

VAPOR CLOUD EXPLOSION BLAST MODELLING**Experimental investigation of the key parameters and blast modelling**

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Abstract

The Multi-Energy method for vapor cloud explosion blast modeling is presented and demonstrated in a case study. The Multi-Energy method constitutes an alternative for conventional TNT-equivalency methods which are unsatisfactory in several aspects. The Multi-Energy concept as it is, however, is only a framework which has to be completed with additional data. These data can be generated in various ways dependent on the available time and budget. In particular, the use of computational fluid dynamics within the Multi-Energy framework enables an increasingly sophisticated approach in vapor cloud explosion hazard analysis.

1. INTRODUCTION

The many vapor cloud explosion incidents from the past indicate that the presence of a quantity of fuel constitutes a potential hazard for its environment. When an amount of fuel is released, it will mix with air and a flammable vapor cloud is the result. If this cloud meets an ignition source, it will be consumed by a combustion process which - under appropriate conditions - may develop an explosive intensity and blast effects.

The potential explosion hazard of a vapor cloud can be quantified as being its explosive power upon ignition. The explosive power of a vapor cloud can be expressed as an equivalent explosive charge whose blast characteristics - the distribution of the blast wave properties in its vicinity - are known.

How to relate the quantity of fuel available in a vapor cloud to an equivalent charge expressing its explosive power? Up to this day TNT-equivalency methods are widely used for this purpose.

TNT-equivalency methods state a fixed proportional relationship between the weight of the fuel available in the cloud and the weight of a TNT-charge expressing the cloud's explosive power. So strictly speaking, using TNT-equivalency methods, it is implicitly assumed that a fuel-air mixture is explosive in itself.

Gas explosion research during the last decade, however, has shown a completely different picture. It shows that a fuel-air mixture is flammable, indeed, but explosive only under appropriate (boundary) conditions, i.e. only where the mixture is partially confined and/or obstructed. This fact is recognized in the Multi-Energy method for vapor cloud explosion blast modeling. The Multi-Energy method, however, is only a framework which has to be completed with additional data.

In this paper, this modern alternative for TNT-equivalency methods is demonstrated in a simple case study. In this case study a vapor cloud explosion hazard assessment is performed with regard to a storage site for liquefied hydrocarbons.

Statement of the problem

A view of the storage site is represented in Figure 1. Three storage spheres, each containing 20 tons of liquefied propane are situated next to a large butane tank of 50 m diameter and a height of 30 m. To diminish heat inflow from the soil, the butane tank is placed 1 m above the earth's surface on a concrete pylon forest (Figure 1). In this environment, a sudden rupture of one of the spheres and a subsequent massive release of propane is anticipated. What blast effects are to be expected if the propane forms a large flammable cloud blanketing the storage site and meets an ignition source?

2. THE MULTI-ENERGY CONCEPT

Presently, the belief is gaining ground that it is hardly possible to detonate an unconfined vapor cloud, originating from an accidental release of hydrocarbons in the open. The point is that the inhomogeneity of the fuel-air mixture, which is inherent to process of atmospheric dispersion, prevents a possible detonation from propagating (Van den Berg, 1987).

The heavy vapor cloud explosion on December 7, 1970 at Port Hudson (MO) where a substantial part of a large unconfined propane-air cloud detonated (Burgess and Zabetakis, 1973), should be blamed on a highly exceptional coincidence of circumstances. Lingering in a shallow valley under calm atmospheric conditions,

a dense propane-air cloud had the opportunity to homogenize sufficiently by molecular diffusion during an exceptionally long ignition delay (Van den Berg, 1987). This incident is unprecedented, so far.

Therefore, in a vast majority of cases, the assumption of deflagrative combustion is a conservative and sufficiently safe approach in a vapor cloud explosion hazard assessment. In general, the initial stage in the process of deflagrative combustion in gas explosions is more or less laminar. Laminar flame propagation is largely determined by molecular transport of heat and species. Therefore, laminar flame propagation is a slow process. Flame velocities in stoichiometric hydrocarbon-air mixtures are of the order of meters per second while attendant overpressures are less than 1 kPa. How can slow laminar combustion develop into an intense, explosive and blast generating process? The key to this problem can be found in the phenomenon of turbulence.

