermodynamic package with physical properties of many elements and compounds. A number of different equations of state are also included. The simplest model makes a discrete description of each phase (ideal gas, correlations for the density of liquid and solid phase as a function of temperature). Third order equations of states are also available such as Peng Robinson and Redlich-Kwong-Mathias-Koperman. For the VCE and the Hot BLEVE cases the discrete description of each phase was used whereas for the Cold BLEVE case the Peng Robinson equation of state was used.

Regarding the VCE and Hot BLEVE cases where combustion occurs, a one-step reaction mechanism is assumed. Transport equation for each species which is involved in the combustion process (i.e. Propane, Oxygen, Water and Carbon dioxide) is solved. In the following paragraphs, the models that were used for the reaction rate are presented.

Vapor cloud combustion modeling

VCE is a premixed type of combustion. The main issue in premixed combustion modeling is the estimation of the reaction rate which appears in the equation of species as source term. The "Multi-phenomena turbulent burning velocity" model [8] is used. The model is based on the turbulent flame speed concept. The fuel reaction rate is modelled as follows:

$$\bar{R}_f=\rho_u S_t\left|\nabla q_f\right| \tag{5}$$

The main concern in this type of models is the calculation of the turbulent flame speed. The turbulent flame speed is calculated based on a modification of Yakhot's equation [10], and accounts for all the main physical mechanisms which appear in deflagrations such as the turbulence generated by the flame front itself, preferential diffusion and fractal structure of the flame front:

$$S_t=\Xi_k\cdot\Xi_{lp}\cdot\Xi_f\cdot S_u\cdot\exp\left(\frac{u'}{S_t}\right)^2 \tag{6}$$

The Ξ factors are not included at the original form of Yakhot's equation. These factors accounts for the various mechanisms which accelerate the combustion process. Details about the implementation in the ADREA-HF can be found in [2].

Hot BLEVE combustion modeling

Hot BLEVE is simulated as a diffusion flame because fuel and oxidizer (air) are initially separately. The Eddy Dissipation Concept (EDC) model [9] is used. EDC model has been used with success in similar cases [11][12][13]. The main idea of the model is that the rate of combustion depends only by the mixing of fuel and oxidizer. The mean reaction rate is calculated by the formula:

$$\bar{R} = C_{EDC}\rho\frac{\varepsilon}{k}\min\left[\frac{q_{f,v}}{\nu_f MW_f},\frac{q_{O_2,v}}{\nu_{O_2} MW_{O_2}}\right] \qquad (7)$$

where the model constant C_{EDC} was set equal to 4 [9]. $q_{f,v}$ and $q_{O_2,v}$ are the vapor mass fraction (i.e. kg of species vapor to kg of mixture) of fuel and oxygen respectively.

Numerical details

ADREA-HF uses the finite volume method on a staggered Cartesian grid. The pressure and velocity equations are decoupled using a modification of the SIMPLER algorithm. For the discretization of the convective terms in the momentum equations a second order accurate bounded central scheme was used while in the conservation equations of species and energy a second order accurate bounded linear upwind scheme. The implementation was carried out using a deferred-correction approach via the source term. For the time advancement, the second order accurate Crank-Nicolson numerical scheme was chosen. The time step is automatically adapted according to prescribed error bands and the desired CFL number. CFL maximum value was lower to 1.0 in all cases.

PROBLEM SETUP

The tunnel was modelled (Figure 1) with accuracy based on its actual geometry. The number of the vehicles that were placed inside the tunnel was estimated based on the traffic data. 59 vehicles were placed in total from which 12 vehicles were trucks and the rest cars. A simplified rectangular geometry of the vehicles was considered (Figure 2). The point of the accident where the explosion occurs was set at 536 m from the beginning of the tunnel (approximately in the middle of tunnel).

Vapour Cloud Explosion

In this scenario a realistic accident involving a propane transport vehicle is considered. The propane leaks from of the storage tank and mixes with the surrounding air forming a flammable cloud. Two simulations were made for this scenario. At first, the release and dispersion of propane was simulated in order to estimate propane concentrations inside the tunnel. Then, the explosion simulation was made by igniting the flammable cloud. The cloud is ignited at the time when the total flammable volume of the propane becomes maximum. This is considered as the worst case scenario. The total mass of the propane is equal to 23100 kg and the storage tank has a volume of 55000 m^3. The mass flow rate is equal to 36 kg/s. The injection point has square geometry of 50 x 50 mm^2 area. The propane at the release point is considered to be in liquid state. The release velocity was estimated equal to 28.69 m/s and its duration equal to 641.67 s. The release direction is horizontal towards the vertical wall of the tunnel (towards +y axis, Figure 1).

