A STUDY ON VAPOUR CLOUD EXPLOSION MODELLING TO PREDICT VARIOUS CAUSATIVE FACTORS

A DISSERTATION

Submitted in partial fulfilment of the
requirements for the award of the degree
of
MASTER OF TECHNOLOGY
in
CHEMICAL ENGINEERING
(With Specialization in Industrial Safety and Hazards Management)

By

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CANDIDATE'S DECLARATION

I hereby declare that the work which is being presented in this dissertation titled **"A STUDY ON VAPOUR CLOUD EXPLOSION MODELLING TO PREDICT CAUSATIVE FACTORS"**, in partial fulfillment of the requirements for the award of the degree of Master of technology in Chemical Engineering with specialization in "**Industrial Safety and Hazards Management**", and submitted to the Department of Chemical Engineering, Indian Institute of Technology, Roorkee, is an authentic record of the work carried out by me during the period July 2007 to June 2008, under the guidance of **Dr. C. BALOMAJUMDER**. The matter embodied in this work has not been submitted for the award of any other degree.

Date: 30/06/2008
Place: IIT, Roorkee

(ANITA)

CERTIFICATE

This is to certify that the above statement made by the candidate is correct to the best of my knowledge.

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(ANITA)

ABSTRACT

The vapour cloud explosion can generate after a incidental release of a flammable gas or volatile liquid which upon ignition will explode if surrounding will favour an explosion. In recent years the vapor cloud explosions at chemical or petro-chemical industries are the pre-dominant cause of the losses. There are many gaps in the knowledge on vapor cloud explosions and no satisfactory theoretical model is available to explain it, although much progress has been made in vapour cloud explosion modelling. Work on fundamental models has been described by a number of authors. Other work has been directed to the correlation of experimental results and to develop the semi empirical models. Some major accidents due to vapour cloud explosion give lessons that there is still much to be learned systematically from past accidents if new technologies or chemical plants are to be designed with regared to safety.

The long list of vapour cloud explosions from the past indicates that the presence of a quantity of fuel constitutes a potential explosion hazard. If a quantity of fuel is released, it will mix with air and a flammable vapour cloud may result. If the cloud meets an ignition source, the flammable mixture will be consumed by a combustion process which, under appropriate conditions, may develop an explosive intensity and heavy blast. Therefore, safety measures are desirable.

In the present work empirical model has been used to predict over pressure generated by vapour cloud explosion, which is the most causative factor. The Over pressure determined by TNT – equivalency method and Multi – energy method.

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Chapter 1

INTRODUCTION

The most dangerous and distructive explosions in the chemical process industries are vapour cloud explosion. It occurs by a sequence release, dispersion and ignition. If a cloud of flammable vapour burns, the combustion rises to an overpressure. If there is no overpressure, the event is a vapour cloud fire or flash fire and if there is overpressure, it is a vapour cloud explosion. A vapour cloud explosion is one of the most serious hazards in the process industries. Vapour cloud explosions do occasionally occur and they tend to be very destructive. A feature of a vapour cloud is that it may drift some distance from the point where the leak has occurred and may thus threaten a considerable area. Safe stand-off distances should be exercised between locations where large quantities of fuels are stored or handled and places where people live or work. Control buildings at chemical plants or refineries and safety related structures of nuclear power plants, for instance, should be designed in such a way that they can withstand the destructive power of a vapour cloud explosion in their vicinity.

As the flame accelerates the pressure waves generated by the flame front begin to coalesce into a shock front of increasing strength. If the explosion occurs in a medium of low initial turbulence, is fully unconfined, and there are no obstacles present then the generated over-pressure is very low. If obstacles are present then expansion-generated flow, created by the combustion, of the unburnt gas passing through the obstacles will generate turbulence. This will increase the burning velocity by increasing the flame area and enhancing the processes of molecular diffusion and conduction, and this will in turn increase the expansion flow which will further enhance the turbulence.

The pressure generated by the explosion will depend on speed of the flame and expansion of the pressure from the vapour cloud. The consequences of vapor cloud explosions range from no damage to total destruction. Experimental studies indicate that the maximum explosion pressure is usually not effected by changes in volume and the maximum pressure and the maximum pressure rate are linearly dependent upon the initial pressure this shown in figure 1 and figure 2.

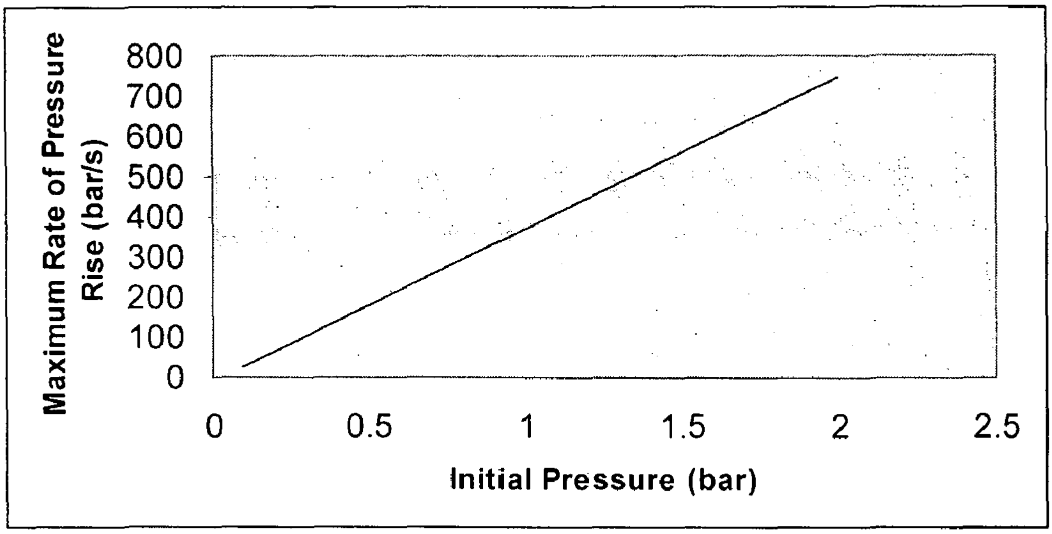


Figure 1 – Effect of initial pressure on maximum rate of pressure rise [12].

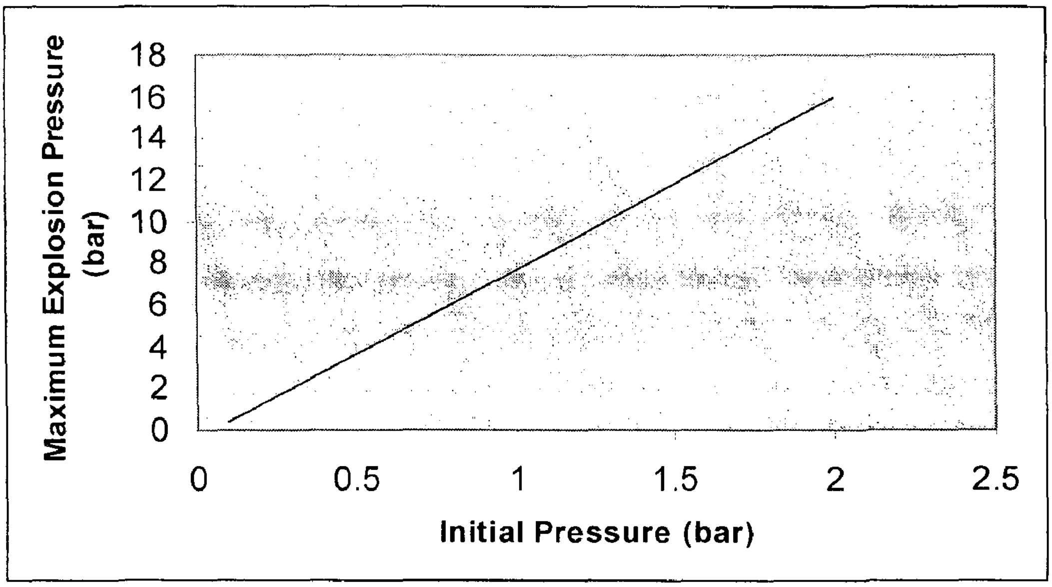


Figure 2 – Effect initial pressure on maximum explosion pressure [12].

The flame can propagate in two modes through the flammable cloud. These are:

(i) deflagration

(ii) detonation

The deflagration is common. A deflagration propagates at subsonic speed relative to the unburnt gas, typical flame speeds (i.e. relative to a stationary observer) are of the order of 1-1000 ms^{-1}. overpressure in a vapour cloud deflageration shown in the figure 3.

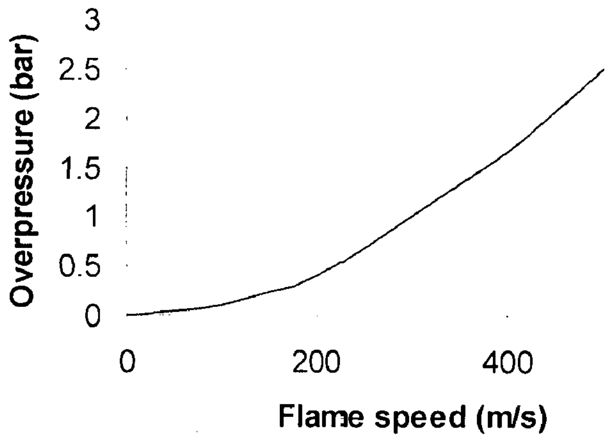


Figure 3. overpressure in a vapour cloud deflageration as a function of flame speed [19].

A detonation wave is a supersonic (relative to the speed of sound in the unburnt gas ahead of the wave) combustion wave. A detonation occurs much faster, within approximately 1/10,000 of a second. In a fuel-air cloud a detonation wave will propagate at a velocity of 1500-2000 ms^{-1} and the peak pressure is about 15-20 bar [34].

The consequences of a vapor cloud explosion will depend on:

- type of fuel and oxidizer .
- size and fuel concentration of the combustible cloud
- location of ignition point
- strength of ignition source
- size, location and type of explosion vent areas
- location and size of structural elements and equipment
- mitigation schemes

Vapour cloud explosions may be very sensitive to changes in these factors. Therefore it is not a simple task to estimate the consequences of a vapor cloud explosion. Vapour cloud explosion behavior depends on a large number of parameters. A summary of more important parameters is shown in Table 1.

Table 1 - Parameters significantly affecting the behavior of vapour cloud explosion.

S. No.	Parameters
1.	Quantity of material released.
2.	Fraction of material vapourized.
3.	Probability of ignition of the cloud.
4.	Distance travelled by the cloud prior to ignition.
5.	Time delay before ignition of cloud.
6.	Probability of explosion rather than fire.
7.	Existence of threshold quantity of material.
8.	Efficiecy of explosion.
9.	Location of ignition with respect to release.

LITERATURE REVIEW

Roger A. Strehlow (1976) usually defined properties of blast waves are introduced. The classical point source or ideal wave is used to discuss scaling laws. They give general explanation of non-ideal blast wave behaviour.

1. Extant theoretical work on blast waves from non ideal sources.
2. Different non ideal source properly effect.
3. Atmospheric and ground effects.

General characteristics of explosions including wave properties like energy, residual energy in the atmosphere, kinetic energy of source material, potential energy of the source, radiation. The authors include that explosions are always non ideal they are significantly different than point source or chemical explosive (TNT) detonations because of their low energy density and the slow addition of energy.

B.J. Wiekema (1984) the approach is based on the accidents that happened in the past. In 87 out of 165 incidents the distance within which ignition occurred. Greater than 60% of 87 vapour clouds were ignited within 100 meters from the location of the spill only 2% of these cases did the vapor cloud drift more than 1 km before ignition. In 150 out of 165 incidents whether an explosion or flash fire according to their report nearly 60% of these cases the explosion occurred and in 40% flash fire. 143 out of 165 incidents about 40% of these incidents there were no fatalities and 25% no was hurt. The spill range 1 to 100 tones for the investigated results. Explosion occurred in semi confined situation not in unconfined.