Premixed combustion induces expansion, a flow field. If the boundary conditions to this expansion flow field are such that turbulence is generated, the flame - which is convected in this flow field - will interact with the turbulence. The turbulence increases the flame front area - the interface between reactants and combustion products - by which the combustion process intensifies. More reactants are converted into combustion products per unit of volume and time resulting in stronger expansion flow. Higher flow velocities go hand in hand with more intense turbulence which, in turn, intensifies combustion etc., etc.

A positive feed-back coupling is triggered by which the process develops more or less exponentially.

A deflagrative gas explosion may be well defined as a process of combustion-driven expansion flow in which the turbulent structure of the flow field acts as an uncontrolled positive feed-back (Figure 2).

The consequence is that a turbulence generating environment is required for the development of explosive, blast generating combustion. This important conclusion determines the concept of a vapor cloud explosion which underlies the method of blast modeling. This basic concept, called the Multi-Energy concept, states that blast is generated in vapor cloud explosions only in the parts of the vapor cloud which are obstructed and/or partially confined and that the unobstructed and/or unconfined parts of the cloud hardly contribute (Van den Berg, 1985). This concept is increasingly supported by experimental data e.g. Zeeuwen et al. (1983), Harrison and Eyre (1987) and Van Wingerden (1989). So, contradictory to conventional methods, in which a vapor cloud explosion is regarded as an entity, in the Multi-Energy concept a vapor cloud explosion is rather defined as a number of sub-explosions corresponding to the various partially confined/obstructed areas in the cloud.

Application

The space underneath the butane storage tank is the only location at the storage site where blast generating (boundary) conditions are found. The space underneath the storage tank is an outstanding example of a combination of partial confinement by extended parallel planes and obstruction by the pilon forest which pre-eminently is a turbulence generating environment. On the other hand, the space underneath and in between the propane spheres, for instance, is relatively open and unobstructed. Therefore, the Multi-Energy concept, applied to this situation, indicates that if the entire storage site is blanketed in an extended flammable cloud, only the explosive combustion which can develop underneath the storage tank is responsible for the blast produced upon ignition of the cloud.

The blast effects produced by this gas explosion are mainly determined by the quantity of combustion energy present in the space underneath the butane tank and the intensity of the combustion process. Both are primarily determined by the size, the shape and nature of this partially confined and obstructed space. The reactivity of the fuel-air mixture is a factor, indeed, but of secondary influence.

3. BLAST MODELING

3.1 The blast model

How should the blast produced by the gas explosion developing underneath the storage tank be modeled? TNT-equivalency methods use experimental TNT-blast data to represent the blast properties in the vicinity. However, the use of TNT-blast data for this purpose is unsatisfactory in several respects:

- TNT-blast does not correspond with gas explosion blast. In the analysis of many vapor cloud explosion incidents, a lot more TNT was required to model the far-field effects than the near-field effects (Brasie and Simpson, 1968). In other words: TNT-blast decays faster than vapor cloud explosion blast. The introduction of a virtual distance (e.g. Prugh, 1987) is only a limited solution to this problem.
- Contradictory to TNT-detonations, gas explosions are variable in strength. This variability in strength is a feature which can hardly be represented by TNT-blast data. In particular, the blast due to low strength gas explosions is hard to model by TNT-blast.

Therefore, in this approach fuel-air charge blast data are used to model blast effects from gas explosions.

Figure 3 shows the peak overpressure as well as the positive phase duration of the blast wave produced by a hemispherical fuel-air charge at the earth's surface dependent on the distance to the blast center in a Sachs scaled representation. This blast model is generated by numerical simulation of spherical steady flame speed gas explosions. The blast model exhibits basic features of gas explosion blast. The strength is a variable

expressed as a number ranging from 1 for insignificant to 10 for detonative strength. In addition, the model gives an indication for the blast wave shape.

The blast produced by the gas explosion underneath the butane tank can now be modeled by the blast from an equivalent hemispherical fuel-air charge which is characterized by a size and a strength.