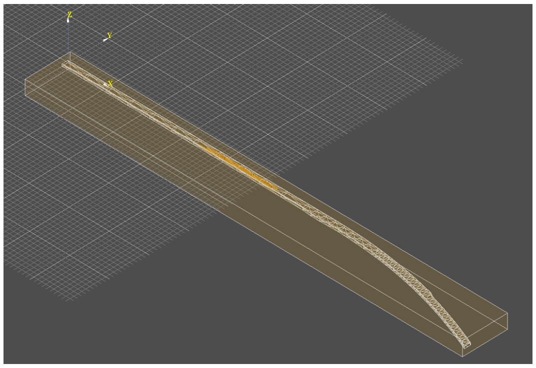

Figure 1 Geometry of the tunnel (white area inside the rectangular box)

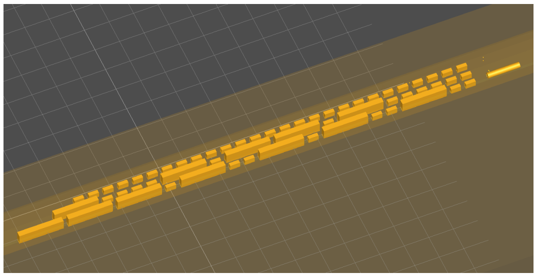

Figure 2 Vehicles inside tunnel. The cylinder represents the fuel tank.

Based on the meteorology data of the tunnel area, -2.15 m/s external wind exists (opposite to the cars' movement). The external wind opposes to the flow field (piston effect) that the car movement generate. The wind from the piston effect was estimated equal to 2.55 m/s based on the traffic of the tunnel. As a result, a total wind field of 0.4 m/s exists inside the tunnel. This value was used as initial and boundary condition in a preliminary simulation in order to predict the initial flow field inside the tunnel for the propane dispersion simulation. However, as the traffic of the cars reduces because of the accident, the piston effect reduces too. Consequently, the external wind became equal to piston effect and eventually overcomes it. This was taken into account, by considering variable boundary condition for the wind strength at the dispersion simulation. As a result the wind boundary condition is varied linearly from 0.4 m/s at the beginning of the dispersion simulation to -0.8 m/s at the end of the leakage.

In Figure 3 the numerical grid on the xz plane at the area close to the release point for the dispersion problem is presented. The total number of active cells is equal to 374,100. Cells get denser close to the release point. Cells get also denser near the ground, in order to capture the stratification of the propane. Propane is heavier than air and as a result it is expected to be accumulated on the ground. The height of the cells near the ground is equal to 0.2 m. For the combustion simulation, a denser grid of 500,000 cells was used. Denser grids were also tested without having significant effect on the results. Several domain sizes were also tested in order to ensure that the boundary conditions do not affect the generated overpressures. The domain size of 1580 x 350 x 20 m was chosen.

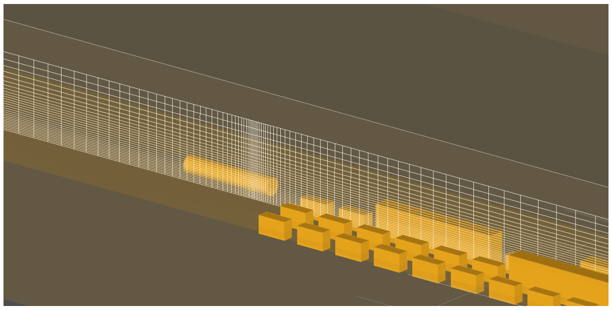

Figure 3 Numerical grid at the area close to the release on xz plane.

Cold BLEVE

In Cold BLEVE case, the total loss of confinement of a tank containing high pressure liquid CO_2 is considered. The sudden loss of confinement of the tank leads to a violent depressurization which causes sudden expansion of CO_2 because of liquid to vapor phase transition. A realistic case scenario is considered. 20440 kg of CO_2 are considered in a volume of 29 m^3. The storage pressure is 57.34 bars and the temperature is the ambient (20^0C). A rectangular geometry of the tank was considered. The tank position is the same with the tank position of the VCE case. Three grids of total number of active cells equal to 480,000, 780,000 and 935,000 were tested without having significant changes in the results. The results with the densest grid are presented next. The tank was discretized using 30 x 9 x 9 cells. Several domain sizes were tested. The domain size of 1290 x 250 x 20 m was chosen.

