

**ACCIDENTAL VAPOR PHASE EXPLOSIONS
ON TRANSPORTATION ROUTES
NEAR NUCLEAR POWER PLANTS**

**Final Report
January - April 1977**

T. V. Eichler H. S. Napadensky

IIT Research Institute

**Prepared for
U. S. Nuclear Regulatory Commission**

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FOREWORD

Final report J6405 is the result of a research study conducted for Argonne National Laboratory by the IIT Research Institute under Contract 31-109-38-3776. This report is entitled "Accidental Vapor Phase Explosions on Transportation Routes Near Nuclear Plants", and covers the contract period January 26, 1977 to April 25, 1977.

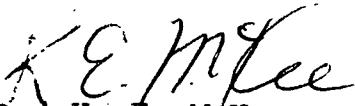
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Respectfully submitted,
IIT Research Institute



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ABSTRACT

This report presents the results of a study of the potential blast effectiveness of vapor cloud explosions for hydrocarbons released under accident conditions associated with transportation routes near nuclear plants. The objective is to provide a methodology for estimating TNT equivalency of accidents of this type in order that safe standoff distances for nuclear plants can be evaluated.

Results are presented that establish the maximum blast effectiveness that can be attributed to fuel-air explosions on the basis of thermodynamics and experimental data. A review of accidental vapor cloud explosions is included and comparisons are made to determine a realistic basis for evaluating an accident's potential destructiveness. It is hoped that this study contributes toward the resolution of the many inconsistencies that appear on this subject.

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ACCIDENTAL VAPOR PHASE EXPLOSIONS ON TRANSPORTATION ROUTES NEAR NUCLEAR PLANTS

1. INTRODUCTION

Vapor clouds consisting of a hydrocarbon-air mixture have formed and exploded following accidents in the transportation of potentially explosive cargo. In order to determine safe standoff distances so nuclear power plants are not endangered by this type of accident, it is necessary to estimate their potential blast effects realistically and with confidence.

This can be accomplished in an efficient manner if the concept of TNT equivalency can be shown to be relevant and a proper methodology developed. It is the objective of the present study to examine the nature of accidental vapor cloud explosions, develop a properly defined concept of TNT equivalency, calibrate it from the available controlled test data, and evaluate its significance against accidental blast damage data.

1.1 Background

Vapor cloud explosions are violent deflagrations or detonations that release their energy of chemical reaction to the surroundings in a manner that generates substantial overpressure and causes blast damage. This type of explosion involves incredibly complex phenomena ranging from the chemical kinetics of the energy release and turbulent flame propagation to the air mixing dynamics of two-phase flows and atmospheric dispersion.

The accident environment ensures that a very large number of variables will be involved such that, if it were desired to experimentally test accident scenarios to develop an adequate statistical base, the number of experiments required would be impossibly large. Thus, the very existence of accidental vapor cloud explosions represents their significance as a major hazard.

The probability of a vapor cloud explosion on a transportation route near any particular site is, however, very small. Davenport (1) in a recently completed compilation of confirmed

vapor cloud explosions lists seven rail tank car and three tanker truck incidents in which significant overpressures were created. Documentation by the National Transportation Safety board exists for the last three tank car incidents occurring in 1972 and 1974.

Numerous other vapor cloud incidents have been documented for spills from pipelines, storage tanks, and, mostly, industrial process vessels or equipment. Vessel failure accounts for nearly two-thirds of transportation releases compared with only about one-third overall, the remainder being mostly piping, valve, or fittings failures. Davenport (1) lists 33 such confirmed explosions and 17 vapor cloud incidents in which overpressures were not created. Strehlow (2) lists 69 explosions out of 108 vapor cloud ignitions of combustible material.

Accident analysis of vapor phase blast effects has been pioneered by Brasie and Simpson, Burgess, Strehlow, Brinkley and others. In spite of their excellent work, however, there exist substantial inconsistencies and false impressions with regard to vapor cloud explosions. For example, Brasie and Simpson (3) used the overpressure-distance curve for a nuclear energy release as their reference damage relation. This inconsistency results in TNT equivalence values almost 100% larger than those corresponding to the TNT curve.

Thus, a rational basis for evaluating the damage potential of accidental vapor phase explosions must be established in order to apply the existing knowledge to a successful regulatory process. This basis must also provide a quantitative understanding of inherent limitations and margins of error.

