Modeling and Mitigating the Consequences of Accidental Releases of Hazardous Materials

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Unconfined Vapor Cloud Explosions: A New Perspective

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Abstract

A modern perspective on the problem of vapor cloud explosions is given. Particular emphasis is placed on the important practical problem of detonation hazards. Significant advances in our fundamental understanding of detonation and flame acceleration have occurred in the last decade. We review these developments in large scale experimentation and numerical modelling of reacting flows. Results of recent large scale experiments on flame acceleration and deflagration to detonation transition are discussed. It has been found that the important factors determining the possibility of detonation include the intrinsic chemical sensitivity of the fuel-air system, the extent of confinement, the location of obstacles within the cloud, and the presence of jet ignition sources.

Direct initiation of detonation is unlikely for most fuel-air systems in a typical accidental release situation.

Deflagration to detonation transition is considered to be the most likely mean of detonation initiation. This has been observed only for the most sensitive fuel in truly unconfined mixtures lacking flame interaction with nearby walls or obstacles.

A technique for estimating detonation hazards in gaseous releases is proposed. This technique is based on evaluating the intrinsic sensitivity of an explosive gas through a combination of lab experiments and numerical simulation of the detailed chemical kinetics. Examples are given for a variety of fuel-air systems.

Overview

The majority of explosion related research efforts during the la
cused on the following areas:

- Flame acceleration mechanisms
- Deflagration to detonation transitions
- Direct initiation of detonations
- Overpressure levels within the combustion zone
- Effects of pressure rise time dependency on structures vs.
- Minimum amount of mass sufficient to sustain a UVCE
- Explosion efficiencies

The original attempt at understanding the properties and chara
UVCE's was presented in 1946 by G. I. Taylor. Taylor's combus
used a piston concept (an infinitely extensible spherical piston) to
vapor cloud, thereby compressing it and simultaneously impartin
to it to establish a shocked condition.

This concept, which is based on the similarity of such a piston mo
the exothermic reaction during the flame propagation of an ign
cloud, has been widely used and modified by subsequent investiga

Many subsequent modelling studies, according to Zalosh [49], have
on simplified, and perhaps unrealistic, assumptions of cloud for
ignition - such as a centralized ignition of a homogeneous hemispher

The quantitative evaluation of the decay properties of the shock fr
begins to decay when the combustion process is complete and the
consumed all of the flammable vapor, has not been resolved sati
These decay properties are, of course, of particular importance i
analysis or in risk analysis, as they would define the differences
UVCEs and TNT-like explosions.

Gugan [12] presents a general discussion of the fundamentals of co
as they relate to the development of unconfined vapor clouds upon
In Appendices, Gugan also provides a theoretical treatment of the f
of vapor clouds and of the blast waves developed after ignition.

Wiekema [47] develops a model to estimate the blast overpressure an
phase duration on the basis of the sensitivity to flame accelerati
combustible mixture.

Lee and Moen [21] present a scholarly experimental/theoretical study of the transition mechanisms from deflagration to detonations in UVCES. Their principal conclusion is that this transition requires flame acceleration by large-scale turbulence during all stages of the combustion process.

Marshall [23] conducted theoretical studies of the size of flammable clouds in terms of the mechanisms controlling dispersion, momentum, buoyancy, and atmospheric turbulence.

Geiger [10] discusses several areas of investigation of UVCEs in Germany, with particular emphasis on detonation-like explosive modes.

Strehlow [40] presents a survey paper on ideal and non-ideal blast waves from accidental explosions. Most accidental explosions will produce non-ideal blast characteristics because of the way that energy is added to or is initially distributed in the source region, and by implication, the degree to which the burning flame accelerates; this acceleration is required for the explosion to develop a blast wave similar to that produced by a condensed phase explosion.

According to Strehlow, when the flame subsequently decelerates to a velocity of less than about 1/16th of the velocity of sound, then the lead shock wave is reduced to a simple compression wave propagating away from the source region. This is an important concept, which provides a sound explanation for reduction in the decay of overpressure in the far field (relative to TNT-type explosions), or, subsequently, the transformation of the shock-like overpressure wave to an acoustic wave.

Phillips ([32] and [33]) discusses research in the U.K. on the mechanism of vapor cloud explosions, and on the dispersion of the cloud. In particular, mechanisms for the acceleration of the flame front by turbulence, by semi-confinement of the cloud, and by a postulated two-fluid model for burnt and unburnt gases moving at different velocities are considered.

Hasegawa and Sato [13] studied the development of the blast wave from UCVEs in deflagration using both theoretical and small-scale experimental methods. The theoretical approach was based on a piston analogy, and provided a reasonable comparison with the experimental results.

Koch, et al. [9] present an excellent summary of previous theoretical and experimental studies in UVCE explosions, with particular emphasis on the likelihood and requirements for transition of a deflagration to a detonation. The conclusions reached in the study are that detonation may occur in cases of jet ignition, but otherwise detonation need not be postulated in safety studies.