Hot BLEVE

In Hot BLEVE case, the total loss of confinement of a tank containing high pressure liquid propane is considered. Similar to the Cold BLEVE case, the depressurization and the sudden expansion of the propane leads to the development of high overpressures. In Hot BLEVE case, the combustion of propane assists to the further increase of the generated overpressures. A realistic case scenario is considered. 23100 kg of propane occupies a volume of 46 m^3. The storage pressure is 18 bars and the temperature is the ambient (20^oC). A rectangular geometry of the tank was considered. The tank position is the same with the tank position of the Cold BLEVE cases. Three grids of total number of active cells equal to 218,000, 514,600 and 943,300 cells were tested without significant changes in the results. The results with the 514,600 cells are presented next. The tank was discretized using 18 x 6 x 11 cells. The same domain size as the Cold BLEVE case was used.

RESULTS AND DISCUSSION

Vapor Cloud Explosion

In Figure 4 the propane volume fraction is presented on xz and xy planes at 600 s. We observe that propane has been spread to the entire length of the tunnel. However it mainly occupies the lower part of it. In the same figure the liquid mass fraction of propane is presented at the height of 0.5 m. We observe that liquid propane exists only in a small area around the release point. The liquid propane absorbs heat from the surrounding air and the tunnel walls and evaporates. The flammable volume reached its maximum value at 1250 s (which is approximately twice the release duration). This is the time when the ignition of the explosion was considered.

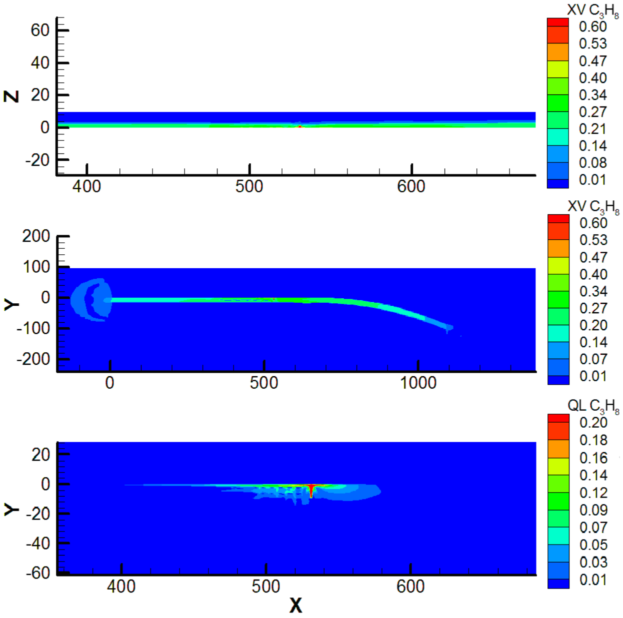

Figure 4 Propane volume fraction on xz (up) and xy (middle) plane and liquid propane mass fraction on xz plane (bottom) at 600 s.

The ignition point was placed near the release point. Figure 5 presents the overpressure time histories across the tunnel for various distances from the ignition point. The maximum value of the overpressure is approximately equal to 500 kPa. We observe that the overpressure profile remains the same until the distance of 230 m from the ignition point. After that distance the overpressures are getting smaller. We also observe that the pressure increases only after 2 s from the ignition. Furthermore we observe that there is no sharp pressure peak but high values of pressures are maintained for large period of time (approximately 2 s). The reasons for the large time-scales are: a) the small laminar flame speed of propane b) the very large amount of fuel and c) the large length of the tunnel and d) the fact that the fuel is spread in its whole length. Finally, We should mention that the pressure is approximately the same in every point of a tunnel cross section (it changes only along the tunnel). In Figure 6 the pressure and temperature contours are presented at 3.4 s. Temperature contours give an indication of the position of the flame front. We observe that at 3.4 s the flame front is outside the tunnel.