3.2 The charge size

A safe and conservative estimate for the size of the charge can be made by assuming that the whole space underneath the tank is filled with a stoichiometric mixture which as a whole contributes to the blast. Consequently, the radius of the hemispherical charge is approximately 10 m which corresponds with an energy of 7330 MJ. (Heat of combustion of stoichiometric hydrocarbon-air mixtures is approximately 3.5 MJ/m^3)

3.3 The charge strength

A good estimate for the strength of the blast is a more difficult problem which can be overcome in a variety of ways depending on the accuracy required and the available time and budget.

Safe and conservative data

A safe and conservative estimate for the strength of the charge for near-field blast effects is 10 i.e. the assumption of detonative combustion. For far-field blast effects, on the other hand, the assumption of any strength higher than or equal to number 6 is sufficient because far-field effects are independent of the charge strength whether the explosion was a strong deflagration (number 6) or detonation (number 10). This is clearly demonstrated by the blast characteristics of the fuel-air charge model in Figure 3.

If the substitution of safe and conservative data is considered to be not accurate enough, the estimate for the strength could be refined by, for instance, experimental data.

Experimental data

Since more than a decade ago, an increasing amount of experimental data on flame propagation in partially confined/obstructed environments becomes available. Many parameters were varied such as:

- geometry (channel-like, cylindrical, spherical)
- obstacle parameters (shape, pitch, blockage ratio)
- fuel reactivity (gas composition, type of gas)
- scale

This growing body of experimental data offers the opportunity to compare real situations with experimental set-ups. For a good interpretation of the mostly small-scale experiments, a solid understanding of scale effects in gas explosions is a necessity. It would be desirable to collect the data in a data base which can be searched by means of a retrieval system.

Experiments which could give a first indication for the overpressure to be expected from the gas explosion in the space underneath the butane tank are reported by Van Wingerden (1989). A large number of obstacle configurations between parallel planes were investigated with regard to their blast generating capabilities. On the basis of these experimental data, a first estimate for the overpressure of 50 kPa to 200 kPa would be reasonable.

In addition, a good understanding of scaling effects offers the possibility of physical modeling i.e. the estimation of overpressures by an experiment in a scaled down version of the real situation. In this connection, Van Wingerden (1989) showed that simple scaling is possible for flame speeds lower than 100 m/s. This means that, if only low flame speeds are anticipated, the physical modeling can be confined to the same fuel and a similar experimental set-up as considered in the real situation. If higher flame speeds are anticipated, Catlin and Johnson (1990) suggest various techniques to compensate for scale effects. For very high flame speeds, quenching of combustion by turbulence becomes a determining mechanism. This can be compensated by the use of oxygen-enriched mixtures (Catlin and Johnson, 1990). The use of more reactive fuels for this purpose was suggested by Taylor and Hirst (1988), although on the basis of different considerations.

Computational data

An approach which seems very promising for the near future is numerical simulation with advanced computational fluid dynamic computer codes such as FLACS (Hjertager, 1982 and 1989) and REAGAS (Van den Berg et al., 1987 and Van den Berg, 1989). These codes are capable of simulating the basic mechanism of a gas explosion, i.e. the feed-back coupling in the interaction of combustion, flow and turbulence. The mathematical model which underlies these codes can be outlined as follows:

- The gas dynamics is modeled as a gaseous fluid which expands as a consequence of heat addition. This is expressed in conservation equations for mass, momentum and energy.

- The energy addition is supplied by combustion which is modeled as a simple one-step conversion process of non-reacted material into combustion products. This is expressed in a conservation equation for the mixture mass fraction with a negative source term for the combustion rate.
- The combustion rate, which is fully controlled by turbulent mixing of combustion products with unreacted material, is modeled by the Bray-Libby-Moss Unified Probability Function model (Bray, 1980).
- The feed-back in the interaction is closed by a k - ϵ model for turbulence which consists of conservation equations for the turbulent kinetic energy k and its dissipation rate ϵ .

Here, the REAGAS-code is utilized to simulate the gas explosion in the space underneath the storage tank. For that purpose the pilon forest between two parallel planes is simplified into a two-dimensional obstacle environment. The obstacles are placed in 11 concentric circles according to the pilon lay out (Figure 4a). In a first approach, a centrally ignited gas explosion in this configuration is simulated in a 130×65 nodes grid. The results are represented in Figure 4a which shows the temperature distribution in the expansion flow field at a few points of time. The temperature distribution is visualized by a pattern of isotherms, one for each increase in temperature of 150 K.