Wingerden and Berg [48] evaluated three blast wave simulation codes: a low flame speed (≤ 100 m/s) Piston model and two gasdynamic-equation-based codes which are applicable for higher flame speeds. Each of these models are based on a spherical symmetric blast wave, although the piston model w investigated for applicability to pancake-shaped vapor clouds. Comparis to small-scale experiments included reasonable simulation of the shape of th blast wave, but only fair prediction of the decay of the blast wave.

Some analytical work has been done on the effects of the shape and symmet of the vapor cloud, prior to its ignition, on the subsequent characteristi of the blast wave. Geiger [10] compares the pancake-shape of dense vap releases with the more normal acceptance of a hemispherical cloud shape a concludes that the decay of overpressure beyond the cloud edge is more rap for a pancake-shaped cloud than for a hemispheric cloud. (Other investigato have also reached this conclusion - see Pickles and Bittleston below). A discussed subsequently, this is not consistent with damage analyses.

Pickles and Bittleston [34] have analyzed the asymmetric blast wave fro an elongated (ellipsoidal) cloud ignited at one end, and, using a numeric procedure based on an acoustic theory approximation, concluded that th asymmetry of the blast wave can be pronounced, with overpressures in th direction of flame propagation being four times greater than in the rever direction, even at long range. They also concluded that the overpressu levels in any direction would be less than those from a hemispherical cloud the same volume. Again, this is not consistent with damage analyses in th far field.

Taylor [41] showed that the Pickles and Bittleston results for an elongat cloud with edge ignition could be developed in analytic form.

It seems fair to conclude, as Strehlow [40] does, that "the acoustic theo for high aspect ratio source regions shows conclusively that deflagative con bustion as such cannot produce the damaging blast waves that have bee observed as the result of UVCES."

This implies that very high-speed deflagrations or detonations must occ within vapor clouds that result in large blast pressures. For this reason, rece research on UVCEs has focussed on mechanisms for the production of hig speed or accelerated flames and the possibility of deflagration-to-detonati transition (DDT) occurring in unconfined or partially confined clouds. Whi this research has been very productive, there are many outstanding problen such as how to scale up experiments done in the laboratory, and developi numerical predictions of DDT that can be used for hazard assessment. Due t these unresolved issues, large-scale experiments have been and will contin to play a very important role in assessing hazards.

Obstacles and Confinement Effects

The two main issues addressed in experiments and models have been the role of confinement and obstacles in accelerating flames and causing DDT. One key observation from experiments on unconfined flames (spherical or hemispherical clouds with central ignition) is that transition to detonation is exceedingly difficult for completely unconfined configurations. Only with the addition of grids or screens in the path of the flame was DDT produced in sensitive fuel-oxygen mixtures (Wagner et al. [8]). Even with large-scale (10 m diameter) clouds, merely low speed (20-50 m/s) flames were produced in completely unconfined fuel-air mixtures (Brossard et al. [5]). There appear to be two significant factors contributing to the ineffectiveness of flame acceleration for completely unconfined flames. First, the natural instability mechanisms of flames only cause a moderate growth in the flame surface area. Second, the lack of confinement results in a substantial decoupling between the upstream fluid motion and the flame motion. This corresponds to rapid decay ($1/r^2$) of the velocity and pressure fields in spherical source flows.

Another key fact is that the addition of obstacles to confined flames produced dramatic accelerations (flame speeds up to 400 m/s) within a short distance for both tubes (Wagner [45]) and cylindrical (pancake) geometries (Moen et al. [25], Moen et al. [26]). While initial studies were with sensitive fuel-oxygen mixtures in small-scale, large-scale experiments (Moen et al. [27]) demonstrated that similar effects could be obtained with insensitive fuel-air mixtures if the scale was increased sufficiently. Using periodic obstacles (orifice plates) or spirals within a tube, (Lee et al. [18]) were able to obtain sufficient flame acceleration to produce DDT in H_2-air and C_2H_2-air mixtures and flame speeds of up to 800 m/s in methane-air mixtures within 5-10 tube diameters of the igniter.

The flame speeds produced in confined clouds, i.e., within tubes, suggests that such processes might be possible in unconfined clouds. A number of studies have been directed towards this possibility over the past decade. Many of these tests have emphasized complex geometries combining partial confinement and obstructions. While these situations are clearly not just simple unconfined vapor clouds, many industrial accidents involving fuel-air explosions do occur near or within process equipment and structures, and these studies are relevant to these common situations.

Work in small-scale by Chan et al. [7] and Urtiew et al. [43] demonstrated the significance of confinement for producing substantial accelerations and also showed the importance of the flame-vortex interactions. Experiments have also been performed with pancaked-shaped fuel-air mixtures at various scales through "forests" of obstacles (van Wingerden and Zeeuwen [44]). Ultimate flame velocities were increased by a factor of up to 8 by confining the flame to a cylindrical channel but only moderate terminal velocities (50 m/s) achieved. These experiments demonstrated that the early stages of f acceleration in hydrocarbon-air mixtures could be scaled on the basis single parameter, the laminar flame speed.