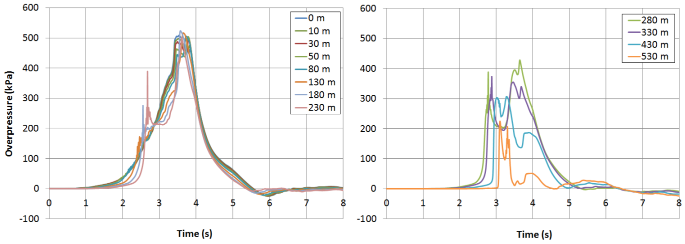

Figure 5 VCE - Overpressure time histories along the tunnel for various distances from the ignition point.

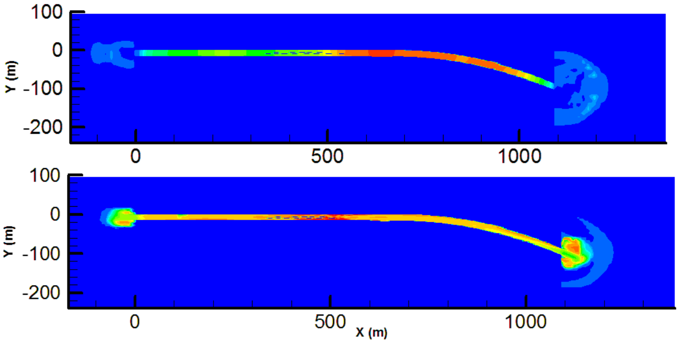

Figure 6 VCE - Pressure contours (up) and temperature contours (bottom) on plane z=3.0 m at 3.4 s. Pressure varies between 1.0-6.5 bars and temperature between 240-2700 K.

Cold BLEVE

In Figure 7 the overpressure time histories for the Cold BLEVE case are presented. Opposite to the VCE case, the overpressure is not the same at every point of the cross section where explosion occurred. The maximum value of overpressure is observed at the right wall and is approximately equal to 3300 kPa. We observe that the overpressure at 15 m from the accident has been greatly reduced. After that point the pressure reduces with smaller rate. The generation of a pressure wave is clearly evident.

In Figure 8 the pressure and temperature contours are presented at 0.4 s. The existence of a pressure wave is also evident here. In the temperature contours we observe that a low temperature area is formed. This is caused by the evaporation of CO_2. High temperature regions are also formed due to compression.

Hot BLEVE

In Figure 9 the overpressure time histories for the Hot BLEVE case are presented. We observe that, similar to the Cold BLEVE case, the pressure is not the same at every point of the cross section where explosion occurred. The maximum value of overpressure is equal to 2000 kPa. We observe that the maximum overpressures at the explosion point are lower compared to the Cold BLEVE case. The lower pressure that propane is stored compared to CO_2 along with the fact that propane has smaller expansion ratio (ratio of liquid to vapor densities) lead to this difference. On the other hand the overpressures are maintained longer in time in Hot BLEVE case. The reason for this is the greater amount of propane compared to the amount of CO_2. The combustion of the propane contributes also to maintain the overpressure values high. The overpressures are gradually decreased as we move away from the explosion point. A pressure wave propagates through the tunnel. The overpressure peaks of this wave have larger values compared to the Cold BLEVE case. Again, the generated heat from the combustion of propane is responsible for this. Combustion of propane leads to high temperatures and as a result high overpressures.

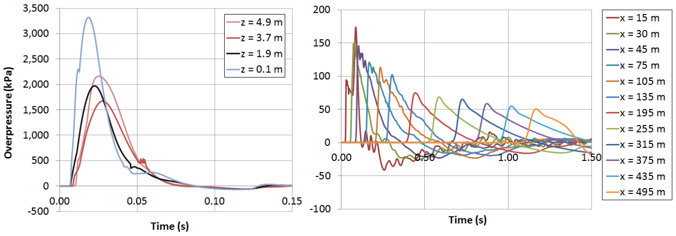

Figure 7 Cold BLEVE - Overpressure time histories at various heights on the right wall of the cross section where the explosion occurred (left) and at the ceiling for various distances from the area of the explosion (right).