H. Giesbretch (1988) Though unconfined vapour cloud explosions can proceed in many different ways, each single one must be investigated to obtain more insight into their causes, and to increase our knowledge about the possible and probable spectrum of such incidents. Following some general remarks on the techniques and problems of damage analysis, the procedure is demonstrated by reference to an explosion in an ethylene plant in Germany in 1985. The explosion of the "Rheinische Olefinwerke Wesseling", Germany, in 1985 was "typical" for the following reasons. Some 4 to 5 tons of propylene had escaped from a leak, the greater part being contained in a flat cloud close to the ground. Higher pressure up to 0.2 bar was found only in the immediate neighbourhood of the more confined part of the plant section. Though the pressure decreased rapidly with increasing distance, explosions of such extent can still cause considerable glass breakage at distances up to 500 m.

D. K. Pritchard (1989) The ability to reliably predict the blast damage from vapour cloud explosions finds use in the safety assessment of hazardous installations and also in the design of such installations. The basic knowledge and terminology necessary to understand the characteristics of blast waves, the way they interact with structures and the response of structures to blast loading is presented. Methods that can be used for predicting the blast wave from a vapour cloud explosion, the blast loading and the structural response are outlined and their limitations discussed.

A. C. Van den Berg et. al. (1993) they described and demonstrated two methods –

1. TNT equivalency method.
2. The multi – energy method.

According to them, the full pressure time history of the blast wave should be specified at any location in vapour cloud explosion's environment. They explain a blast model defines a peak overpressure, while the under – ambient pressure effects are neglected. But these parameter s are minimally required to calculate the behaviour of structures under blast loading or to asses blast explosion damage.

A wide distribution of TNT equivalency (0.02% - 15.9%) with a median value 3% was observed, 97% of the cases was covered by a TNT equivalency lower than or equal to 10% . covering 60% of the cases the mean vale observed was a TNT equivalency of 4%.

The value of 10% corresponds to approximately a TNT equivalent of 1 Kg of TNT for every Kg of hydrocarbon release and to 5 Kg of TNT for every Kg of hydrocarbon mixed with air between the flammability limits. TNT equivalency methods for vapour cloud explosion modeling should only be used for the assessment of blast effects in the far field where the over pressure is 30 KPa. In the near field their use can lead to over design of structure. A French authority safety rule recommends the 10% equivalency for safety calculation and the French chemical industry recommends the 4% equivalency, both based on the full amount of fuel released.

A. Koshy et. al. (1995) their analysis is also based on the past accidents. According to this paper which occurred in less than a minute shows –

1. Most of the chemicals involved are reactive in nature.
2. The mode of chemical release was either as pressurized gas or as a two phase mixture.

Vapour cloud explosions occurring later than 2 min after chemical release, the chemicals are generally non reactive and flammable.

They mentioned when diluted with inert gas, hydrogen (flammable limits 4% - 75.6%) it can burn with less than 5% oxygen. Dispersion calculations for dense gas cloud reveal that the lower flammability limits can be reached within the first few minutes, they assumes a wind speed of 2-3 m/s, the cloud would have traveled 120-18 m before ignition.

R. P. Cleaver et. al. (1997) they describes the number of model produced linked together to predict the consequences of a confined region on a processing (gas) or storage site. They used phenomenological model. Spherical symmetry may be assumed for central ignition of a compact region until the flame first reaches the edge of the region. A calculation is carried out to determine the pressure that is generated by the combustion of the vapour cloud. A method of calculating the propagation of the resulting pressure away from the source region is then applied and this information is used to estimate the loading received by other structures on the site outside of the congested region.

The combination of the correlations and the mathematical relationships produce a predictive model for the source pressure as a function of time for the case of the central ignition of vapour cloud occupying a compact, congested region, provided suitable values can be defined for the geometric parameters. This approach has the advantage that the speed of each part of the wave is predicted to increase with increasing pressure.

Pritchard, Freeman and Guilbert (1996) the code has been used for prediction of explosion over-pressure in a series of small-scale baffled and vented enclosures.

Pritchard, Lewis, Hedley and Lea (1999) stressed that great care must be taken when applying models to other gases than the one for which the model has been "tuned", or calibrated. They found that the agreement between calculations and experiments was poor when changing gas from methane, the gas for which the model was calibrated, to propane. contains a detailed discussion on the deficiencies with the ignition model and the thin flame model implemented in CFX-4.

A.C. Van den Berg et. al. (2000) This paper describes the developments in vapour cloud explosion blast modeling. TNT equivalency methods are used for simple vapour cloud explosion but presently TNO multi energy method is more reasonable as a simple and practical method. The application of multi energy method requires knowledge of two parameters –

1. Charge size – The heat of combustion of the flammable mixture actually contribute to the blast.
2. Charge strength – The explosion overpressure produce.

J.S. Puttock et. al. (2000) The SCOPE 3 model (Shell Code for Overpressure Prediction in gas Explosions) has been developed to predict the overpressures which could be generated by gas explosions in vented enclosures, such as offshore modules. SCOPE 3 attempts, wherever possible, to model the underlying physical processes in an explosion. This phenomenological approach gives greater confidence in predictions for full-scale events than methods based simply on correlations of experimental data. A phenomenological modelling approach can provide a useful tool in the range of methods applied for the prediction of explosion overpressures. With less need for details of the small objects in the geometry, screening runs can be done earlier or more easily than when using CFD. Furthermore, computer run time is short; so large numbers of sensitivity runs can easily be performed. SCOPE 3 has been validated against data from over three hundred explosion experiments.

VAPOUR CLOUD EXPLOSION MODELING

Although there are many gaps in the understanding of vapour cloud explosions, considerable progress has been made in modelling such explosions [16].

Following approaches considered as modelling have been described [25].

(1) Point source models
    i. TNT equivalent model,
    ii. Self-similarity model;
(2) Fuel-air cloud model;
(3) Bursting vessel model;
(4) Piston model
    i. Constant velocity piston model,
    ii. Accelerating piston model.

In the TNT equivalent model the explosion is taken to be equivalent to that of a TNT explosion with the same energy of explosion. This model is therefore an empirical one, but it was for some time virtually the only practical model available. The TNT equivalent model has a single parameter, the mass of TNT. It can be made more flexible by the introduction of a second parameter, the height above ground zero at which the explosion occurs. The effect of increased height is to reduce the overpressures near the centre. The use of an arbitrary assumed explosion height is useful in obtaining better fits to overpressures assessed from damage in actual explosions.

In the self-similarity model, the blast parameters such as peak overpressure are correlated in terms of the ratio radial distance per time. In its simplest form the model gives a power law relation for the variation of peak overpressure with distance.

In the fuel-air cloud model it is assumed that a detonation propagates through the fuel-air mixture without any expansion of the cloud. A shock wave with a high peak overpressure is produced at the cloud boundary. At the completion of the combustion, subsequent decay of the shock wave is similar to that for the point source models. Another approach is to assume that the fuel-air mixture undergoes combustion in a hemispherical Vessel, defined by the cloud boundary, and that when combustion is complete, the vessel bursts. The state of the gas, after combustion but before bursting, is determined by standard methods. Subsequent decay of the shock wave may be calculated by numerical solution of wave propagation equations.

The modeling of the consequences and the effects of the accidental release of dangerous materials is an important issue. Most explosion models still use the simplified TNT-equivalency approach although it is common knowledge that the typical characteristics of a vapor cloud explosion is modeled unsatisfactorily. There are a wide range of class of models available - from empirical and phenomenological, which are Computational Fluid Dynamics (CFD) based. There is a range of modelling approaches available, each with their own strengths and weaknesses. In order to establish greater confidence in model predictions, it is clear that the improvements in the physics and the numeric's are required for the future.

Table 2 - Some principal vapour cloud explosion incidents [16].

Some incidents involving vapour cloud fires and explosions				
Date	*Location*	*Chemical*	*Mass* released (te)	*TNT equivalent* (te)
1939	Newark, NJ	Butane		
1943	Ludwigshafen, Germany	Butadiene, butylene	16.5^d	
1945	Los Angeles, CA	Butane		
1948	Ludwigshafen, FRG	Dimethyl ether	30	20
1949	Detroit, IL	Propane, butane	1.6	
1951	Baton Rouge	HCs		
1953	Campana, Argentina	Gasoline		
1954	Portland, OR	LPG	$250\ m^3$	
1955	Freeport, TX Wilmington, CA	Ethylene Butane	0.68-1.36	
1956	Baton Rouge, LA	Butylene	10	
	North Tonawanda, NY	Ethylene	2.5	
1957	Sacramento, CA	LPG		
1958	Ardmore, OK Augusta, GA	Propane LPG		
1959	Meldrin, GA	LPG	18	
1961	Freeport, TX Lake Charles,	Cyclohexane Butane	18	0.025
1962	Berlin, NY Fawley, UK Houston, TX	Propane Gasoline	14.3	
	Ras Tanura, Saudi Arabia	Propane	1.1	
1963	Plaquemine, LA	Ethylene		0.9
1964	Jackass Flats, NV	Hydrogen	0.09	0.027
	Liberal, KS	Propane		1.0
	Orange, TX	Ethylene	0.18	0.27
1965	Baltimore	Benzene		
	Baton Rouge, LA	Ethyl chloride	19.3	135-180
	Escambia, USA Lake Charles, LA	Hydrogen, carbon monoxide Methane or	(0.070)	(0.012)
1966	Raunheim, FRG	Methane	1-1.5	2.7
	Scotts Bluff, LA	Butadiene	0.45	
1967	Lake Charles, LA	Isobutylene	9	12
1968	Pernis, Netherlands	Light HCs	55-110	20
1969	Escombreras, Spain	Propane		(0.012)
	Fawley, UK Glendora, MS Houston, TX Texas City,	Hydrogen, naphtha VCM Natural gas Butadiene	23	

1970	Big Springs, TX			
	Linden, NJ	Hydrogen, HCs	114	45
	Port Hudson, MO	Propane	27-55	45
1971	Baton Rouge, LA	Ethylene	3.6	0.45
	Houston, TX	Butadiene	12	
	Longview, TX	Ethylene	0.45	0.5
1972	East St Louis, IL	Propylene	53.5	2.5
1973	Gladbeck, FRG			
	Noatsu, Japan St-Amand-les-Eaux, France	VCM Ethylene	4.2	0.2
1974	Beaumont, TX	Isoprene	7.6	0.9
	Climax, TX Cologne, FRG	VCM VCM	110	
	Decatur, IL	Isobutane	69	20-125
	Fawley, UK	Ethylene	0.9-2.7	
	Flixborough, UK Holly	Cyclohexane Propane	36	18
	Houston, TX Petal, MO Roumania Zaluzi, Czechoslovakia	Butadiene Butane Ethylene Ethylene	<80	20-57
1975	Antwerp, Belgium	Ethylene	2.5	
	Beek, Netherlands Cologne,	Propylene Hydrogen,	5.5	2.2
	Eagle Pass, TX	LPG	18.2	
	Rosendaal, Netherlands	Gasoline	25-50	1.0
	Watson, CA	Hydrogen	0.3	0.018
1976	Longview, TX Los	Ethylene		
1977	Baytown, TX Brindisi, Italy	Gasoline Light HCs	300	
	Dallas, TX Port Arthur, TX	Isobutane Propane	68.2	1.6
1978	Abqaiq, Saudi Arabia Denver, CO	Methane, then LPG Propane		24
	Immingham, UK Pitesti, Roumania Poblado Tres, Mexico	Syngas Propane, propylene Natural gas	0.2-0.3	0.03
1979	Texas City, TX Torrance, CA Ypsilanti, MI	Propane C_3-C_4s Propane	3.1	0.9
1980	Borger, TX	Light HCs		
	Enschede, Netherlands	Propane	0.11	
	New Castle, DE	Hexane, propylene	12.7	
1981	Czechoslovakia	Syngas		
	Gothenburg, Sweden	Propane	30^0 m^3	
1982	Philadelphia, PA			

1983	Port Newark, NJ	Gasoline		
1984	Romeoville, IL	Propane		
	Sarnia, Ontario	Hydrogen	0.03	0.91
1985	Cologne, FRG	Ethylene		4.1
	Edmonton, Alberta Lake Charles, LA Mont Belvieu, TX	NGL Propane Ethane, propane	4900 m^3	
1987	Pampa, TX	Acetic acid, butane		
	Ras Tanura, Saudi Arabia	Propane	300 m^3	0.9
1988	Beek, Netherlands	Ethylene		
1988	Norco, LA	Light HCs	9	
	Rafnes, Norway	VCM Ethylene dichloride	25 30	
1989	Baton Rouge, LA Minnebeavo, USSR	Ethane, propane, butane Propane		11-14
	Pasadena, TX	Isobutane	37.8	
	Ufa, USSR	NGL		10000
1990	Cincinnati, OH Maharastra, Bombay Porto de Leixhas, Portugal Tomsk, USSR	Xylene, solvent Ethane, propane Propane Gas		
1991	Kensington, GA Pajaritos, Mexico Seadrift, TX	Butadiene Propane Ethylene oxide		

3.1 Empirical models

Empirical models also referred to as quasi-theoretical are based on limited experimental data. These considered the most simplified method for estimating the blast effects from vapour cloud explosions.