Later work at large scale showed the possibility of acceleration leading to l for H_2- air mixtures in partially-obstructed and vented channels, (Sher et al. [39] Sherman et al. [38], Tieszen et al. [42]). These tests demonst that venting can have both a negative and positive effect on flame acce tion. With a small amount of venting from the top of a channel confine the remaining three sides, the flows induced by venting contributed to fl acceleration. Increasing the venting (percentage of open area) results in eventual reduction of the flame acceleration and inhibits transition to det tion completely if the venting is large enough. Moen et al. [28] demonstr DDT in C_2H_2-air mixtures in a channel, vented on the top and filled wit array of pipe obstructions. The flame speed just prior to transition was m/s. Flame speeds up to 200 m/s were observed in propane-air mixtures a quasi-steady-state propagation rate was achieved within several meter the ignition source.

It is important to note that in the large-scale experiments of Moen et DDT was observed in only the most sensitive mixtures. These experime were essentially unconfined but highly-obstructed, designed to simulate accident within a pipe-rack or a portion of a processing plant. The fail to produce DDT or substantial flame acceleration in less sensitive mixtu reinforces the notion that it is extremely difficult to obtain detonation in c pletely unconfined vapor cloud explosions, even when numerous obstructi are present.

Jet Ignition Effects

It has been known for a decade that it is possible to initiate detonation high-speed turbulent flame-jets or combustion product jets. The first demo stration by Knystautas et al. [16] of this important mechanism for shockle initiation of detonation was in small scale with sensitive fuel-oxygen mi tures. Later studies by Schildknecht et al. [35], Moen et al. [29], and Mack et al. [22] have concentrated on the initiation of sensitive fuel-air mixtur at large (1-10 m) scales. These experiments have demonstrated that tran tion to detonation can be induced in essentially unconfined fuel-air mixtur of moderate sensitivity (H_2 and C_2H_2). Such tests are a dramatic confi mation of the modern notions that the absolute dimensions and method ignition play a key role in determining the ability to initiate detonation Even though detonation was not produced in less sensitive fuel-air mixtur such as ethylene and propane, substantial overpressures (1-6 bar) were produced by these explosions. This indicates the hazardous nature of flame-jet ignition, a common scenario in industrial accident analysis. Criteria for jet initiation of detonations are less clear but the absolute velocity of the jet and the jet turbulence parameters appear to be the most important factors.

TNT Equivalence Analysis

Although the characteristics of the blast wave from a vapor cloud explosion are known to differ substantially from those resulting from a TNT explosion, it is common in explosion investigations to establish an "equivalent TNT yield" for the vapor cloud explosion. The principal reason for this is that the characteristics of TNT explosions, including the blast effects and the relation of the overpressure wave to the distance from the center of the explosion and to the charge weight of TNT have been well established from extensive experiments and weapons tests. These TNT data can be used, therefore, to estimate the quantity of explosive material involved in the accidental release, or the effective source strength of the vapor cloud explosion.

The equivalent TNT yield is based on two factors: first, the ratio of the heat of combustion of the combustible gases in the vapor cloud to the heat of detonation of TNT; and, second, the efficiency of the vapor cloud explosion. An equivalent mass of TNT is calculated using the following equation:

$$\frac{M_{TNT}}{M_{cloud}} = \frac{\Delta H_c}{1155} \times E_f \qquad (1)$$

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:

$$X = 0.3967 \times M_{TNT}^{1/3} \ \exp\left[3.5031 - 0.7241\ln(O_P) + 0.0398(\ln O_P)^2\right] \qquad (2)$$

where:

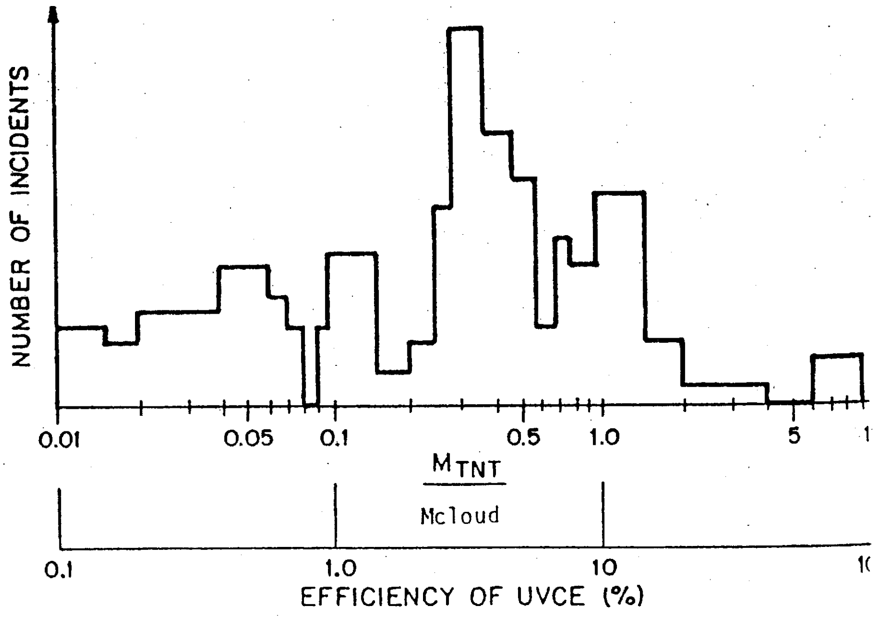
X = Distance to given overpressure, m

O_p = Peak overpressure, *psi*

The first of these is simply the ratio of the total energies available per mass of material. For most hydrocarbon materials, this ratio is about Thus, on a mass basis, a hydrocarbon release has ten times as much poten explosive energy as TNT.