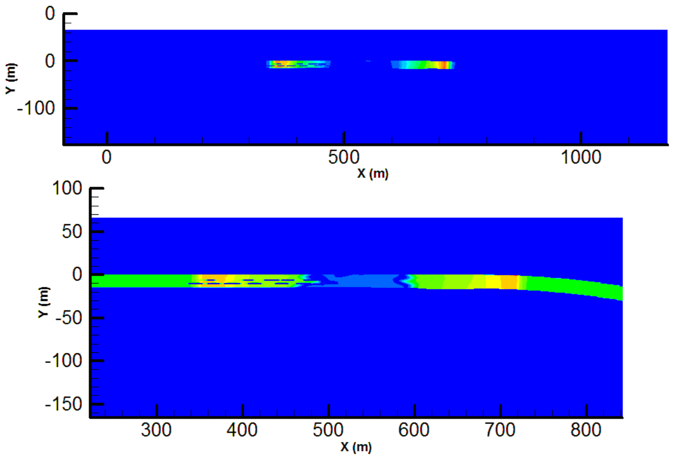

Figure 8 Cold BLEVE - Pressure contours (up) and temperature contours (bottom) on plane z=3.0 m at 0.4 s. Pressure varies between 1-2 bars and temperature between 180-400 K.

In Figure 10 the pressure and temperature contours are presented at 1.0 s. The existence of a pressure wave is also evident here. To compare with the Cold BLEVE case, the area where high overpressures occur are larger. The combustion of propane is responsible for this, maintaining the pressure high in a large area. In temperature contours we observe that low (below ambient) and high values of temperatures are formed because of propane evaporation and combustion respectively.

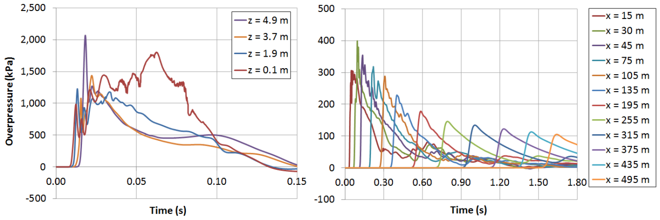

Figure 9 Hot BLEVE - Overpressure time histories at various heights in the right wall of the cross section where the explosion occurred (left) and at the ceiling for various distances from the area of the explosion (right).

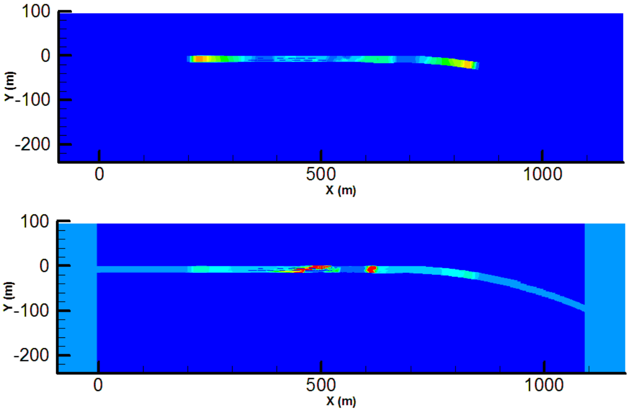

Figure 10 Hot BLEVE - Pressure contours (up) and temperature contours (bottom) on plane z=3.0 m at 1.0 s. Pressure varies between 1-2.5 bars and temperature between 200-800 K.

CONCLUSIONS

Three explosion cases in a large tunnel were studied: A Vapour Cloud Explosion (VCE) of propane-air premixed gas mixture, a Cold BLEVE case caused by the total loss of confinement of a tank with liquefied CO_2 and a Hot BLEVE case caused by the total loss of confinement of a tank filled with liquefied propane. Realistic parameters were selected for each case. CFD simulations were carried out in order to predict the generated overpressures and the temperature distribution inside the tunnel.

The worst case in terms of maximum overpressures was the Cold BLEVE case. The VCE case gave smaller maximum overpressures compared to BLEVE cases. The reason for that behaviour is the different physics between the two phenomena. In VCE case, a flame front exists which travels through the premixed mixture which occupies the whole length of the tunnel. The pressure in this kind of explosion (non-detonation case) is usually increased progressively. Furthermore, the duration of the explosion is larger compared to the BLEVE cases. On the other hand, BLEVE are more violent explosions with short duration. The main mechanism which generates the overpressures is the sudden expansion of the liquefied gas due to phase change. This phenomenon is very rapid and occurs in a small area, around the liquefied gas. As a result, the generated overpressures take great values but have shorter duration compared to the VCE case. A pressure wave front is formed which propagates throughout the tunnel. Finally, significant differences are observed in pressure values between near distances, especially at the points which are located near the explosion.

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