3.1.1. TNT Equivalency method

The TNT equivalency method is based on the assumption that explosive power of a vapour cloud explosion can be related to the mass of the TNT that can produce the same explosive power [36]. However, there are substantial differences between gas explosions and TNT. In the former the local pressure is much less than for TNT detonations. Furthermore, the pressure decay from a TNT detonation is much more rapid than the acoustic wave from a vapour cloud explosion. The TNT equivalency model uses pressure-distance curves to yield the peak pressure, [2].

The equivalent TNT yield is based on two factors:

1. the ratio of the heat of combustion of the combustible gases in the vapor cloud to the heat of detonation of TNT,
2. the efficiency of the vapor cloud explosion.

An equivalent mass of TNT is calculated using the following equation:

$$\frac{M_{TNT}}{M_{cloud}} = \frac{\Delta H_c}{1155} \times E_f \tag{1}$$

Where

M_{TNT} - TNT equivalent mass, (kg)

ΔH_c - Lower heat of combustion, kcal/kg

M_{cloud} - Mass in cloud, (kg)

E_f - Efficiency

The distance to a given overpressure is then calculated from the equation:

$$X = .3967 \times M_{TNT}^{1/3} \exp\left[3.5031 - 0.7241 \ln(O_P) + 0.0398(\ln O_P)^2\right] \tag{2}$$

Where

X - Distance to given overpressure, m

O_p - Peak overpressure, psi

The first of these is simply the ratio of the total energies available per unit mass of material. For most hydrocarbon materials, this ratio is about ten. Thus, on a mass basis, a hydrocarbon release has ten times as much potential explosive energy as TNT. The second factor relates to how well or efficiently the vapor cloud behaves as an explosive material upon ignition.

The basic TNT curve relating the peak overpressure of the blast wave from a TNT explosion to the scaled distance parameter, in accordance with the Hopkinson scaling, is shown on both figures 4 and 5.

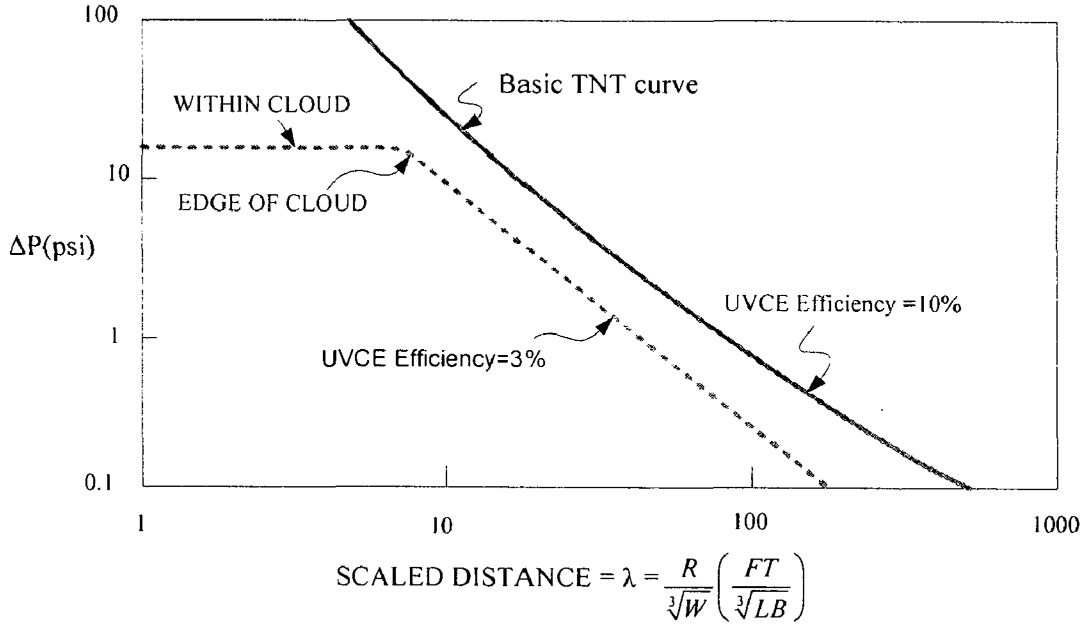


Figure 4- Free-field overpressure vs. scaled distance: TNT and UVCE explosions [2].

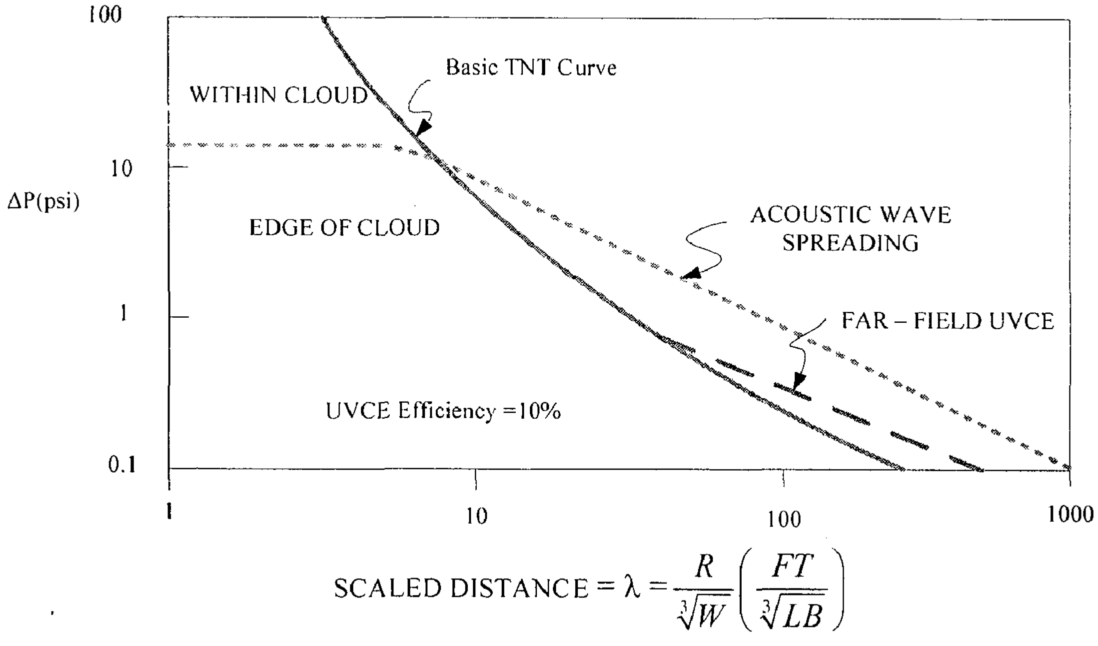


Figure 5 - Free field overpressure vs. scaled distance for different spreading assumptions [2].

This curve is based on a series of experiments and weapons tests carried out over many years, and represents the peak overpressure, for a TNT explosion on the ground surface, which generates an overpressure blast wave which radiates into a hemispherical space [2]. The shape of overpressure profile according to the TNT equivalent model and to some possible models of vapour cloud explosions is shown in figure 6.

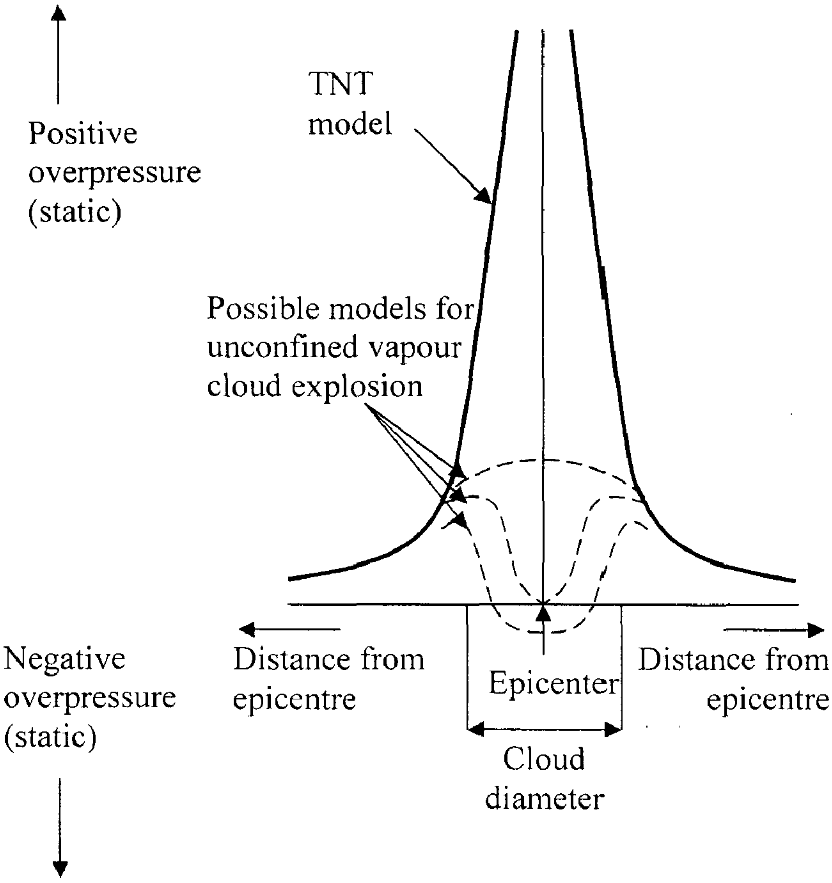


Figure 6. Overpressure given by the TNT equivalent model and by some possible models of vapour cloud explosion [16].

3.1.2 The TNO multi-energy method

The model is based on the assumption that vapour cloud explosion can occure only within that portion of a flammable vapour cloud that is partially confined. Applying the Multi-Energy method, a blast should be modeled by the specification of an equivalent hemi-spherical fuel-air charge, which is directly related to the heat of combustion of the flammable mixture actually contributing to the blast, and strength which is defined as the maximum explosion overpressure produced [19]. According to TNO recommendations, the charge energy should be taken equal to the full heat of combustion of the flammable mixture present within the partially confined, obstructed area in the cloud, assuming that the fuel is stoichiometrically mixed with air and strength is assumed to be maximum. If the assumption of maximum strength results in unacceptable overestimates of blast effects, the approach may be refined on the basis of correlation with experimental data. The explosion centre can be defined as

$$\overline{R} = R^{*}(P_0 / E)^{0.33} \tag{3}$$

$$E \approx 3.5V_{cloud}, \tag{4}$$

Where,

$\overline{R}$ - scaled distance from the charge,(dimensionless)

R - distance from the charge, m

P_0 - ambient pressure (pa)

E - charge combustion energy, joules

V_{cloud} - Volume of vapour cloud in the congested area,m^3.

The point is that the inhomogeneity of the fuel-air mixture, which is inherent to the process of atmospheric dispersion, prevents a possible detonation wave from propagating [39].

3.1.3 Baker-Strehlow Method

The **Baker-Strehlow** method, [4], was developed to provide estimations of blast pressures from vapour cloud explosions. The model was further extended by [5]. The methodology consists of a number of steps, assessing flame speed, fuel reactivity, confinement, etc.

- Walk through plant identifying potential explosion sites
- Decide on the dimensionality of the confined areas to work out flame speed
- Calculate burning velocity for fuel mixtures

The blast pressure and impulse are the read from a series of graphs. The revisions proposed by **[5]** were the results of experience gained from plant hazard assessments.