The second factor relates to how well or efficiently the vapor cloud behave an explosive material upon ignition. The efficiency is dependent upon sev conditions, including the quantity released, the rate of release, the direct of release, wind and atmospheric stability at the time of the release, the ti between the initial release and ignition of the cloud, and degree of turbul mixing of the released vapor with air.

Figure 1: TNT equivalent of unconfined vapour cloud explosions [1



Unlike TNT or other high explosives which are designed specifically to produce a highly efficient explosion, the dispersed vapor cloud even under the most favorable conditions will be relatively inefficient. A study of over one hundred vapor cloud explosions which have occurred in recent years led to the graph shown on Figure 1, which indicates the relative frequency of occurrence of values of the efficiency (and the TNT equivalent, assuming an energy ratio equal to 10) of these explosive events. As the Figure indicates, efficiencies of three to four percent are most common, while an efficiency range of one to ten percent accounts for a significant percentage of the explosions studied.

Another important factor in defining the efficiency and the equivalent yield parameters is related to the percentage of the total released material which should be included in the calculation. If the vapor cloud is dispersed extensively before ignition occurs, then some of the vapor is diluted below the lower flammable limit, and some, near the source of the release, may be above the upper flammable limits. Therefore, only that portion of the vapor cloud within these limits will be within the flammable range.

Historically, the estimates of UVCE efficiencies, such as those shown on the figure, have been based on the total mass released. Obviously, for most, if not all, of these events, the calculated efficiency would increase if the mass of the flammable cloud were used in the calculation, and it is likely the wide scatter of efficiency values shown in Figure 1 is at least partly explained by the wide ratio of the actual flammable mass to the total released mass of these events.

Although it would be preferable to estimate explosion efficiencies on the basis of the flammable mass, such a process introduces still another assumption into the calculations, since for most accidental releases, the total amount released is more readily estimated than the amount in the flammable range.

As the methods and models available for dispersion analyses improve, and thus the estimation of the flammable mass of a hydrocarbon release becomes more accurate, then consideration should be given to developing estimates of the UVCE efficiency on the flammable mass.