The sequence of pictures shows a very characteristic behavior of gas explosions, namely: a slow start followed by a more or less exponential development in flame speed and pressure once the feed-back coupling in the process of flame propagation is triggered. This characteristic behavior can be readily recognized in the overpressure transients sampled at various locations in the flow field and represented in Figure 4b. The computations show that an overpressure of more than 40 kPa is generated during the development of this centrally ignited gas explosion. This maximum overpressure is observed more or less throughout the partially confined space.

However, the assumption of central ignition is unrealistic. It is more likely that the vapor cloud will meet an ignition source somewhere at the storage site outside the partially confined area. Then the combustion process in the obstacle configuration will be initiated from its edge and the flame propagation has a substantially longer path available to speed up than in the centrally ignited case.

As a consequence, it must be held realistic that the maximum overpressure generated in the space underneath the storage tank may be substantially higher than 40 kPa.

To check whether the effect of edge-ignition can be simulated by the REAGAS-code, the combustion process was initiated halfway between center and edge. The results, represented in Figure 5a and 5b, confirm the expected behavior. Since the combustion products are vented out of the obstacle configuration at an earlier stage now, the feed-back is triggered later but the considerably longer path available for the combustion process to speed up results in a maximum overpressure of more than 70 kPa. The maximum overpressures that are attained now, are less homogeneously distributed in the space underneath the tank.

A further increase of the maximum overpressure is to be expected if the combustion process would have been initiated closer to the edge but, unfortunately, this is not well possible with the present version of the REAGAS-code. Therefore, a maximum overpressure of approximately 100 kPa generated by the gas explosion underneath the tank is considered realistic. This overpressure corresponds to a blast strength of number 7 of the fuel-air charge blast model.

3.4 Far-field blast effects

With the vapor cloud's explosive potential expressed as an equivalent fuel-air charge of a radius $R_0 = 10$ m ($E = 7330$ MJ) and a strength of number 7, the potential blast effects of the vapor cloud explosion can be graphically represented by substitution of these data in the Sachs scaled fuel-air charge blast model. Figure 6 shows the blast peak overpressure as well as the duration of the blast wave's positive phase dependent on the distance to the charge center. It shows that such a charge is capable of producing a blast wave of about 1 kPa overpressure and a 60 ms duration up to almost 1000 m distance.

3.5 Near-field blast effects

The representation of blast effects by means of a spherical model results in an idealized picture which may hold only for the far-field at best. Blast effects produced by a partially confined space of such a large aspect ratio (length/height) as in the present situation are largely determined by the size of the opening through which the explosion pressure is vented from the confinement into free space. In addition, the partial confinement by extended parallel planes induces a preferential direction in the combustion process. The consequence is that near-field blast effects from gas explosions are often highly directional, a well known fact from the literature. In addition, near-field blast effects are largely influenced by the interaction with near-by structures and objects. For the gas explosion in question the near-field blast wave propagation is largely determined by the presence of the butane storage tank itself.

These effects can be approximated by numerical simulation. In this paper, these effects are simulated with

the BLAST-2D code (Van den Berg, 1990). This code is capable of computing blast effects by the solution of the Euler equations in a two-dimensional space. The Euler equations describe the conservation of mass, momentum and energy for inviscid flow of a perfect gas. Flux-Corrected Transport (Oran and Boris, 1987) is used to capture and preserve shock phenomena.

For the problem in question, the code is initialized with a perfect gas in the space underneath the storage tank, pressurized up to a pressure and temperature that a 100 kPa overpressure blast wave is formed on the burst. The computation is performed in a cylindrical grid consisting of 300*300 nodes. The results are represented in Figure 7a and 7b. At a few consecutive points of time the pressure distribution in the flow field is represented in Figure 7a. The pressure distribution is visualized by a pattern of isobars, one for each change in pressure of 2.5 kPa.

Shocks are present where isobars accumulate. In addition, the overpressures sampled at various locations at the earth's surface as well as at the tank's wall and roof are represented in Figure 7b. The Figures 7a and 7b show some features which are very characteristic for blast from gas explosions.