1.2 Accident Conditions

The ultimate goal of the accident hazard evaluation is to estimate the probability of occurrence of a vapor cloud explosion having given blast effects at a given site. Thus,

$$\begin{aligned} P(\text{specific blast effects at specific site}) = \\ P(\text{specific blast effects/vapor cloud explosion} \\ \text{at specific site}) \\ \times P(\text{vapor cloud explosion at specific site}) \end{aligned}$$

The last probability is extremely low whereas the conditional probability relates to the nature of vapor cloud explosions and is of concern in the present study.

The probability of achieving specific blast effects is essentially one of determining the nature of the energy coupling to the mechanisms that produce these specific effects, both symmetric and asymmetric. The primary accident conditions controlling the explosive energy release and blast energy coupling are

- material involvement
- ignition-explosion process
- topographical and meteorological conditions

1.2.1 Material Involvement

Only the material released to the atmosphere prior to an explosion event can be potentially involved in the energy release. The spill rate depends on the tank conditions, material properties, ambient temperature, and rupture size. For a pressurized liquid, flash vaporization rates and the initial momentum of the spill can be readily estimated. Hardee and Lee (4)* show for a specific case that flash vaporization of liquid propane results in 30% of the total mass in a vapor phase after isentropic expansion; this is compared in Figure 1 with an experimental release having a final quality of 27% vapor phase.

Initial momentum releases for several pressurized liquids are shown in Figure 2. This momentum is released very rapidly, in about a quarter of a second for propane. It should be noted that liquid propane at 70°F generates an initial spill velocity of about 400 miles per hour. Applying continuity and momentum requirements to the expansion process gives the tank dump time in terms of the contents and rupture size.

$$t_d = \left(\frac{\phi}{P_{\text{tank}} - P_{\text{atm}}} \right) \frac{W}{A_r} \quad (1.1)$$

* Their calculations for cloud growth contain several apparent inconsistencies; therefore, only the information presented here is used from their report.

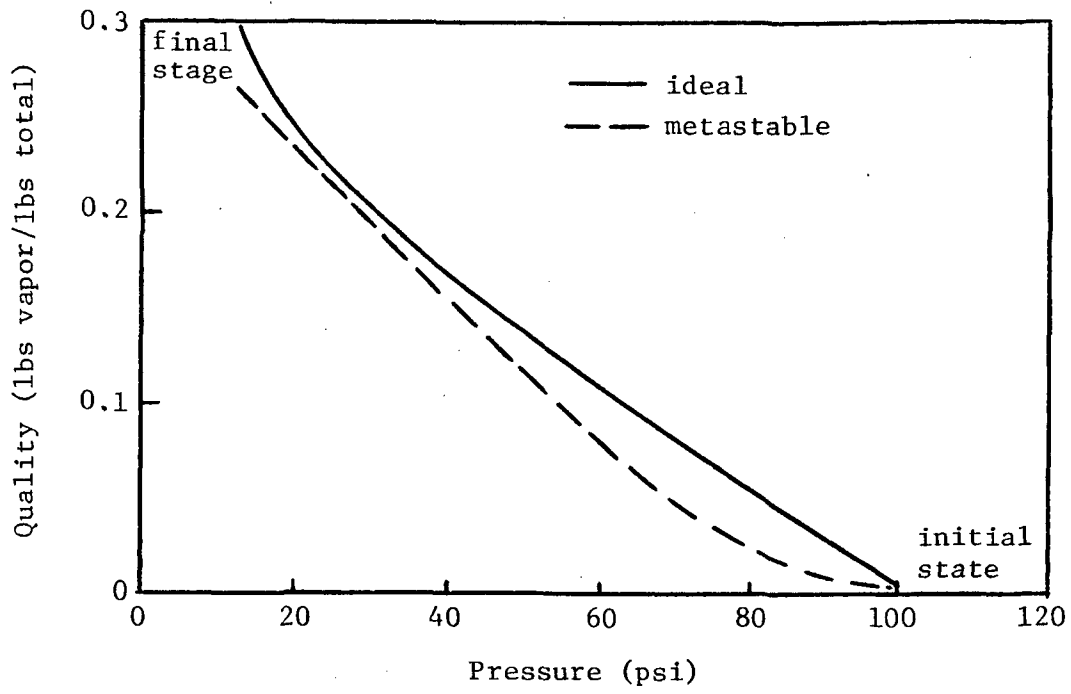


Figure 1 Pressure-quality curve for propane showing ideal and actual expansions (4)