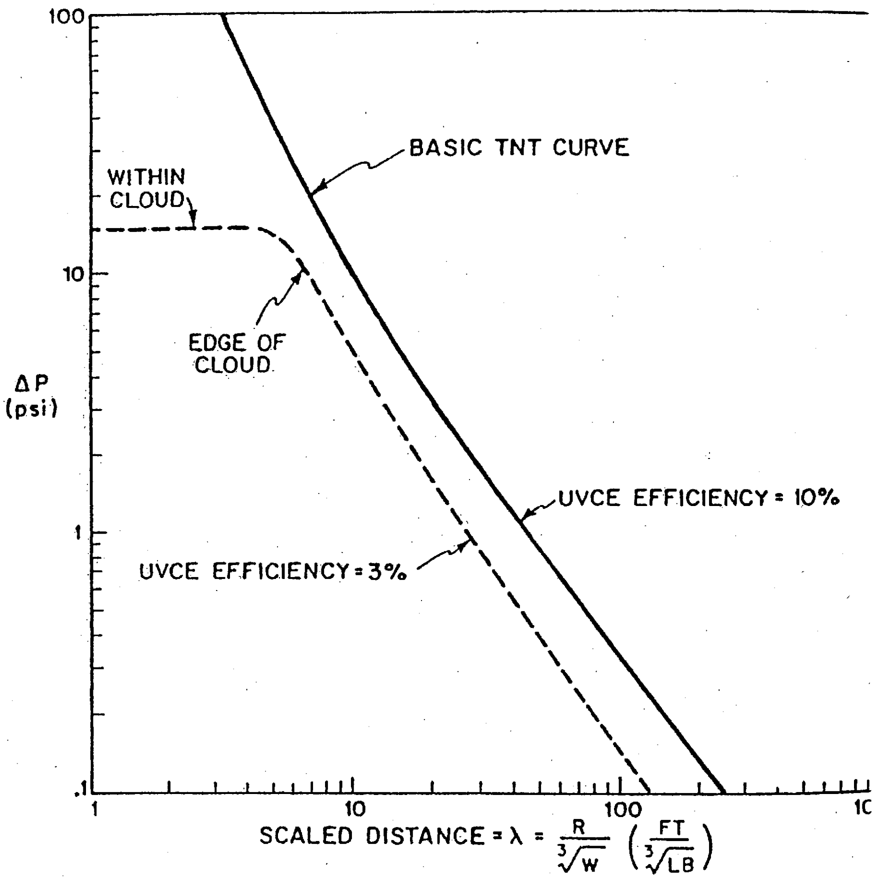


Figure 2: Free-field overpressure vs. scaled distance: TNT and UVCE exp] sions

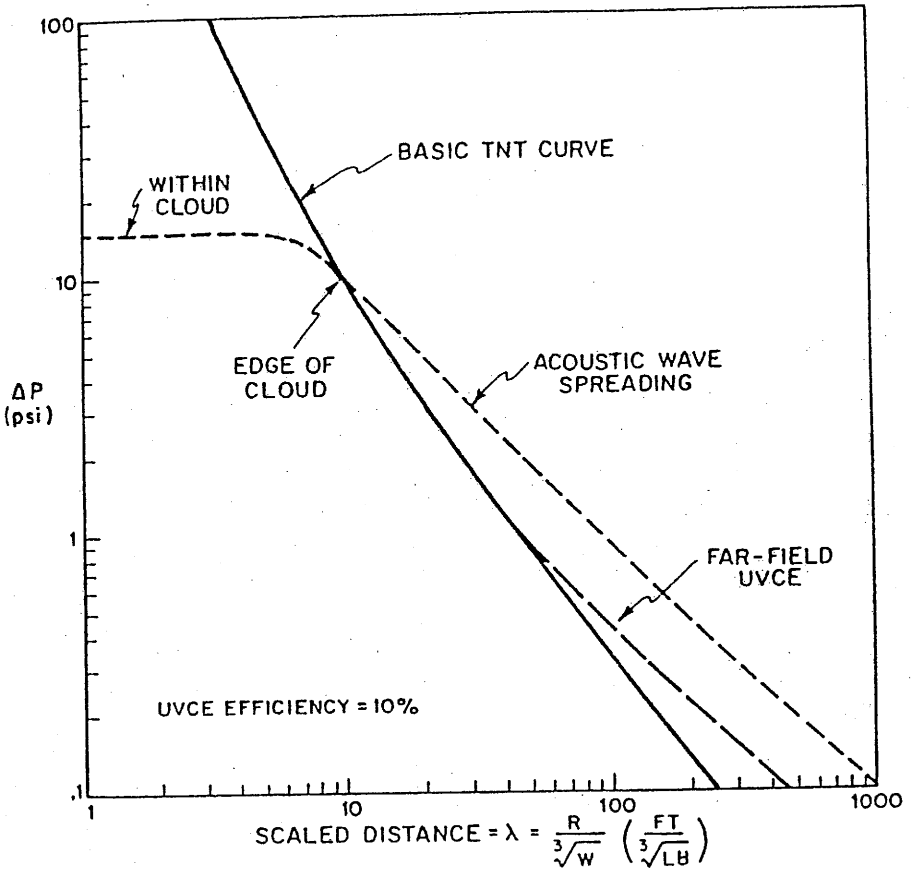


Figure 3: Free field overpressure vs. scaled distance for different spreading assumptions

The basic TNT curve relating the peak overpressure of the blast wave fro a TNT explosion to the scaled distance parameter, in accordance with t Hopkinson scaling, is shown on both Figures 2 and 3. This curve is bas on a series of experiments and weapons tests carried out over many yea and represents the peak overpressure, for a TNT explosion on the grou surface, which generates an overpressure blast wave which radiates into hemispherical space.

Little is known about the peak overpressure (or, of the entire time-histor resulting from vapor cloud explosions. Based on explosion damage anal ses together with some small-scale experiments and theoretical analysis, it thought that the corresponding curve for vapor cloud explosions is appro mately similar to the basic TNT curve with the following exceptions:

1. Within the vapor cloud, it is considered likely by many investigato that the peak overpressure does not exceed 15 psi. At the edge of t cloud, the overpressure is likely to be 10 psi or somewhat less.
2. Outside the cloud, the decay in overpressure is assumed to follow gene ally the trend indicated for the basic TNT curve. On Figure 2, a dec curve is shown for a vapor cloud efficiency of three percent, a val frequently assumed for design and analysis. On Figure 3, a curve f ten percent efficiency is shown; this curve is superimposed on the TN curve, on the basis that the ratio of the total energies of the hydrocarb vapor cloud and an equal weight of TNT is ten.
3. In the far-field, with peak overpressures of, say, 0.5 psi or less, it considered likely that the vapor cloud overpressures decay less rapid than the TNT overpressures. In this region, the vapor cloud overpre sure blast wave behaves more like an acoustic wave, thus decaying b geometric spreading only. The consequence of this is that higher va ues of overpressures occur from vapor cloud explosions than from TN explosions of equivalent weight at far locations.

On Figure 3, acoustic wave spreading is shown for the far-field assumptio for all distances beyond the 1.0 psi overpressure, and, for comparative pu poses, for the case where the overpressure decay is only due to acoustic-ty spreading losses at all locations outside the cloud itself.

The difference between TNT curve decay and acoustic-type decay in the fa field is significant in damage analyses. For example, a 0.2 psi damage estima (say, by window damage analysis) at a range of 5000 feet implies a equivale charge of 20 tons if the TNT curve is used, and an equivalent charge of le than 5 tons if the acoustic decay curve is used.

