A DIRECT SOLUTION FOR PREDICTING THE EFFECTS OF UNCONFINED VAPOR CLOUD EXPLOSIONS

By

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SUMMARY

A direct solution for predicting the effects of Unconfined Vapor Cloud Explosions on structures has been developed and verified against empirical data. Methods such as the TNT-equivalency model are still being widely used to simulate such explosion effects, however, many limitations exist in using these models especially close to the source. Use of flawed models could potentially lead to loss of property and/or life due to an underestimation of the destructive effects. This should be of interest to not only manufacturers of hazardous materials, but also to insurers who must understand the nature of the risk that is being underwritten, organizations involved in analyzing and mitigating explosive risks, government safety compliance organizations and law firms involved in litigation as a result of explosion accidents.

The computer model, CMBWAT, directly calculates the results of detonations and deflagrations for both chemical and nuclear explosions. It computes the strength of the incident and reflected shock wave and the attenuation of those waves over distance. Included in this model is the capability of analyzing various structural configurations and their ability to withstand the explosion effects.

Systems Integration Corporation developed this code and verified it against actual test data. A graphic demonstration has been developed in concert with Forensic Technology International, Inc. which visually displays the explosion, reaction zone and wave attenuation over distance. At this time, the Canadian Occupational Safety and Hazard Administration and the US Nuclear Regulatory Agency are reviewing this approach for incorporation into their regulations.

INTRODUCTION

A series of analytical studies based upon physical principles resulted in the development of a methodology and computer program which evaluates explosive phenomena for both chemical and nuclear processes. The objective is to provide an analysis of the physics of the explosion rather than to correlate to the highly inaccurate TNT-equivalency method developed by the US Army[1]. TNT-equivalency has since been abandoned by the Army but is continued to be used by industry. An example of the inaccuracy of the TNT-equivalency is as follows: For hydrogen (H_2) storage volumes in excess of 3,500 scf, the TNT-equivalency models are likely to be significantly unconservative. For very large gaseous H_2 (15,000 scf or more) explosion effects can exceed the TNT-equivalency predictions by a factor of 2 to 4. To emphasize the criticality of the problem, it has been reported that Unconfined Vapor Cloud Explosions (UVCEs) represent 50% of the overall dollar loss due to industrial accidents. In fact, of the 10 largest property losses in the process industry, 7 have been due to UVCEs [2]. clearly, with this type of potential exposure, accurate means of evaluating these blast effects would be in demand.

This methodology was developed specifically for the analysis of UCVEs and the resulting structural response given a particular design. It analyzes both the initiating detonation and attenuation of the resulting shock wave with time and distance. The code solves the non-steady state, non-steady flow and non-isentropic flow relations to compute static and stagnation pressure, velocity and the shock wave impulse delivered to the target surfaces within the flow field as a function of time, both for the incident and reflected wave.

The methodology has been accurately compared to actual test data and has been successfully used in several explosion litigation cases. A previous paper [3] has elicited much interest from companies involved in risk analysis, law firms and regulatory agencies.

TNT-EQUIVALENCY LIMITATIONS

The TNT-equivalency model is the traditional analysis tool for characterizing blast effects. The combustion energy of the explosion is converted to an equivalent TNT mass and yield. These have been used to estimate the potential damage that could occur from UCVEs [4]. However, the TNT-equivalency method has many limitations and can greatly underestimate the damage caused by non-TNT explosions. For example, TNT-equivalencies for gaseous hydrocarbon explosions in air overestimates the overpressures, underestimates impulses and grossly underestimates reflected pressure multipliers.

Despite these serious limitations, the TNT-equivalency still used because of its ease and requires only limited assumptions for determining the initial release size and yield factor. Various versions of TNT-equivalency methods (such as providing new correlation factors) have been developed, however the basic limitations remain.

DESCRIPTION OF THE NEW METHODOLOGY

The new model was developed from basic physical principles [5]:

1. The shock wave strength is determined from the calculated stagnation temperature across the propagated wave as it moves through the reaction zone;
2. The attenuating incident and reflected shock waves are calculated from conservation of mass, energy and momentum;
3. The reflected pressure multiplies is determined without the poor assumptions of steady state, steady flow and isentropic conditions.