3.1.4 Congestion Assessment Method (CAM)

This model was developed at Shell Thornton Research Centre [11]. The model has been enhanced and further extended by [26,27]. A decision tree procedure as guidance for estimating the source pressure, taking into account the layout of the plant [11], e.g. degree of confinement and congestion and the type of fuel involved. The accuracy of the estimations was variable, but the method was designed to yield conservative pressures.

The method comprises three steps:

1. An assessment of the congested region is carried out to assign a reference pressure, which is an estimation of the maximum over-pressure generated by a deflagration of a vapour cloud of propane.
2. The type of fuel is taken into account through a fuel factor, which is then multiplied by the reference pressure worked out in step to determine the maximum source pressure.
3. It is now possible to estimate the pressure experienced at various distances from the ignition point. A simple decay law inversely proportional to the distance [11]. Pressure decay curves generated by fitting polynomials to detailed computations [26].

3.2 Phenomenological models

Phenomenological models are simplified physical models. The greatest simplification made is with respect to the modelled geometry. Generally, no attempt is made to model the actual scenario geometry, which is instead represented by an idealised system.

3.2.1. SCOPE (Shell Code for Over-pressure Prediction in gas Explosions)

The SCOPE model was initially designed for modelling explosions in offshore modules. However, the model may be applied to any geometry where a single flame path may be identified. It is based on the original version of SCOPE [11].

a. SCOPE 2

The SCOPE code seeks to model gas explosions by representing the essential physics in a simplified form. Models of this type are to be distinguished from empirical models that are nothing more than 'fits' to existing experimental data and are of limited applicability. The model is one-dimensional and is based on the idealised geometry of a vented vessel containing a series of obstacle grids. The external over-pressure calculated by the model is related to the vent flow (which in turn is related to the box internal pressure) when the flame has traversed 70 % of the box length. The ratio of the external pressure to the internal pressure also depends on the vent area. the maximum internal pressure is determined by

$$P_{\max} = P_{emerg} + 0.7 P_{ext} \qquad (5)$$

where V is the box volume, P_{ext} is the external explosion over-pressure, and $P_{0.7}$ is the maximum internal pressure for $X/L \leq 0.7$.

b. SCOPE 3

Generally objects will be of mixed scale and in characterising these objects in terms of a blockage ratio and a shape (round or sharp edged) information has been lost. The main effect of obstacles of various sizes is on the flame surface area which increases as it passes between the objects; the flame area affects the consumption rate of the unburnt gas. SCOPE 3 will allow rear venting, in addition to the side and main vents allowed by

SCOPE 2. SCOPE 3 has been validated against more than 300 experiments. Further developments of SCOPE 3 involves modelling of un-confined but congested plant, with central ignition, and modelling the effect of water deluge on explosion development, [28]. The overall structure of the model is shown in the figure 7.

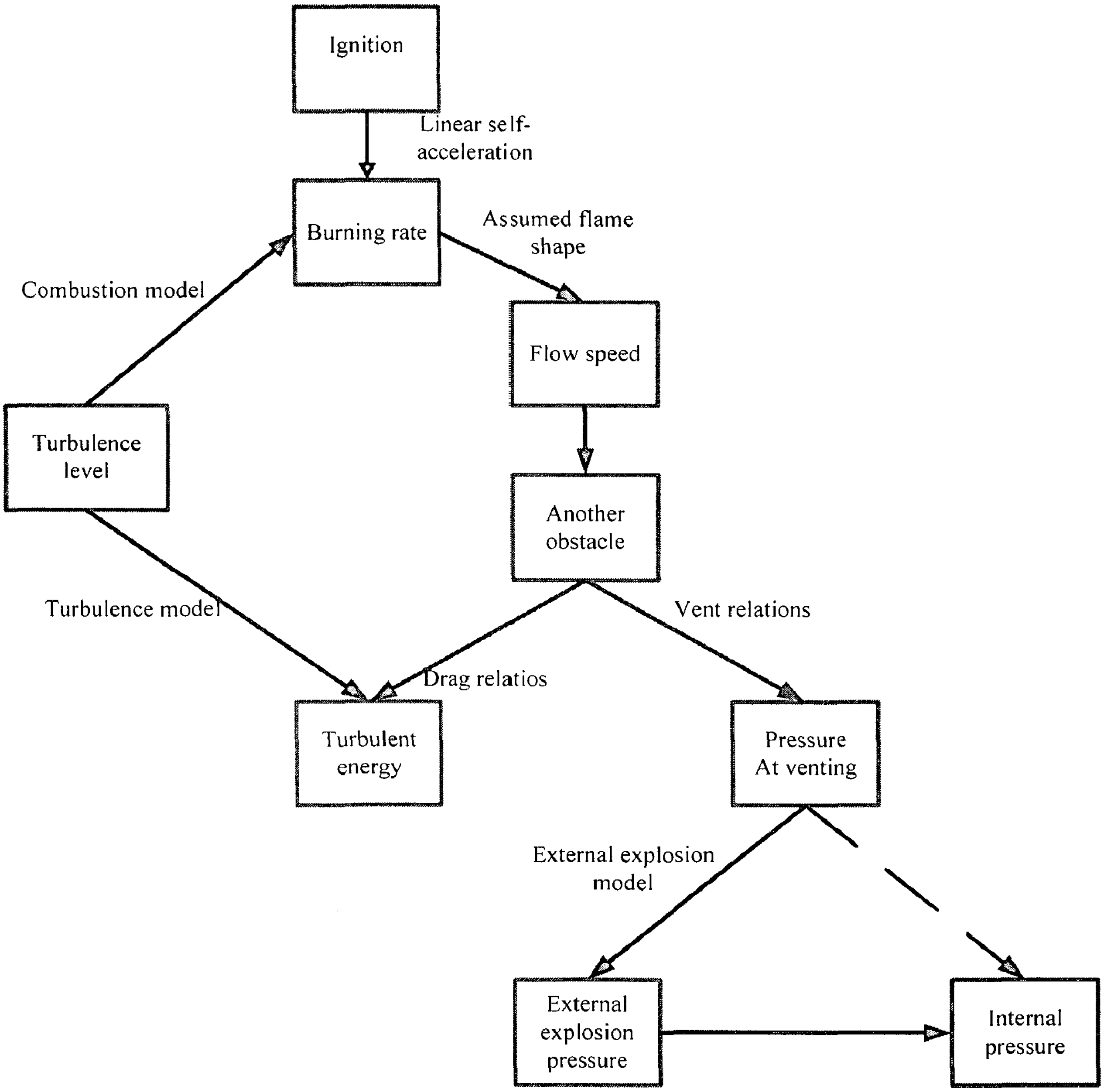


Figure 7 - The overall structure of the model [28].

3.2.2. CLICHE (Confined LInked CHamber Explosion)

The CLICHE (Confined **LI**nked **CH**amber **E**xplosion) code has been developed by Advantica Technologies Ltd. The status of its present development is unknown. CLICHE was developed to study confined explosions in buildings but its use has been extended to modelling explosions in off-shore and on-shore plant. The basis of CLICHE is well established in applications to vented vessels explosions [15,12]. The explosion model formulation used in CLICHE was developed by applying the conservation laws to the unburnt and burnt gas volumes in each chamber, assuming that the properties within each chamber are uniform and that any momentum changes occur only at the perimeter of these volumes. Equilibrium properties are assumed for the burnt gas and taking into account the pressure and temperature dependence.

3.3. Computational fluid dynamics (CFD) Models

CFD models find numerical solutions to the partial differential equations governing the explosion process. Solutions obtained with **CFD** codes contain a great wealth of information about the flow field, i.e. velocities, pressure, density, species concentrations, etc. Surface pressure data can be used for structural analysis. The Navier-Stokes equations, which govern the fluid flow, and the sub models used to represent the terms which are not modelled exactly.

3.3.1. EXSIM (Explosion SIMulation)

The EXSIM (Explosion SIMulation) code is under continuing development at the Telemark Technological R&D Centre (Tel-Tek) in Norway and Shell Global Solutions in United Kingdom. The current version of the EXSIM code is version 3.3. EXSIM is a structured Cartesian grid, semi-implicit, finite volume code that relies on the Porosity / Distributed Resistance method for the representation of small-scale objects. The main effect of these obstacles is to obstruct the flow and generate additional turbulence. A box shaped domain is specified, the subsequent geometry being built up by the addition of variations of eight basic objects. These objects are:

1) Large box, resolved by the grid.

2) Cylinder aligned with one of the co-ordinate directions.
3) Pipe bundle in the form of a box.
4) General porous box.
5) Louvered wall
6) Box beam or box that is not resolved by the grid.
7) Sharp edged beam.
8) Grating.

3.3.2 FLACS (FLame ACceleration Simulator)

The FLACS (FLame ACceleration Simulator) code has been developed at the Christian Michelsen Research Institute in Norway, now CMR-GEXCON. FLACS is a finite volume code based on a structured Cartesian grid. The Porosity / Distributed Resistance approach is used to model sub-grid scale obstacles. Obstacles which are not resolved by this grid are represented as an area blockage and a volume blockage. Walls and decks may be modelled in four different ways: solid unyielding surface, porous surface, blows out / explosion relief panel, or open. There have apparently been further developments in the FLACS code [35] i.e. to the laminar and turbulent combustion modelling, to the modelling of turbulence generation at walls and implementation of a subgrid model describing turbulence length scale as a function of obstacle size.

3.3.3. AutoReaGas

AutoReaGas is the result of a joint venture, between Century Dynamics Ltd. and TNO, that began in 1993. The gas explosion solver is a three dimensional finite volume CFD code based on a structured, Cartesian grid. Present development work is concerned with improving important aspects of the solver; in particular a higher order numerical discretization scheme will be implemented in the near future. A new improved combustion model will also be implemented. In addition, a wall friction model will be incorporated for modelling gas explosions in geometries with no sub-grid scale obstacles. In the longer term a number of developments are planned; these include:

1. A dynamic structural response capability coupled with the explosion and blast processor.

2. Gas dispersion modeling and Multi-block mesh, which allows a more efficient grid structure to be used.

3.3.4. CFX

The explosion modified code models the three important stages in the growth of an explosion.

1. There is ignition and the establishment of an initial flame.
2. The flame front expands initially laminar and then weakly turbulence zone.
3. If the flame encounters obstacles, or the turbulence level in the unburnt gas ahead of the flame otherwise increases, the flame will accelerate, propagating as a thick, highly turbulent reaction zone.

Quenching of a flame is the reduction in reaction rate due to either flame stretch or turbulent time scales. Quenching due to flame stretch has been accounted for in both the thin flame and eddy break-up combustion models by a simple expression based on the Damköhler number [23].

Initially, the combusting region will be small compared to the volume of grid cells it occupies. A simple model treats this early flame as a laminar fire ball, which allows the fuel consumption rate to be estimated analytically as a function of time. The flame is assumed to be spherical and to burn at the laminar rate. The radius of the ignition region (*RIg*) is fixed and it is from this that the ignition time is determined

$$t_{Ig} = \frac{R_{Ig}}{u_f}$$

The fuel mass fraction source term within the ignition region is given by

$$\bar{\omega}_f = \begin{cases} -\rho \dfrac{Y_f}{t_{Ig}} \left(\dfrac{t}{t_{Ig}} \right)^2 \exp\left(-\dfrac{t}{t_{Ig}} \right) & for\, t \le t_{Ig} \\ 0 & for\, t > t_{Ig} \end{cases}$$

The flame propagates as a thin or quasi-laminar reaction zone. The actual physical width of this reaction zone (i.e.. for a real laminar flame) is likely to be smaller than the grid spacing. However, the simulated width of the reaction zone cannot be less than one cell, therefore it is necessary to model the heat release rate. Consider the reaction process to be characterised by a single progress variable (c) where, in this case, $c = 1$ is a property of the unburnt mixture.

Now consider a set of values for this progress variable (ci) at distances along a line normal to the flame front separated by spacing's of Δ_i.

$$\frac{dc_i}{dt} = \begin{cases} -\frac{c_i}{t_B} & for\, c_{i-1} \leq \alpha \\ 0 \quad for & c_{i-1} > \alpha \end{cases}$$

where

t_B - The burning time and is a constant bounded by zero and unity.