- The blast waves show a very pointed negative phase.
 - At the rim of the vent opening, a vortex structure is generated.
 - Such a flow phenomenon is characterized by a substantial pressure dip in its center.
 - The formation of a secondary wave. Blast is the result of fast expansion of combustion products. Because of the inertia of the expanding fluid, the combustion products overexpand, while generating under-ambient pressures in the blast center.
- Consequently, the flow reverses which results in recompression of the fluid in the blast center. The subsequent expansion produces a secondary wave.

These phenomena come alive in the sequence of pictures in Figure 7a and can be traced in the overpressure samples in Figure 7b.

3.6 Blast loading

In addition, numerical simulation of blast may reveal all details of the blast loading endured by any object of any shape at any distance from the explosion. To demonstrate this, in Figure 8a and 8b the results are presented of a numerical simulation in a 350*150 nodes grid of a blast wave of 10 kPa overpressure and 60 ms duration falling in at two buildings located close behind one another. It is to be expected that the blast loading at these buildings will be considerably influenced by one another's presence.

In Figure 8a the pressure field is represented which develops as a consequence of the blast wave reflection at the configuration. At some consecutive points of time the pressure distribution is visualized by means of an isobar pattern, one isobar for each increase in pressure of 0.5 kPa. The pictures give a clear view of how the blast loading is the result of a combination of wave reflection and lateral rarefaction of reflected overpressures. In particular, they show how in between the two buildings a complicated wave pattern develops, a consequence of various reflections and wave interactions. The overpressures sampled at three different locations at each building are graphically represented in Figure 8b. In the overpressure transients, the complicated wave pattern can be readily recognized. The overpressure build-up in transient number 3, for instance, sampled at the back wall of the first building shows a sequence of 4 shock phenomena which can be traced in the plots. The first corresponds with the passage of the shock of the infalling blast wave, diffracted around the building. The second corresponds with the same wave, reflected by the ground. The third corresponds with the infalling shock wave, reflected directly from the second building. This shock phenomenon is immediately followed by a fourth which is the result of reflection by the second building and subsequently by the ground.

The computation shows that the blast load at the front of the second building is considerably less than the reflected overpressure of the undisturbed blast wave endured by the front of the first building. In this way the effects of blast load reduction by sheltering effects can be quantified.

4. CONCLUSION

The Multi-Energy method for vapor cloud explosion blast modeling is presented and demonstrated in a case study. The Multi-Energy method constitutes an alternative for conventional TNT-equivalency methods which are unsatisfactory in several respects.

Contradictory to TNT-equivalency, in the Multi-Energy concept the fuel-air mixture is considered to be explosive only in partially confined, congested/ obstructed areas of the cloud. This result of more than a decade of experimental research leads to an alternative approach in vapor cloud explosion hazard analysis. If a release of fuel is anticipated somewhere, the environment should be investigated with regard to the presence of blast generating (boundary) conditions.

The Multi-Energy framework is a flexible concept which makes it possible to incorporate current experimental data and advanced computational techniques into the procedure of vapor cloud explosion blast modeling. In particular, the application of computational fluid dynamic codes such as REAGAS and BLAST-2D are shown to contribute to a more and more sophisticated approach in vapor cloud explosion hazard analysis.

Although the computational results presented in this paper were obtained with two-dimensional methods, three-dimensional versions of the codes are fully operational at TNO.

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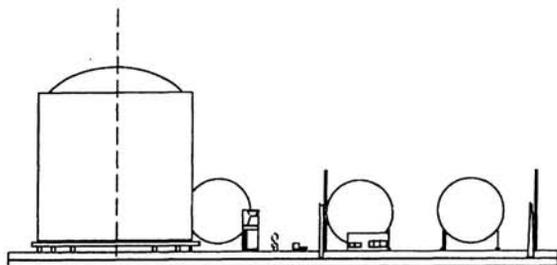