Explanation of Shock Waves

Explosives generate shock waves in a system by the addition of a large amount of internal thermal energy over a short time and distance. A shock wave created by an explosion will have an initial overpressure that is a function of the change in stagnation temperature occurring inside the reaction zone. As the wave moves away from the reaction zone boundary, this peak overpressure is attenuated with distance. The damage assessment for such events has typically been determined using peak overpressure, and increasing this overpressure by a factor of two when an object which reflects the incident wave is encountered. The damage that is caused by a shock wave is really a function of the integrated area under the wave pressure-time curve. The peak overpressure is only the initial value of this pressure *vs.* time curve; pressure actually goes negative at the end of most true wave pressure-time curves. The major damage from a wave is usually caused by the positive phase of the reflected wave.

The integration of the wave pressure-time curve is called the impulse. Impulse is thus a function of the wave peak pressure and the length of the wave (a direct function of the mass of the reacting substances). For this reason, explosions caused by different substances will result in different levels of damage even when the overpressure measurements are similar. The following provides an explanation of this phenomena:

Visualize a small object (say one inch long and one quarter in diameter) traveling at six thousand miles per hour which passes within two feet of your house. You may hear the crack *of the supersonic wave, but no damage will occur. Now, keeping the object velocity and distance the same as before (i.e., peak overpressure is the same for both cases), make the object one hundred feet in diameter and four hundred feet long. You will not hear the crack, because your house would be obliterated. The difference in result is caused by the difference in duration of the overpressure. The overpressure lasts much longer in the second case, so the impulse is much larger.*

An example of an overpressure vs. time history and thus the impulse is given in Figure 1.

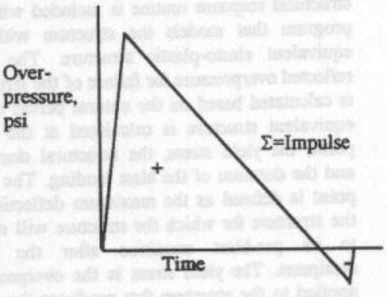

Figure 1- Overpressure Time History

Shock Wave Calculations

Each phase of the shock wave affects structures differently so all must be computed. The total reacting mass is vital to this calculation. For example, TNT reacted in 100% theoretical air yields 4.21 unit masses of products for each unit mass of TNT. Hydrogen, on the other hand, yields 35 unit masses of products per unit mass of gas or over 8 times as much. TNT has a higher initial overpressure with much less mass, while H_2 has a lower initial overpressure (due to a lower stagnation temperature of the products). Thus, the integrated impulse (and the damage potential) for hydrogen is over 30 times that of TNT per unit mass. This is characteristic of most UVCEs and has been effectively used by the military. When explosive energy is not allowed free expansion, such as in a pipeline, the damage effects go up dramatically. With a spherical expansion, the energy is dissipated in all three directions, whereas in situations with fewer degrees of freedom, the energy is concentrated.

Reflected Pressure Multiplier

All of this is further complicated by the fact that when the incident wave encounters any structure, it is reflected. This reflected wave is *always* stronger than the incident wave. Blast wave analyses in the past have usually used reflection factors of about 2 for determination of the reflected wave strength. However, the factor are only near 2 when the incident wave is near a Mach number of one and is stagnated against the wall under reversible, isentropic, steady state and steady flow conditions. This assumption is not bad at longer distances from the event center where these conditions are not far off. The real behavior of this reflected wave, however, is neither steady state, isentropic, nor reversible. Reflection factors can be as much as five, and sometimes more. When two reflected waves intersect (forming a shock stem), the multiplier can be over ten. The reflected wave pressure, temperature, velocity and impulse history must therefore, be determined. The reflected wave thus has the greatest potential for damage. Again the positive, negative and total impulse of this wave must be determined.