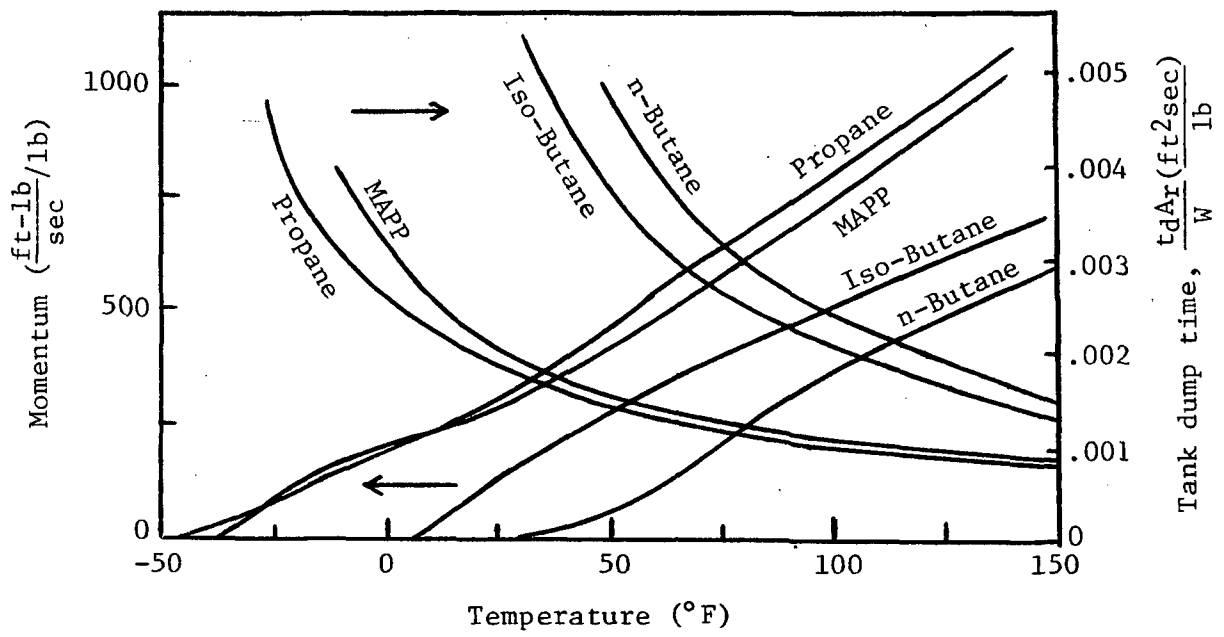


Figure 2 Momentum release per pound of fuel and tank dump time versus temperature (4)

where W = tank contents (lbs)
 P_{tank} = tank pressure (psi)
 ϕ = momentum release per pound of fuel (ft-lb/sec/lb)
 t_d = tank dump time (sec)
 A_r = rupture area (ft²)

Normalized tank dump times for several materials are given in Figure 2. As an example, assume a tank car cargo of 150,000 pounds (30,900 gallons) of liquid propane at relatively warm temperatures. The tank dump time as a function of rupture area is, from data in Figure 2, given as

$$t_d = 180/A_r \quad (1.2)$$

Thus, the contents would be completely released in 10 minutes for a 7½ inch diameter puncture hole, corresponding to a spill rate of 3090 gallons per minute, and in just 1 minute for a 23½ inch hole.* The release of pressurized propane can, therefore, be very rapid and about 25% to 30% of the spill appears almost immediately in the undiluted vapor phase. The remaining 70%-75% exists as a fine spray of liquid droplets.**

As this two-phase mixture is turbulently mixed with entrained air, liquid droplets are heated and vaporize.*** It requires the heat capacity of about 9 pounds of ambient air to vaporize 1 pound of liquid propane at its boiling point, -42°C. Thus, 1 pound of pressurized propane will give a vapor phase-air mixture of roughly 13% by weight, 9% by volume, propane at -42°C. This mixture is about one-third denser than surrounding ambient air at 68°F.

* Using the formula given by Brasie (5) for the combined weight flux of vapor and liquid yields a release rate for propane over twice the values computed from equation 1.2.

** This spray is apparently ignored by Junglaus (15) as contributing to the vapor cloud material involvement.

*** Not all of the liquid droplets will, of course, form vapor or spray; Kletz (6) suggests using an amount equal to the adiabatic flash, but this is a nonsupported estimate.