The burning velocity is given by

$$u_B = \frac{\Delta_i}{t_B \ln\left(1/\alpha\right)}$$

The constant determines the thickness of the modelled flame. If this constant is too large then the flame will be spread over several cells, whereas a small value will produce a flame that occupies only the thickness of one cell - yielding an undesirably large burning rate. Hence, a moderate value of this constant is used [7].

The laminar burning velocity of a combustible mixture is a function of the gas composition, its temperature and pressure, and may generally be easily specified. However, a small degree of turbulence will affect the flame propagation velocity greatly.

Table 3 - Merits and demerits of different methods of different models [23].

Name	Merits	Demerits
TNT Equivalency method	• Easy method.	• Non unique yield factor is neede. • Weak gas explosion not well represented. • Information for only the positive phase duration. • The estimation of blast effect in far field (30 kpa), but near field it can lead to overdesign.
TNO multi-energy conept	• Fast method. • Conservative approximation can be made.	• Difficult to accurately represent complex geometries and setting a sensible value for charge strength and total combustion energy. • Not suitable for weak explosions. • Not clear how to deal with congested regions and multiple blast waves.
Baker-strehlow method	• Easy to use and fast. • It gives some geometrical details with respect to confinements. • It can handle multi-ignition points.	• It can be overconservative.
Congestion assessment method	• Easy to use and short run time. • Calibrated against large number of experiments. • It can deal with non symmetrical congestion and long, narrow plant.	• It allows only natural representation of the geometry. • No uniqueness in the specification of level of congestion and level of confinement.
SCOPE 2 and SCOPE 3	• It can handle venting and external explosion. • Validated against small, medium to large experiments. • Contains less geometrical detail than CFD models.	• It can deal with single enclosures only. • Does not provide the information about the flow field as CFD models.
CLICHE	• Allows ignition location anywhere within cuboidal volume. • Based on some fundamental physics and empirical correlations. • Flame distortion effects due to vents included. • Short run time. • Can handle external explosion.	• Simplified representation of the geometry. • Does not provide the information about the flow field as CFD models.

	• It can generate its own input parameters from an obstacle database.	
EXSIM	• User can specify special resolution of obstacles. • Compared against small, medium and large scale experiments. • It can be applied to congested but unconfined geometries and external explosion. • It can read in CAD data.	• Using standard k-ε model. • Does not have a local grid refinement facility.
FLACS	• Compared against small, medium and large scale experiments. • It can be applied to congested but unconfined geometries and external explosion. • Can read in CAD data. • Incorporates a water deluge model.	• Uses k-ε model, but with modifications to deal with near wall flows. • Recent developments not in the open literature.
AutoReaGas	• Compared against small, medium and large scale experiments. • Incorporates a water deluge model. • Can read in CAD data.	• Uses standard k-ε turbulence model.
CFX – 4	• Offers multi-block capability for greater control over the meshing. • A number of turbulence models, including Reynolds stress transport models, are implemented. • Performs adequately for CH_4 and H_2 deflagrations.	• Yields poor agreement with experiments for gases other than methane and hydrogen, to which the model appears to have been tuned. • Uses a thin flame model which is not well suited to explosion modeling. • Uses an ignition model with deficiencies.

Chapter 4

COMBUSTION MECHANISM OF VAPOUR CLOUD EXPLOSION

Typical gaseous detonations show propagation velocities of the order of 2000 m/s and peak overpressures of the order of 20 bar. For a mixture of constant composition the detonation process is steady. After the reaction front has consumed the combustible mixture the shock expands in the ambient air. Since an ordinary building will be demolished at an overpressure as low as a few tenths of a bar, a detonation in the open could cause great damage. However, a detonation in air will not easily be initiated [10]. Unless the fuel is very reactive as is the case with acetylene or ethylene oxide, it requires an intense shock wave. With other fuels such as methane, it is even doubtful whether a vapour cloud detonation is possible, although in closed systems this has been observed. Much easier to initiate are deflagrations. Sparks with an energy content of the order of as little as a milli Joule are capable of starting a deflagration, at least in mixtures of optimum concentration, which are usually near the stoichiometric point. If the mixing ratio approaches the explosion limits the reactivity of the mixture decreases and the minimum ignition energy goes up. In a quiescent fuel-air mixture the flame velocity is of the order of a few metres per second. Due to the free expansion of the hot reaction products in the open the flame velocity is composed of the burning velocity (= velocity of the flame relative to the moving gas) and the expansion velocity (ratio is 1:7 for stoichiometric mixtures). Flames with velocities of the order of a few metres per second-do not produce peak overpressures in the open of any significance. The assumed central ignition of the combustible cloud will result in a deflagration or a detonation depending on several parameters such as the strength of the ignition source, the size of the cloud, the presence of obstacles and, mainly, on the reactivity of the fuel.

Early experimental attempts to reproduce the high overpressures generated in vapour cloud explosion incidents had met with little success, very low flame speeds and negligible overpressures being observed. In hindsight these results were not surprising as the vapour clouds were relatively small, contained no obstacles and were virtually unconfined. More recent experiments, using larger partially confined clouds containing arrays of obstacles, have resulted in very fast flames and overpressures large enough to cause significant blast damage [21]. These experiments clearly demonstrate the need for some degree of partial confinement or obstructions within the cloud for a vapour cloud explosion to produce damaging levels of overpressure. In the case of obstructions or obstacles the flame is accelerated due to turbulence effects; increasing the turbulence increases the burning velocity. For situations where there is a series of obstacles within the cloud, a positive feedback mechanism can lead to a very rapid flame acceleration [37]. Combustion of the vapour, results in expansion, inducing a gas flow ahead of the flame. The gas flow interacts with the obstacles creating a turbulent flow for the flame to propagate into. Turbulence increases the flame burning velocity and hence the rate of combustion, rate of expansion and gas flow ahead of the flame increase. This in turn leads to even higher burning velocities, rates of expansion, etc.

Table 4 – Combustion properties of some hydrocarbon gases and hydrogen in air [19].

Fuel	Flammable range %	Stoichiomertic mixture	T_f K	E	H_{st} MJ/m^3
Hydrogen	4 – 75	30	2318	8.0	3.06
Methane	5 – 15	9.5	2148	7.4	3.23
Ethane	3 – 12.5	5.6	2168	7.5	3.39
Propane	2.2 – 9.5	4.0	2198	7.6	3.46
Butane	1.9 – 8.5	3.1	2168	7.5	3.48
Pentane	1.5 – 7.8	2.6	2232	7.7	3.59
Hexane	1.2 – 7.5	2.2	2221	7.7	3.62
Heptane	1.2 – 6.7	1.9	2196	7.6	3.62
Acetylene	2.5 – 80	7.7	2598	9.0	3.93
Ethylene	3.1 – 32	6.5	2248	7.8	3.64
Propylene	2.4 – 10.3	4.4	2208	7.7	3.59
Butylene	1.7 – 9.5	3.4	2203	7.6	3.64
Benzene	1.4 – 7.1	2.7	2287	7.9	3.62
Cyclohexane	1.3 – 8.0	2.3	2232	7.8	3.85

T_f - Flammable temperature (K)
E - Expansion factor = final volume/initial volume
H_{st} - Heat of reaction per unit volume of stoichiomertic mixture (MJ/m^3)

Method of modelling

5.1. TNT – equivalency method

The basic concept

TNT-equivalency methods, for instance, state a proportional relationship between the quantity of fuel in the cloud and the weight of an equivalent TNT-charge expressing its explosive power. Up to this day, TNT-equivalency methods are widely used for this purpose. However, TNT-equivalency methods are becoming progressively less satisfactory as the understanding of blast generation vapour cloud explosions increases. Methods which utilize an equivalent fuel-air charge to express the potential explosive power may overcome the imperfections of TNT-equivalency blast modelling to some extent. Such a charge can be characterized by, for instance, applying the multi-energy philosophy which reflects the current understanding of vapour cloud explosions. In addition, the multi-energy concept makes it possible to incorporate current experimental data and advanced computational fluid dynamics into the procedure of vapour cloud explosion hazard assessment.

For a long time now, the military has been interested in the destructive potential of high-explosives. Therefore, extensive experimental data on the relation between TNT and damage have been available for many years. Consequently, it is quite obvious that the explosive power of accidental explosions, deduced from the damage patterns observed, was expressed as equivalent TNT-charge weights. Because the quantification of the potential explosive power of fuels was a necessity long before the mechanisms of blast generation in vapour cloud explosions were understood, it is fully comprehensible that the TNT-equivalency concept was also utilized to make predictive estimates for vapour cloud explosion hazard assessment. Basically, the use of TNT-equivalency methods for blast predictive purposes is very simple. If the equivalent charge weight is known, the corresponding blast characteristics can be read from figure 8.

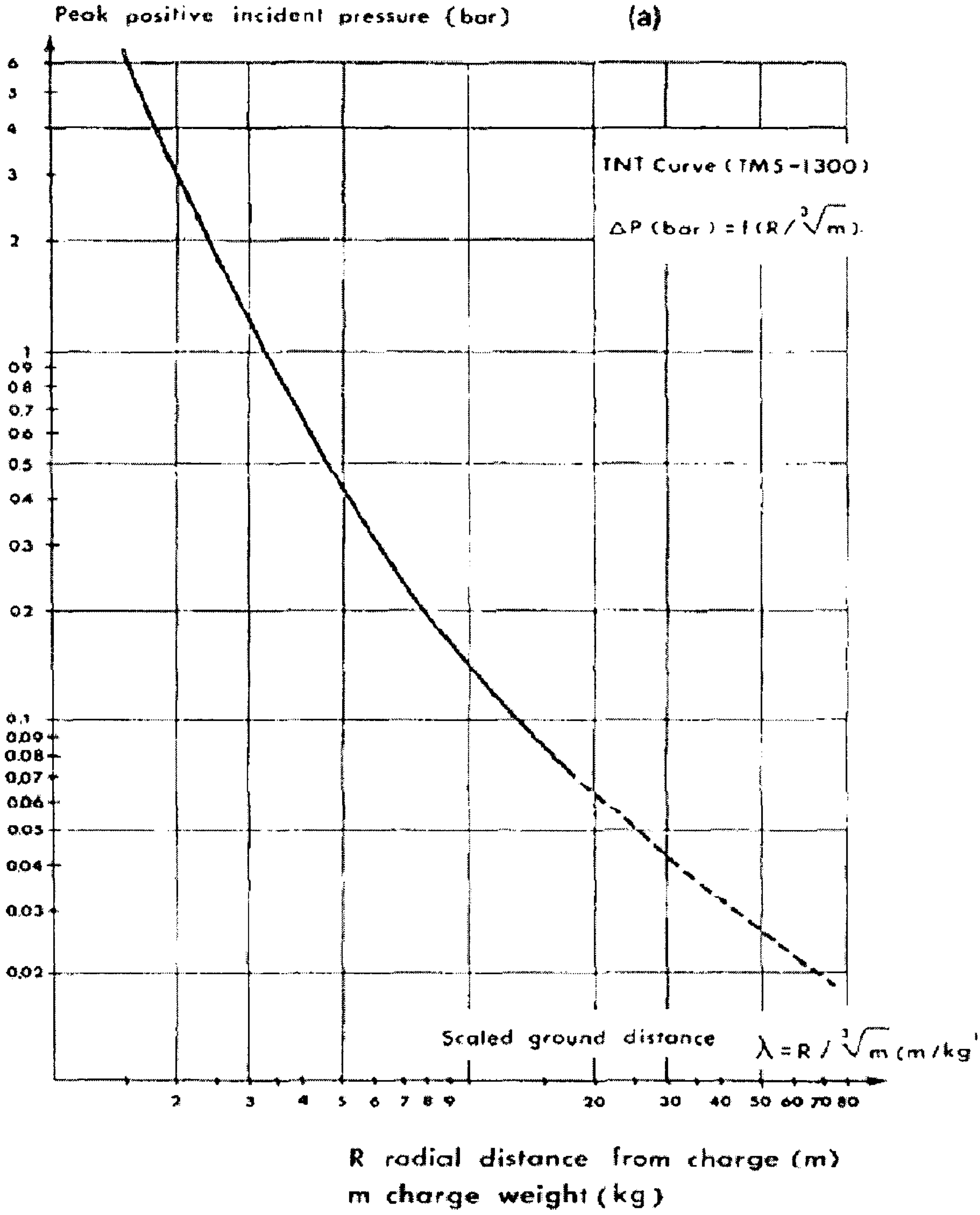


Figure 8 – (a) Blast peak incident overpressure for a hemispherical TNT charge [36].