Wave Attenuation

The incident wave attenuation with distance must be computed. This is important since the wave overpressure decreases with distance while the wave duration gets longer. Therefore, the impulse must be computed with distance since in some cases (such as H_2) the actual reflected positive phase impulse is slightly higher a short distance from the detonation than it is at the edge of the reaction zone. TNT and other solid explosives do not exhibit this characteristic. The total impulse always goes down with distance. However, for reactions with large product production and relatively large negative pressure components, the relation between positive and negative changes with distance especially in the reflected wave. This yields the before-mentioned conditions which exist when only the positive phase impulse is looked at with distance. Vapor and solid explosives have very different characteristics and therefore the scaling laws used for so many years do not apply for vapor explosions in general and for some solid explosions in particular.

BLAST WAVE MODEL

The computer code CMBWAT was developed specifically for the analysis of explosive phenomena, and analyzes both the initiating deflagration or detonation and the attenuation of the resulting shock wave with time and distance. This analysis solves either spherical or hemispherical blast wave for pressure- or temperature-generated supersonic shock waves. Both the incident and reflected waves are calculated for any location in the flow field. The initial stagnation temperature or pressure increase that creates the shock wave is calculated, and then attenuated with distance. The model solves the nonsteady-state, nonsteady-floe and nonisentropic flow relations which compute the static and stagnation pressure, velocity and the shock wave impulse delivered to target surfaces within the flow field, all as a function of time, both for the incident and reflected waves. There are 39 standard types of fuels that can be selected as well as the capability of customizing the input fuel composition. Capability also exists to examine air or pure oxygen as the oxidizer, to constrain the blast wave shape to one-, two- or three-dimensional conditions, as well as a choice of deflagration or detonation.

Basic principles are used in all equation derivations; data fits and scaling are only used if they can be substantiated by those basic principles. The combustion subroutines compute the resulting stagnation temperature using kinetic equilibrium of all major product compounds, the combustion wave, pressure, density, etc. Upon completion of the combustion process, the resulting wave is attenuated with distance. Incident, reflected and expansion waves are computed. The entire pressure, velocity and dynamic pressure-time histories are computed. An example of output for a H_2 detonation is given in Table 1. This table shows the following detonation parameters:

- Overpressure, psi
- Wave velocity, feet per second
- Reflected impulse, psi-s
- Reflected overpressure, psi
- Total positive impulse, psi-s
- Reflected pressure, psi

When the shock wave from an explosion encounters a structure such as a building, the overpressure is increased by reflection of the shock off the wall. The overpressure applied to the wall is a factor of two larger than its free field value if the building is far from the explosion and reach factors of 10 or more above the free field value for hydrocarbon explosions. The blast also induces additional loads on the structure via drag forces from high pressure air flowing around and over the structure.

CMBWAT can be used for analyses of blast loading on buildings and other structures. A structural response routine is included with the program that models the structure with the equivalent elasto-plastic structure. The peak reflected overpressure for failure of the structure is calculated based on the natural period of the equivalent structure is calculated at the yield point, the yield stress, the structural ductility, and the duration of the blast loading. The yield point is defined as the maximum deflection of the structure for which the structure will return to its pre-blast condition after the blast dissipates. The yield stress is the overpressure applied to the structure that produces the yield point deflection. The ductility is the ratio of the deflection at failure divided by the yield point deflection. The structure will fail under the blast loading if the peak overpressure incident on the structure exceeds the failure peak reflected overpressure of the structure.

Table 1 Output For H_2 Case

H_2: 15,000 SCF (79.67 lbm)

20 % Yield = 3,000 SCF (15.93 lbm)

Dist. Ft	Vel., FPS	Press PSI	Imp. PSI-S	Refl Press PSI	Pos Refl Imp. PSI-S	Peak Neg Refl Press PSI
20	4379	238.2	0.369	1474	0.627	-14.1
40	2273	51.7	0.641	206.9	0.815	-14.1
60	1673	20.1	0.399	59.9	0.835	-14.1
80	1442	10.6	0.275	26.9	0.598	-8.1
100	1336	6.6	0.208	15.6	0.432	-4.6
120	1279	4.6	0.167	10.5	0.338	-3.1
140	1246	3.5	0.141	7.7	0.279	-2.3
160	1224	2.8	0.122	6.1	0.239	-1.8
180	1209	2.3	0.108	5.0	0.209	-1.5
200	1199	1.99	0.097	4.22	0.187	-1.3