Figure 1 View of a storage site for liquefied hydrocarbons

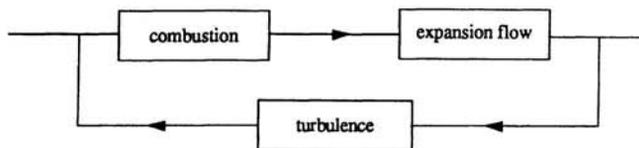


Figure 2 Positive feed-back, the basic mechanism of a deflagrative gas explosion

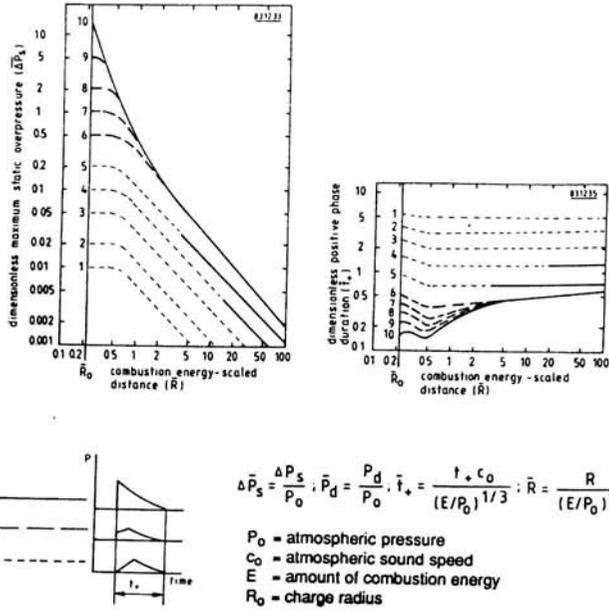


Figure 3 Hemispherical fuel-air charge blast model

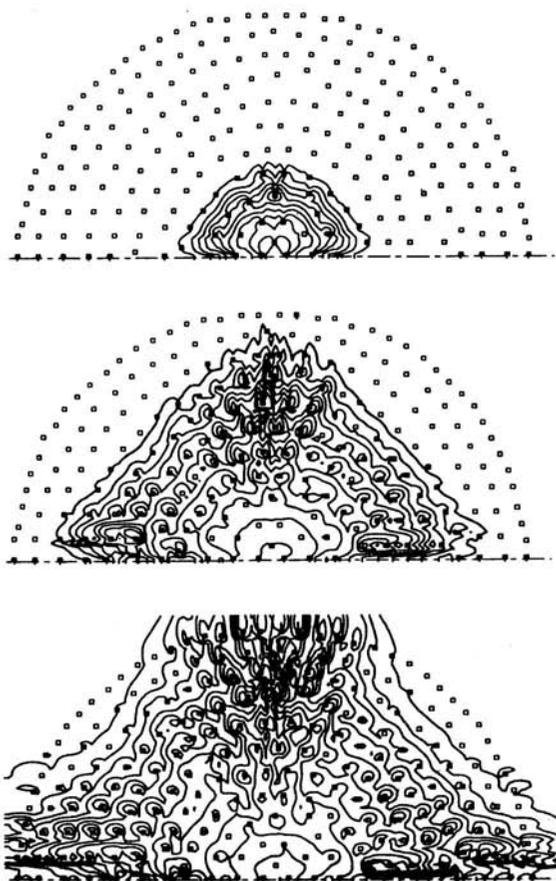


Figure 4a REAGAS simulation of a centrally ignited gas explosion developing in a concrete pilon forest underneath the butane storage tank

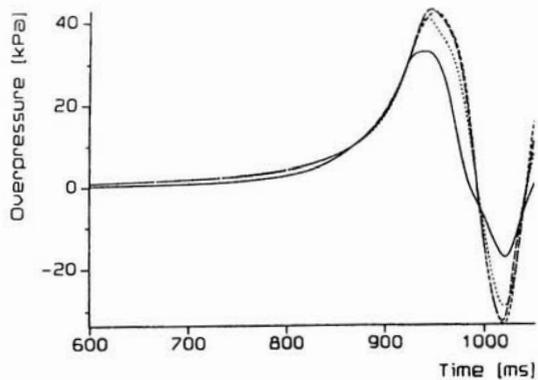


Figure 4b Pressure transients sampled at various locations in the space underneath the butane storage tank