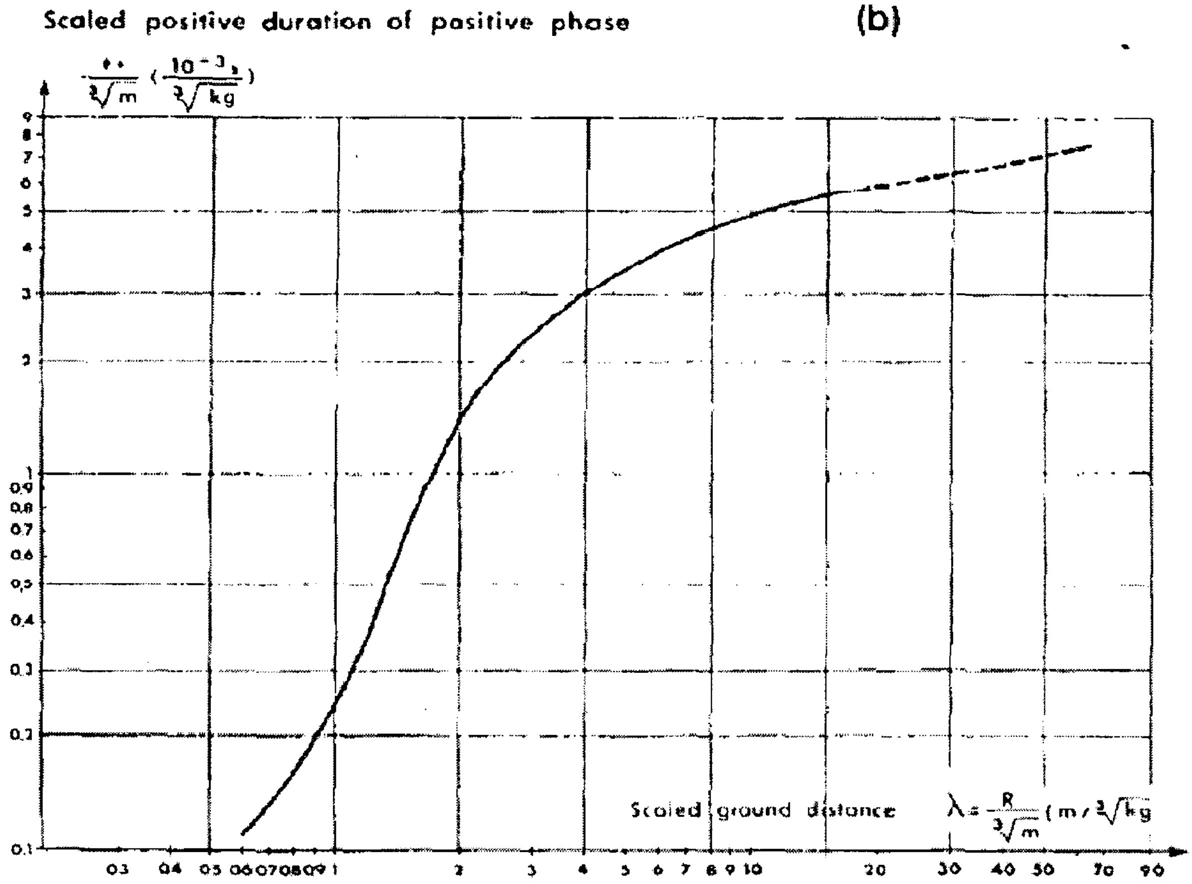


Figure 8 - (b) Blast positive phase &ration for a hemispherical TNT charge [36].

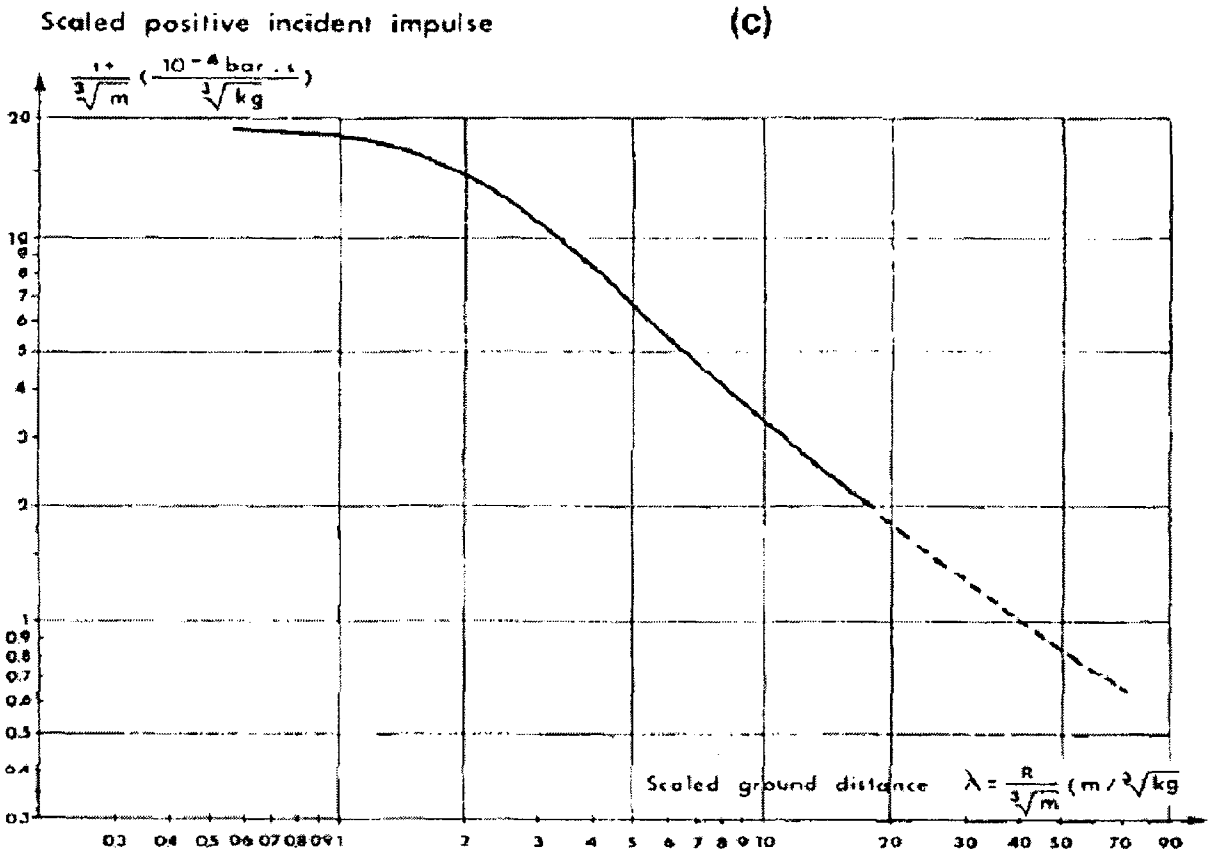


Figure 8 – (c) Blast positive incident impulse for a hemispherical TNT charge [36].

5.2. The Multi-energy method

The basic concept

Presently, the belief is gaining ground that it is hardly possible to detonate an unconfined vapour cloud. The point is that the inhomogeneity of the fuel-air mixture, which is inherent to the process of atmospheric dispersion, prevents a possible detonation wave from propagating TNT-equivalency methods are widely used for simple vapor cloud explosion blast modeling. Presently, however, almost 15 years after its formulation, the TNO Multi-Energy method is increasingly accepted as a more reasonable alternative. The Multi-Energy concept is based on the starting point that, assuming deflagrative combustion, the explosive potential of a vapor cloud is primarily determined by only the obstructed and/or partially confined areas in the cloud. Separate areas produce separate blasts. So, contradictory to more conventional methods, in which a vapor cloud explosion is regarded as an entity, according to the Multi-Energy concept a vapor cloud explosion is rather defined as a number of sub-explosions corresponding with the various partially confined, obstructed areas in the cloud [36].

Applying theMulti-Energy method, a blast should be modeled by the specification of an equivalent hemi-spherical fuel-air charge, which has two characteristics, namely [2]:

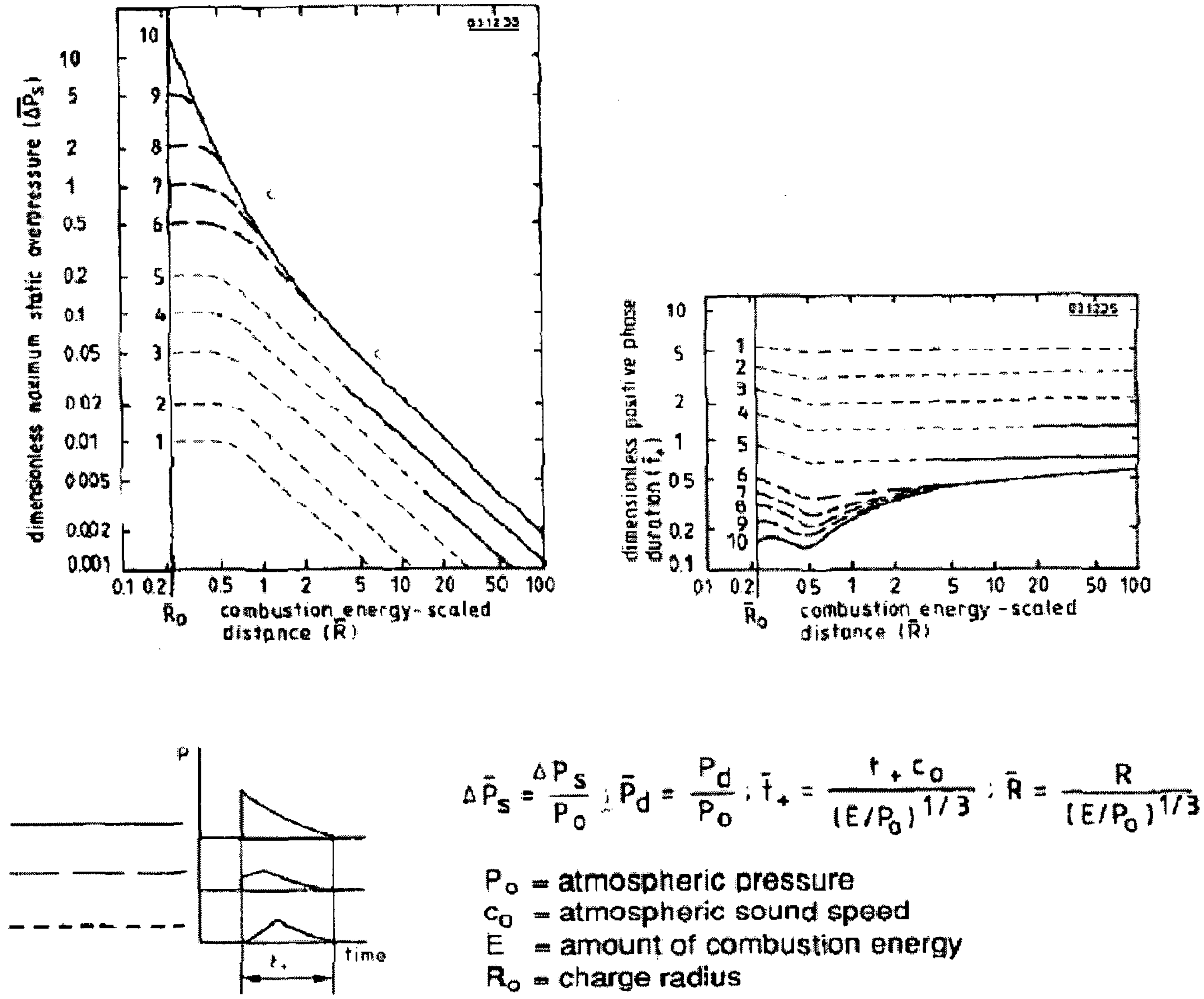
- A charge size, which is directly related to the heat of combustion of the flammable mixture actually contributing to the blast,
- A charge strength which is defined as the maximum explosion overpressure produced.