Thus the manner in which the peak overpressure of the blast wave from

UVCE decays with distance, particularly in the far-field, is important when far-field locations are used in damage analyses.

Unfortunately, the decay characteristics are not well understood in this region, and the usual analysis methodology is to assume that the TNT curve applies. As indicated by the examples, however, this approach can significantly underestimate damage in the far-field, or, alternatively, lead to excessive estimates of equivalent yields from specific damage.

With the substantial uncertainties of the characteristics of the peak overpressure from a vapor cloud explosion both at close-in ranges (greater than 10 psi) and at far-field ranges (less than 0,5 psi), the most useful comparison of vapor cloud explosions and TNT explosions are at mid distances, corresponding to, 0.5 psi up to 10 psi with the least uncertainty in the narrower range of about 0.5 psi to 3 psi. It is in this range that damage analysis is considered most appropriate for estimating the source strength of a vapor cloud explosion.

Detonation Analysis

Detonation is the most hazardous type of UVCE. A detonation in a stoichiometric gas- phase fuel-air mixture in a supersonic wave propagating with a definition velocity between 1800-2400 m/s. The velocity depends on the exact composition (see Table 1), and is experimentally observed to be between 90 and 100 % of the classical value predicted by the Chapman-Jouguet (CJ) theory. The peak (CJ) pressure behind the detonation is approximately 20-30 bars and an expansion wave directly follows the detonation, reducing the pressure to near atmospheric in a time comparable to the sound wave transit time through the burned gas, typically about 1 ms per meter of cloud thickness.

In the far field, the blast wave produced by a detonating vapor cloud has been experimentally demonstrated (Moen et al. [30]) to be identical to that produced by the equivalent mass of high explosive. In the near field, particularly within the cloud, the peak overpressure is lower for the vapor cloud but the pressure pulse duration is much longer than for an equivalent energy high-explosive blast. The differences in near field characteristics of vapor cloud and high explosive detonation result in a failure of the energy equivalence concept for near field damage. In particular, the near field positive-phase impulse is much larger for a vapor cloud detonation than the equivalent high explosive blast. This leads to much larger near field damage than would be predicted on the basis of the energy deduced from far field observations.

Table 1: Detonation Parameters of Common Fuels-Air Systems

Chemical	% (volume) at $\phi = 1$	P_{CJ} (bar)	U_{CJ} (m/s)	Δ (mm)	λ (mm)	(
H_2	29.60	15.6	1968	0.29	15	5
CH_4	9.48	17.2	1801	24.00	300	19.2-105.6
C_2H_2	7.75	19.1	1864	0.27	6	5
C_2H_4	6.54	18.4	1822	2.60	27	48
C_2H_6	5.66	18.0	1825	4.60	55	144-
C_3H_6	4.46	18.5	1809	–	52	216-
C_3H_8	4.03	18.3	1798	4.10	55	240-
C_4H_{10}	3.13	18.4	1796	–	60	240-

Reaction Zone Length

A detonation can be idealized as a nonreactive shock wave followed by ch ical reaction zone. The high temperatures and densities produced by strong shock initiates the reaction between fuel and oxygen. Reaction typical hydrocarbon fuels require many intermediate steps (several hund and species (20-50) before the final products of combustion, CO_2 and are produced. The time or distance required to achieve complete reac is an indication of the detonation sensitivity of the fuel-air system. A parameter is the thickness of the reaction zone, Δ, which can be use rank the sensitivity of many fuels to detonation. The more sensitive the the smaller Δ. These reaction zone thicknesses can be computed (Westb and Urtiew [46]) using detailed chemical reaction network model for m common fuels, some values for common hydrocarbons are listed in Tab together with other important detonation parameters. Note that many of higher hydrocarbons have similar reaction zone thicknesses and would be pected to have comparable detonation sensitivity. Methane is an excepti compound and does not follow this rule, it is among the most insensitiv hydrocarbons but can be detonated if sufficient energy is used.

Cell Size

Experimentally, the shock wave and reaction zone structure is observed (Le to be unstable, resulting in transverse instability waves moving across detonation wave. The instability waves are quasi-periodic and have a ch acteristic spacing λ known as the cell size, after the cellular appearance the spatial structure of the instability wave pattern. The cell size λ and reaction zone thickness Δ are closely related, for common fuel-air mixtu

λ is about 20-50 times Δ (Westbrook and Urtiew [46] Shepherd [36] and [37]). The cell size is also a convenient measure of detonation sensitivity and has the advantage of being experimentally measurable in laboratory-type experiments. Cell sizes have been obtained for many common fuel-air mixtures and are also given in Table 1.