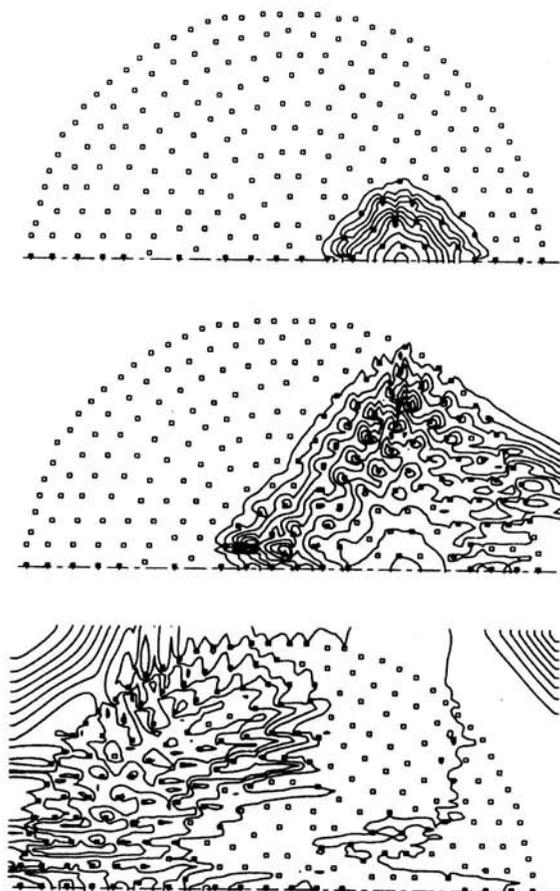


Figure 5a REAGAS simulation of a decentrally ignited gas explosion developing in a concrete pilon forest underneath the butane storage tank

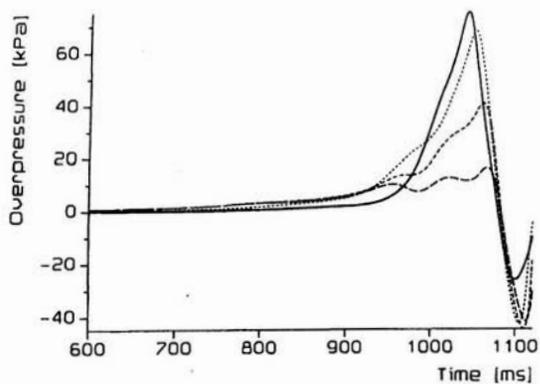


Figure 5b Pressure transients sampled at various locations in the space underneath the butane storage tank

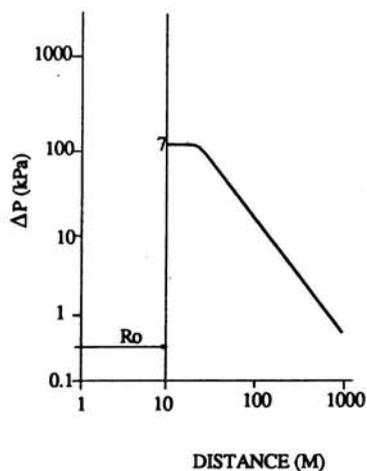


Figure 6a Blast peak overpressure dependent on the distance produced by a fuel-air charge of 10 m radius and strength number 7

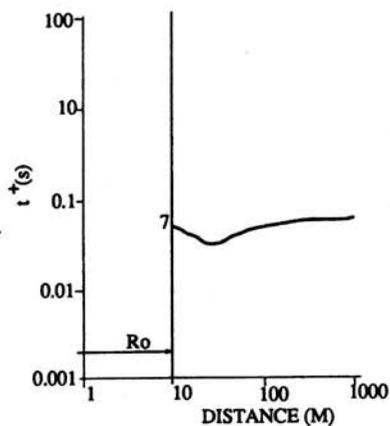


Figure 6b Duration of the blast wave's positive phase dependent on the distance produced by a fuel-air charge of 10 m radius and strength number 7