According to TNO recommendations, the charge characteristics can be specified following a simple safe and conservative approach, namely:

- The charge energy should be taken equal to the full heat of combustion of the flammable mixture present within the partially confined, obstructed area in the cloud, assuming that the fuel is stoichiometrically mixed with air.
- The charge strength is assumed to be maximum.
- If the assumption of maximum strength results in unacceptable overestimates of blast effects, the approach may be refined on the basis of correlation with experimental data.

The heat of combustion of the fuel-air mixture was assumed to be 3.5 MJ/m3, which is representative for an average stoichiometric hydrocarbon-air mixture [17].

Figure 9 shows the peak overpressure as well as the positive phase duration of the blast wave, produced by a hemispherical fuel-air charge of radius R_O at the earth's surface. The blast model reflects basic features of gas explosion blast. The initial blast strength is a variable expressed as a number ranging from 1 for insignificant to 10 for detonative strength. The initial blast strength can be defined as a consistent set of blast parameters at the location of the charge radius R_O. In addition, the model gives an indication for the blast wave shape.



$$\Delta\bar{P}_s = \frac{\Delta P_s}{P_0}\ ;\ \bar{P}_d = \frac{P_d}{P_0}\ ;\ \bar{t}_+ = \frac{t_+ c_0}{(E/P_0)^{1/3}}\ ;\ \bar{R} = \frac{R}{(E/P_0)^{1/3}}$$

P_0 = atmospheric pressure
c_0 = atmospheric sound speed
E = amount of combustion energy
R_0 = charge radius

Figure 9 – Dimensionless positive phase duration vs. combustion energy scaled distance [4].

STATEMENT OF THE PROBLEM

Three storage spheres containing liquefied propane are situated next to a large butane tank. To diminish heat inflow from the soil, the butane tank is placed 1 m above the earth's surface on a concrete pylon forest. In this environment a massive release of 20 tons of propane is anticipated. For a complete description of blast loading, the full pressure-time history of the blast wave should be specified at any location in a vapour cloud explosion's environment. A blast model, on the other hand, defines a blast wave only in terms of the peak overpressure, the positive phase duration and the positive impulse, while the under-ambient pressure effects are neglected. These blast parameters are minimally required to calculate the behaviour of structures under blast loading or to assess explosion damage.

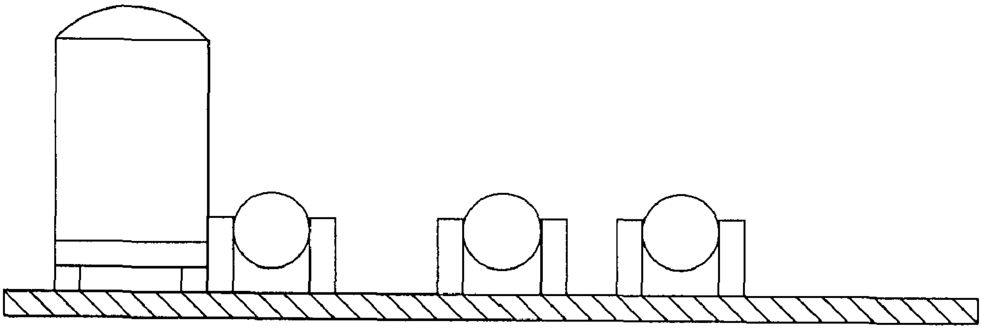


Figure 10 – View for storage site.

6.1. RESULTS

TNT equivalency method and multi energy method used to determine the over pressure generated by vapour cloud explosion, which is occurred by release of 20 ton of propane from the storage tank.

The equivalent charge weight has been calculated with the help of equations 1, 2, 3, and 4. After getting the equivalent charge weight the corresponding blast characteristics read from the figure 8 (a, b, c) and 9. The values evaluated by these methods shown in the table 5 and table 6. According to these data over pressure curve has been plotted with respect to various distance and positive phase duration.

Table 5 – Blast characteristics modelled by TNT-equivalency methods.

Over pressure (kPa)	TNT equivalency			
	10%		4%	
	Distance (m)	Positive phase duration (ms)	Distance (m)	Positive phase duration (ms)
40	170	115	125	60
33	195	118	130	72
25	220	120	150	90
20	250	134	210	98
15	350	140	266	105
11	423	146	314	112
9	490	150	360	115
7	520	154	426	135
6	670	160	510	140

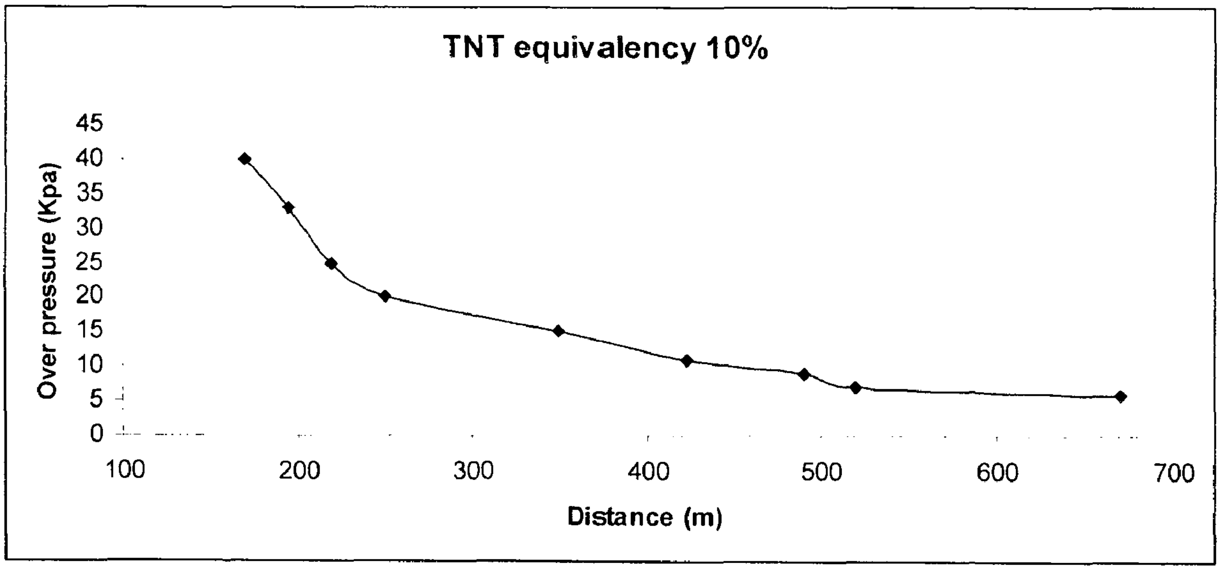


Figure 11 – Over pressure vs. distance at an approximate upper limit (10%) of TNT equivalency.

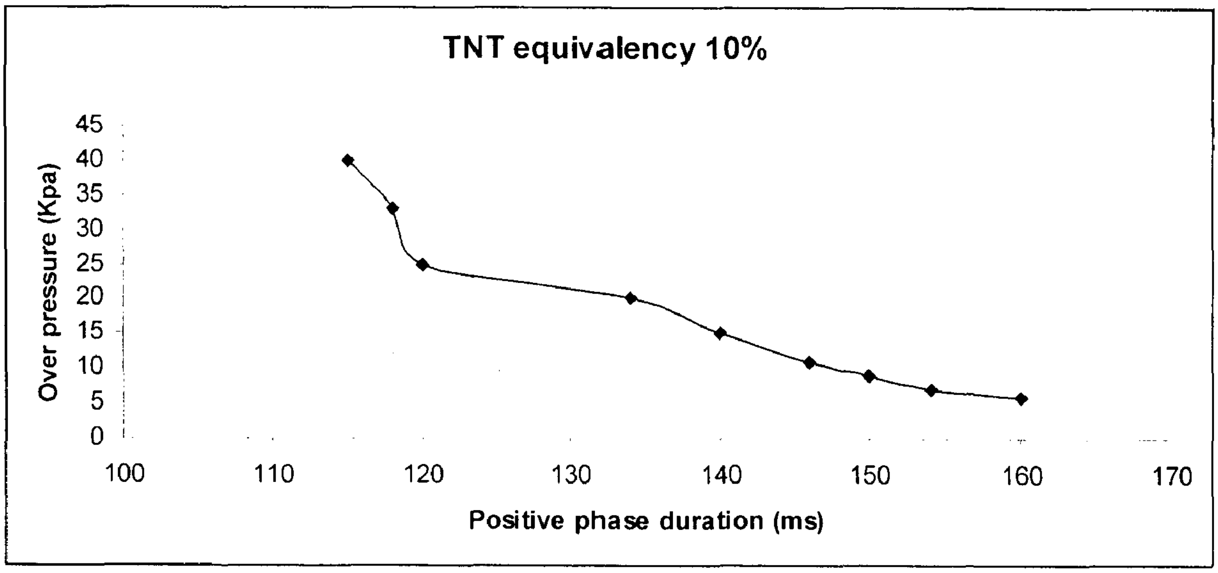


Figure 12 – Overpressure vs. positive phase duration at an approximate upper limit (10%) of TNT equivalency.

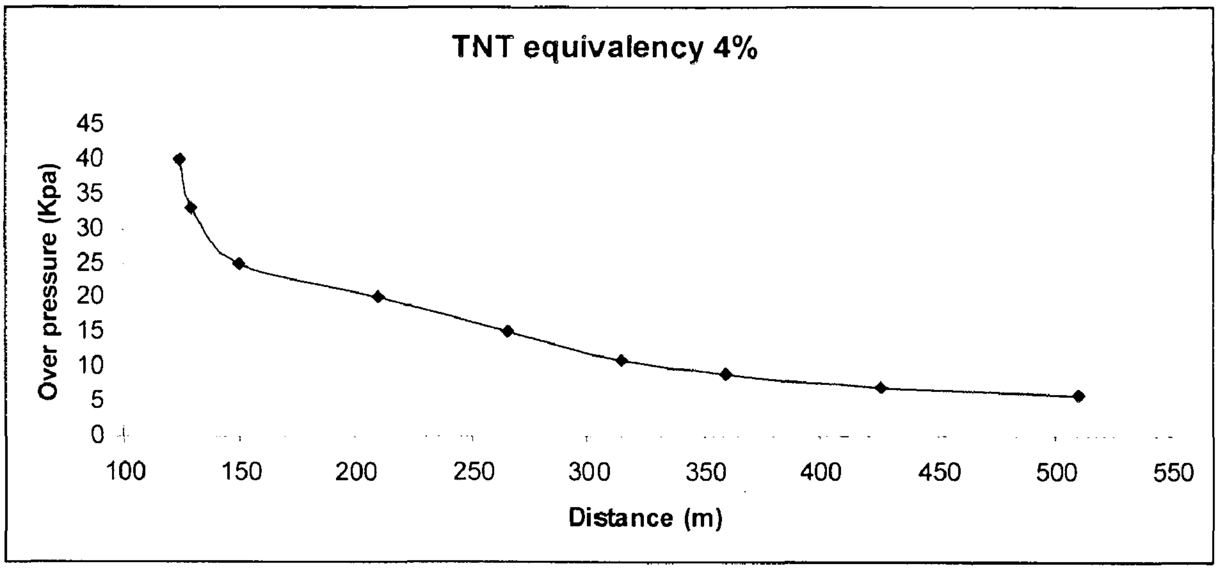


Figure 13 – Over pressure vs. distance at an average limit (4%) of TNT equivalency.