Critical Energy

Extensive experimentation in the last decade, review by Lee [20] , has shown that the behavior of detonations can be directly related to the sensitivity to the mixture, as characterized either by Δ or λ. One the most important relationships for UVCEs is the minimum or critical energy E_c required for direct initiation of detonation. It is found that (Lee [19]) in order to directly initiate detonation, i.e., without a flame acceleration and DDT process occurring, that a large amount of energy must be rapidly (within microseconds) deposited directly within the vapor cloud. Only very rapid energy releases such as from sparks, exploding wires, or high explosives are effective in causing direct initiation. It has been experimentally observed (Bach et at. [1]) that if less than a critical amount of energy is used, detonation will not occur and only a high speed flame will result. The overpressures may be substantial, as in turbulent jet initiation, but a detonation does not occur. Critical energies for direct initiation depend on the fuel type and equivalence ratio and have been experimentally measured for many common fuels. Critical energy values are conventionally given in terms of the equivalent mass of the high explosive tetryl (1 kg of tetryl is equivalent to 4.8 MJ), some data are given for stoichiometric mixtures in Table 1. Note that for the higher hydrocarbons (except methane), the minimum critical energies are all similar and are of the order of 50 - 80 g of explosive. This magnitude of rapid energy release is essentially impossible to obtain in an accident situation and emphasizes how unlikely direct initiation of detonation is for most UVCEs.

Benedick et al. [4] have shown a direct link between the cell size λ and the minimum critical energy E_c:

$$E_c = 490 \rho_0 U_{CJ}^2 \lambda^3 \tag{3}$$

where the quantities are E_c (Joules), initial fuel-air density ρ_0 (kg/m^3), the detonation velocity U_{CJ} (m/s), and detonation cell size λ (m). This relation is very useful in predicting E_c values from laboratory measurements of the cell size. The observed proportionality between cell size and reaction zone length enables predictions or extrapolation of E_c values for fuel-air systems in which the chemical kinetics are well understood.

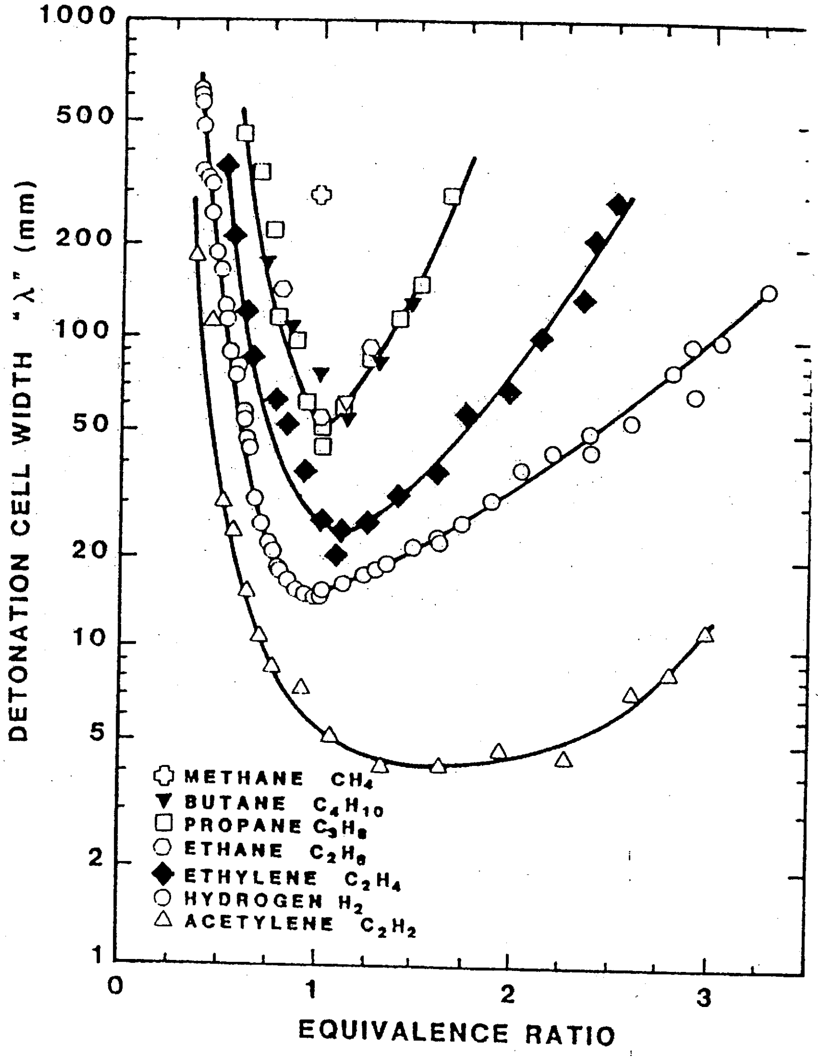


Figure 4: Fuel-air detonation cell sizes

As the equivalence ratio of the mixture departs from stoichiometric, any given mixture will become much more insensitive. This is due to the lower energy release of off-stoichiometric mixtures resulting in lower post-shock temperatures and densities and longer reaction times. The Arrhenius dependence of reaction rate on temperatures and the large effective activation energies of common fuel-air reactions causes a sharp increase in reaction time and reaction zone length as the mixtures varies from stoichiometric. This dependence is reflected in the "U-shaped curves" measured for the dependence of detonation cell size on reaction zone length, shown in Figure 4. As a consequence, nonuniformity within the vapor cloud and the natural concentration gradient that exists due to the mixing processes during the release make direct initiation of detonation even more difficult. Only that portion of the cloud which is within a concentration range that yields modest increases in cell size over the stoichiometric value will be capable of detonation.