COMPARISONS WITH ACTUAL DATA

Results of computer analyses were compared with actual test data. Specifically [5]:

1. Kinney, G. F., and Grahm, K. J. "Explosive Shocks In Air", Second Edition, Springer-Verlag, New York, (1985). Agreement was within 4% for the data published.
2. EPRI NP-4947-SR, "BWR Hydrogen Chemistry Guidelines 1987 Revision", Applicable data compared within 6%.
3. EPRI NP-5283-SR-A, "Guidelines for Permanent BWR Hydrogen Water Chemistry Installations 1987 Revision." Data compared within 5% or better.
4. Air Products Report, "Liquid Hydrogen Storage System Hazardous Consequence Analysis", January 10, 1985. This data compared within 3% or better.
5. US Bureau of Mines Explosion Data. 5% match or better.
6. US Army Technical Manual, where applicable.
7. US Army tests with 4 x 10^6 lbm ANFO
8. US Army tests with 10 x 10^6 lbm ANFO

In addition, a peer review was conducted at Sandia National Laboratory to compare the accuracy of CMBWAT against other test data. Figure 2 shows a comparison of CMBWAT calculations for hemispherical detonations of hydrogen-oxygen-nitrogen mixtures [6].

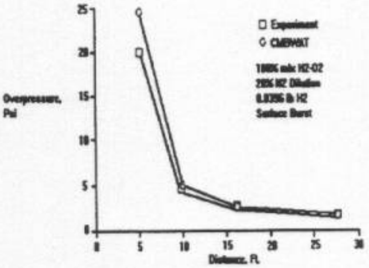

Figure 2 H2/O2/N2 Comparison With Test Data

In general, CMBWAT compares reasonably well with the data except near the cloud. Direct measurements of pressures in the cloud and in the near-field are, at best, difficult to measure. This is because the loading frequency of the pressure increase on the gauge is often near the resonant frequency of the gauge itself and the pressure gauge may not produce a linear response.

Figure 3 shows a comparison of CMBWAT to spherical detonations of methane-oxygen mixtures. Predictions for the near field are similar to those of the previous example. In this comparison, CMBWAT's predictions of the overpressure are both above and below the measured values. Figure 4 shows CMBWAT's pressure/time history predictions of a hemispherical detonation of a propane-oxygen mixture at a fixed distance.

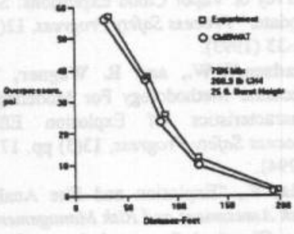

Figure 3- CH4/O2 Comparison With Test Data

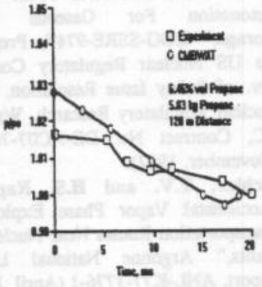

Figure 4- Propane/Air Comparison With Test Data

SUMMARY

A methodology for predicting the characteristics of explosions based upon physical principles has been developed and successfully implemented.

The computer code can analyze many explosion types and configurations and the corresponding structural response. Regulatory changes to require such analyses are under consideration.

LITERATURE CITED

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3) **Madsen,W.W., and R. Wagner,** " An Accurate Methodology For Modeling The Characteristics Of Explosion Effects", *Process Safety Progress*, 13(3) pp. 171-175 (1994).
4) **Elia, F.,** "Explosion and Fire Analysis," *Risk Assessment and Risk Management For The Chemical Process Industry*, Stone & Webster Engineering Corporation, Van Nostrand Reinhold (1991).
5) **Madsen, W.W., D.H. Van Haften, J. Neuman, and R.P. Kennedy,** "Improved Estimates of Separation Distances To Prevent Unacceptable Damage To Nuclear Power Plant Structures From Hydrogen Detonation For Gaseous Hydrogen Storage," EGG-SSRE-9747, Prepared for the US Nuclear Regulatory Commission, Div. of Safety Issue Resolution, Office of Nuclear Regulatory Research, Washington, DC, Contract No. DE-AC07-76ID01570 (November, 1992).
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