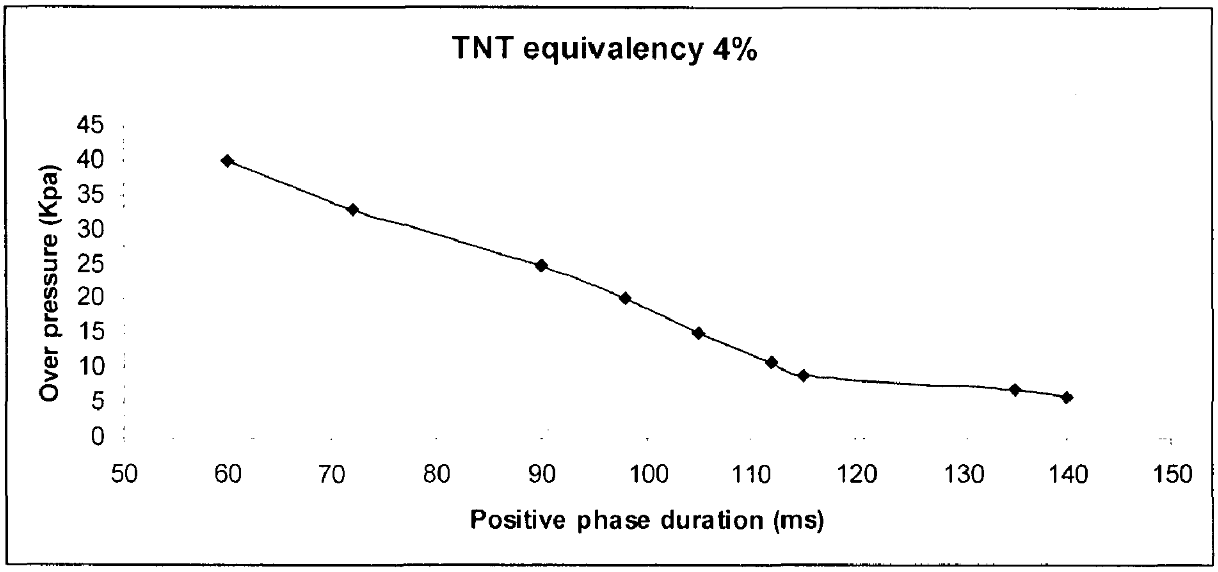


Figure 14 – Over pressure vs. positive phase duration at an average limit (4%) of TNT equivalency.

Table 6 – Blast characteristics modelled by Multi – energy method.

Over pressure (Kpa)	Multi – energy method	
	Distance (m)	Positive phase duration (ms)
40	77	53
33	83	59
25	91	67
20	110	71
15	135	80
11	148	92
9	167	98
7	198	103
6	255	108

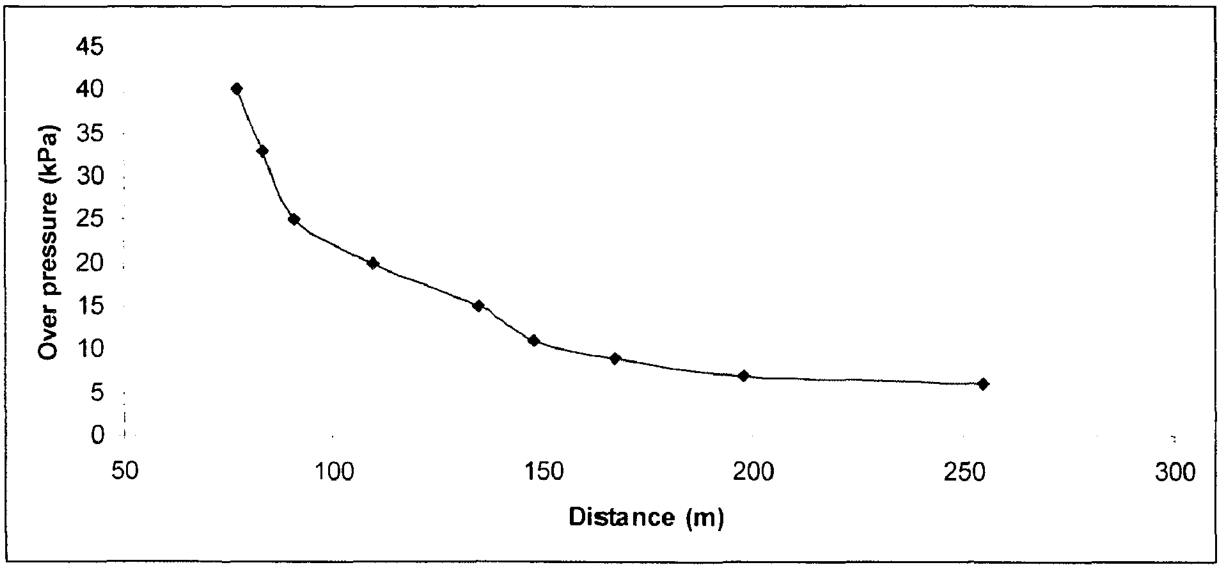


Figure 15 – Over pressure vs. distance for multi energy method.

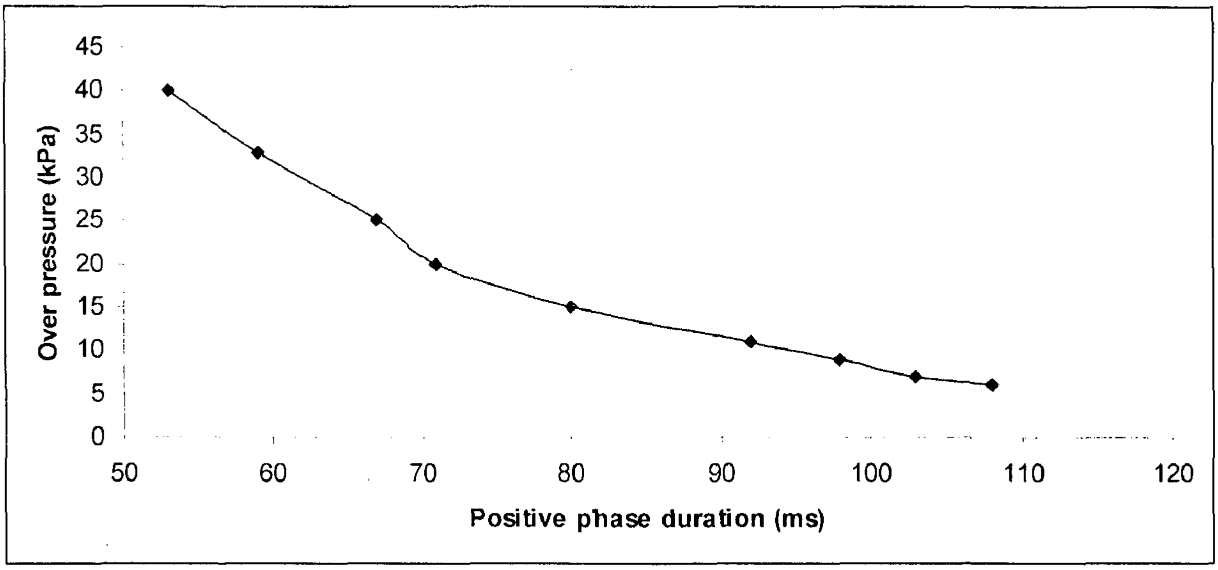


Figure 16 – Over pressure vs. positive phase duration for multi energy method.

To bypass the imperfections of TNT blast as a model for gas explosion blast, in the multi-energy method fuel-air charge blast is used for this purpose.

In TNT equivalency at an approximate upper limit (10%) the over pressure is decreasing as distance increases, showed in figure 11. The variation of over pressure is very large so this method is quite over predictive regarding vapour cloud explosion at a large scale. The over pressure with respect to positive phase duration shown in figure 12. As positive phase duration increases the over pressure of explosion decreases. The positive phase duration is time in mili seconds which is taken by explosion at corresponding over pressure. This is also over predictive for an explosion because the impact of vapour cloud explosion will be more at higher over pressure. When vapour cloud drift to some distance then the concentration of reaction mixture will decrease with the time and distance, so the effect of explosion will be less.

In TNT equivalency at an average limit (4%) corresponds to an average major incident. By using an average value of the TNT equivalency, "average major incident conditions" are extrapolated to an actual situation. Therefore, TNT-equivalency methods give a reasonable estimate of far-field blast effects only if the actual conditions correspond more or less to "average major incident conditions". In this case the variation of over pressure is less and at some small distance it can find higher over pressure, which is the most considering scenario for worst case in vapour cloud explosion with respect to safety. An average limit (4%) of TNT equivalency can be use to predict over pressure, but this is also over predictive at large scale. Figure 13 and figure 14 shows the over pressure curve according to distance and positive phase duration.

In Multi energy method the over pressure against distance and positive phase duration has shown in figure 15 and figure 16. From the data it can be observe that this method can determine higher pressure at very small distance compared to TNT equivalency method and the positive phase duration is also less. Positive phase duration should be less for safety aspect. So Multi energy method is more deterministic to estimate blast characteristics.

TNT blast is a poor model for gas explosion blast. While a TNT charge produces a shock wave of a very high amplitude and a short duration, a vapour cloud explosion produces a blast wave, often shockless, of lower amplitude and longer duration. If the blast modelling is the starting point for the computation of structural response for, for instance, the design of blast resistant structures, TNT blast will be a less satisfactory model. Then the positive phase duration of the blast wave are important parameters which should be considered and the use of a more appropriate blast model is recommendable. A practical value for TNT equivalency is an average, based on a wide statistical distribution of TNT equivalencies found in practice, As a consequence, a predictive estimate with TNT equivalency on the basis of an average value for the TNT equivalency has a very limited statistical reliability.

The heat of combustion of the fuel-air mixture was assumed to be 3.5 MJ/m3, which is representative for an average stoichiometric hydrocarbon-air mixture, The blast model reflects basic features of gas explosion blast. The initial blast strength is a variable expressed as a number ranging from 1 for insignificant to 10 for detonative strength. 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 wholly 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=3.5 MJ/m3). 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 showed in figure 9.

CONCLUSION

The vapour cloud explosion models are present in various degrees of complexity, but they fall into three different groups i.e. empirical models, phenomenological models and CFD models. The limitations of the empirical and phenomenological models are simplified physics and relatively natural representations of the geometry and which can only be overcome through additional calibration. This limits the scope for improvements of the models. The codes include the group of CFD models which are in widespread use, as the phenomenological model SCOPE. Few years before the CFD-based models incorporated realistic combustion models, but now it is able to accurately represent all important obstacles in real, complex geometries and turbulence-combustion interaction. All methods and models, whether they are for predicting overpressures, loads or responses need to be validated against experimental data that is representative of the conditions and scale of events they will be used to predict. To date, data for validation has been obtained on a relatively small-scale and even large-scale experiments that are being proposed will still be one or two orders of magnitude short of full-scale. It is, therefore, important that the limited number of large-scale experiments that can be aimed at set up scaling laws, as once established other effects can be studied on a smaller scale. Good instrumentation is also necessary for very costly large-scale tests.

7.1. RECOMMENDATIONS

In the near future, substantial progress in vapour cloud explosion blast modelling can be made by:

1. The development of a data base containing data on both vapour cloud explosion incidents and gas explosion experiments (small- and full-scale).

2. A further development of software for the computational simulation of the process of turbulent premixed combustion in gas explosions and blast effects.

3. The multi-energy concept applies only if the possibility of unconfined detonation can be ruled out. Therefore, the confidence in the multi-energy method for vapour cloud explosion blast modelling will increase substantially if the conditions under which the possibility of unconfined vapour cloud detonation should be considered, are further specified.

4. In order to establish greater confidence in model predictions, it is clear that, for the future, improvements in the physics and the numeric's are required, particularly for the CFD-based approaches. However, predictive approaches are needed now. It is thus important that the user be aware of the uncertainties associated with the different models.

5. More work is needed to establish the reliability of the combustion models used. Presently, the majority of the explosion models investigated prescribe the reaction rate according to empirical correlations of the burning velocity. However, it should be recognised that these correlations are subject to a large uncertainty. The eddy break-up combustion model should ideally not be used if the flame front cannot be properly resolved or, the resulting errors should be recognized and quantified.

6. The sensitivity of model predictions to the turbulence model used should be investigated. Turbulence modelling has not yet received much attention in the field of explosion modelling.

7. Perhaps the safest thing that can be advised at this point is that it would be unwise to rely on the predictions of one model only, i.e. better to use a judicious combination of models of different types, especially if a model is being used outside its range of validation.

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