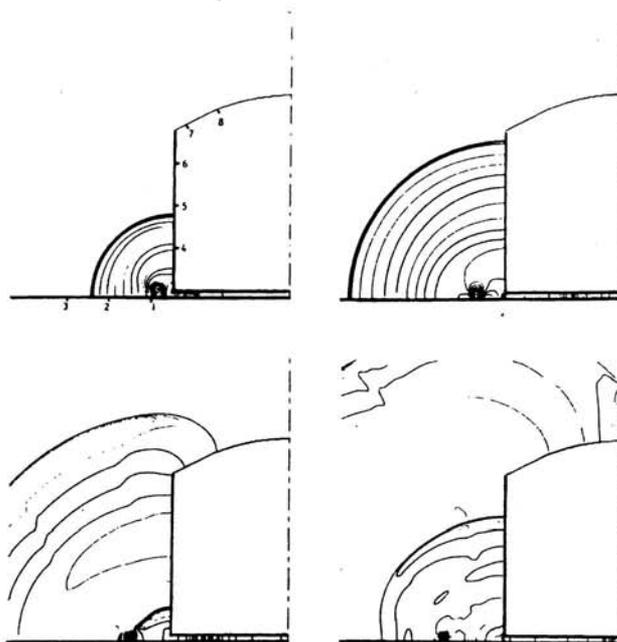


Figure 7a BLAST-2D simulation of the near-field blast produced by the gas explosion underneath the butane storage tank

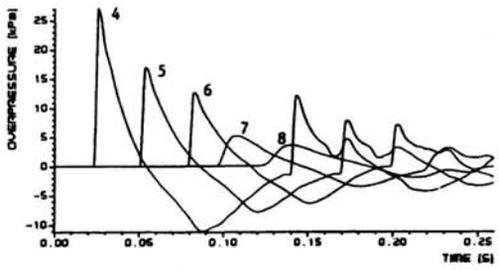
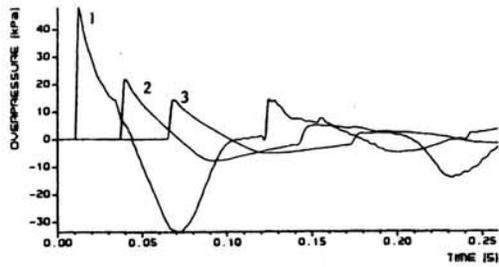


Figure 7b Blast overpressures sampled at various locations in the vicinity of the gas explosion

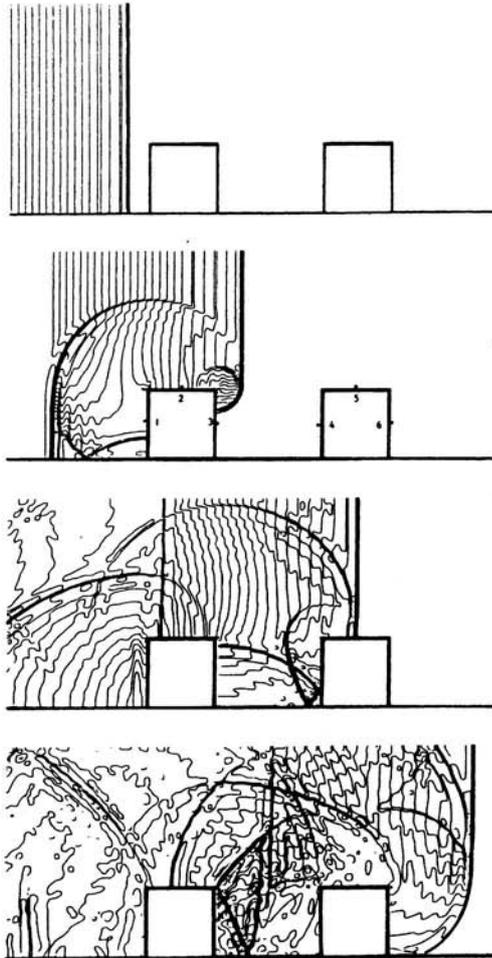


Figure 8a BLAST-2D simulation of the blast wave reflection by a complex of two buildings

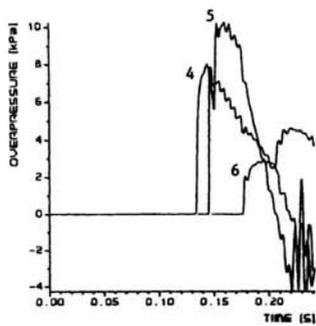
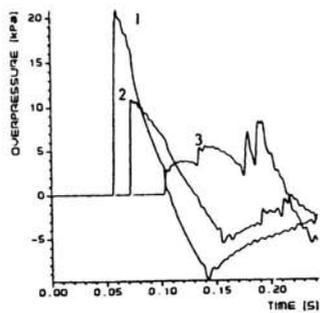


Figure 8b Overpressures sampled in various locations at the buildings