Flame Acceleration Mechanisms and DDT

When flames propagate in obstacle-filled region, the acceleration mechanism is due to the flame-generated flow pulling the flame through the narrow region (throat) at the obstacle locations and the flame is then wrapped up in the vortices shed from the downstream side of the obstacle. The flame shoots out ahead since it is pushed from behind as the pockets of reactants between the obstacles are burned out. In turn, the increase in burning area results in a greater volume flow rate out of the burned region. This pushes the unburned reactants over the obstacles faster, producing more vorticity and setting up a positive feed back mechanism between fluid motion and the flame motion. This is particularly effective in closed tubes (Lee [20]) but will also result in flame acceleration in unconfined but obstructed regions, as discussed previously in the literature review. If the flame speeds and fluctuating velocities become large enough ahead of the flame, then significant pressure fluctuations can occur. These pressure fluctuations will also feed back in the flame propagation process and provide another mechanism for acceleration.

If the flame acceleration process proceeds to a sufficiently high level, it is possible for a sudden transition to detonation to occur. The ability to promote flame acceleration and the tendency for DDT is a function of the several factors (Lee [26]): the reaction and transport rates in the mixture; confinement; obstacle geometry. The following parameters are found to be important:

1. laminar flame propagation velocity.
2. detonation cell size (reaction zone thickness,

3. obstructed area ratio, and
4. minimum transverse dimension of the obstacles or tube.

These factors appear to be significant for both confined and unconfine plosions. The onset of DDT has been observed to be correlated witl sensitivity of the mixture and the minimum size of the orifices withi tube.

Transition to detonation is found (Knystatuas et al. [17], Peraldi et al. to be possible if the detonation cell size λ is less than the minimum trans dimension in the system D_m. In the case of an unconfined cloud, this di sion is the minimum thickness of the cloud. While the data are inconclu a thickness of 3-6 λ appears to be required.

Numerical modeling of DDT has been directed at understanding the f acceleration portion of the process. No method has been developed yet th capable of accurately predicting a complete flame acceleration and trans to detonation event. Hazard assessment for DDT events therefore proc by a combination of experiment, partial numerical modelling, and ju ment. Two principal types of numerical models have been applied to problem: inviscid, incompressible vortex dynamics and flame front trac (Barr [3], Cattolica et at. [6], Barr [2], Lee et al. [20]); finite-difference, c pressible flow with k-ϵ turbulence models and mixing-rate limited chem (Hjertager [15], Hjertager [14], Marx [24]). Each scheme has its peculiar its and deficiencies. Comparisons with experiments indicate that the in stages of flame acceleration can be predicted successfully by either mc Details of the flame-vortex interaction process are well resolved by the vo dynamics technique. The compressible flow models are successful in prec ing the pressure waves produced by high-speed flames in partially confi and obstructed tubes. However, the actual onset of detonation can not treated by the present models. This problem is due in large measure to practical limitations on spatial and temporal resolution in multidimensi computations. However, in current models, a key difficulty also lies in combustion submodel: it is simply not possible to simulate details of reac zones (needed for detonation onset modeling) with the current subgrid-s models of turbulent combustion.

Conclusion

Completely unconfined and unobstructed vapor clouds ignited by low-ene sources burn through a low-speed turbulent flame mechanism that result small blast pressures. In order to produce substantial blast waves and as ciated far-field damage, high-speed deflagrations or detonations must occ

High-speed deflagrations can be produced if the cloud is partially obstructed by obstacles such as pipe racks. Turbulent jet initiation and partial confinement can result in higher flame speeds and blast overpressures. Structural damage from vapor cloud explosions involving high-speed flames can be as severe as those involving actual detonations.

Direct initiation of detonation requires the rapid deposition of substantial amounts of energy (i.e, high explosive detonation) and is an extremely unlikely mode of accidental initiation for almost all common fuel-air mixtures. If detonation does occur in a UVCE, it is most likely the result of accelerated flames or turbulent jet initiation leading to DDT.

At least some degree of confinement, partial obstruction of the flow paths, or a high-speed jet ignition source is required to produce DDT. The less sensitive the explosive (the larger the detonation cell size), the larger the scale and the greater the degree of confinement or obstruction is required to produce DDT. If turbulent flame-jet ignition is used, the velocity and geometric scales must be appropriately large to obtain DDT. Both confinement and obstructions provide a means of feedback between the flame-produced mean flow and the flame itself. Production of vorticity and the reflection of pressure waves are the physical mechanisms by which the feedback occurs.

The sensitivity of a given fuel-air system to direct detonation initiation and DDT can be partially assessed by laboratory measurement of the detonation cell size or computations of the detonation reaction zone length. If necessary, large scale experiments can be used to confirm these predictions of detonability. Altough tentative criteria for DDT and turbulent jet initiation have been identified, more research is needed to quantify the conditions under which DDT occurs in UVCEs.

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