The major conclusions to be inferred are that, for hydrocarbon materials having a high vapor pressure and low boiling point and stored under pressure, the spill mechanism tends to

- promote rapid mixing of large portions of the available fuel,
- produce fuel-air mixtures in the vapor phase close to the upper explosive limit,
- generate a negatively buoyant vapor cloud due to the low temperature of the fuel-air mixture and the weight of the hydrocarbon molecules which strongly influences its subsequent convective dilution.

1.2.2 Ignition-Explosion Process

Ignition in an accident environment can be expected to occur near the cloud boundary by the first source encountered by gases within the flammability limits. The proximity of the ignition source, therefore, controls the size of the vapor cloud and influences the magnitude of the explosion.

Although accident and tank puncture mechanisms can be expected to produce ignition sources near the spill source, and immediate combustion has been observed in many accidents, the close-in rich mixture concentration, high flow velocity, and low temperature provide favorable conditions for vapor cloud growth. If no ignition source is found, the vapor will ultimately disperse harmlessly into the atmosphere. A study of rail tank car accidents (see Section 4.1) indicates that ignition is more likely to occur than no ignition.

Since the cloud seeks an ignition source as it expands, ignition is very site-specific with the probability of ignition-increasing and probability of continued material involvement decreasing as the cloud grows. It can also be expected to be significant with respect to asymmetrical blast effects, but results are not available to determine the relationship.

The blast effects of a vapor cloud explosion are highly dependent on the mode of combustion. Whereas Geiger (7) states

that the probability of the detonation mode occurring is very low, Davenport (1) lists twice as many vapor cloud ignitions creating significant overpressures as those that did not. Also, Strehlow's (2) data can be similarly interpreted. Thus, either detonation or overpressure producing deflagration appear to have the highest probability of occurrence. The quality of available accident data unfortunately does not allow us to establish the exact nature of the energy release and blast coupling mechanism.

The transition from slow combustion to rapid deflagration or detonation is a likely vapor cloud explosion scenario. It is interesting to note here the following description from the NTSB report (8) on the 1972 East St. Louis, Illinois incident.

"Flames were first observed at or near an unoccupied caboose standing on Track No. 19. The flames progressed westward toward Track No. 25 and eastward toward Track No. 15. An orange flame then spread upward, and a larger vapor cloud flared with explosive force. Estimate of the time lapse between these occurrences range from 2 to 30 seconds. Almost immediately thereafter a second, more severe explosion was reported".

This almost certainly describes just such a transition. A very elongated vapor cloud formed, since the spill source was moving, which most probably accounts for the apparent double explosion (it is easy to visualize a concentration discontinuity in this type of cloud geometry). If the two explosions occurred soon enough together, their blast waves would have coalesced!

A detonation wave represents a stable state of combustion characterized by a subsonic flame propagation relative to the precompressed unreacted gas equal to the detonation velocity relative to the ambient gas. A minimum amount of hydrodynamic energy must be available to support its propagation. Similarly, the propagation of any combustion wave requires hydrodynamic energy to support it, and this energy can only come from the ignition source or the chemical reaction.

Flame acceleration is readily observed in all detonable fuel-oxygen mixtures; however, Kogarko (9) using centrally ignited balloons reports no discernible flame accelerations in air mixtures of acetylene, propane, and methane. Therefore, it is important to consider what conditions in the accidental vapor cloud environment are capable of generating flame accelerations.

Lee (10) formulated a criterion for self-initiation which illustrates the relative ease with which mixtures can attain the autoignition limit corresponding to detonation. Taking the chemical energy release per unit mass as 2 to 1 for hydrocarbon-oxygen to hydrocarbon-air mixtures, the turbulent flame speed for self-initiation of the air mixtures is about 755 fps compared with 215 fps for the oxygen mixtures. Therefore, an amplification factor, the ratio of the critical turbulent flame speed to the characteristic laminar flame speed, is 460 for air mixtures and 6 for oxygen mixtures using typical laminar speeds of about 1.6 fps for fuel-air and 32.8 fps for fuel-oxygen. For acetylene and hydrogen-air mixtures, the amplification required is about 150.

Thus, not only are self-accelerating mechanisms present in fuel-oxygen mixtures as a result of their energy density, but the transition to detonation occurs with relative ease due to their low critical turbulent flame speed. Just the opposite is true for fuel-air mixtures, however, and very large flame accelerations must take place. It should be noted that even if transition to detonation does not take place, the very high flame speeds permissible in fuel-air mixtures greatly increase the rate of energy release and, therefore, the propensity to generate blast effects in the surroundings.

In the absence of a strong ignition source, the only mechanism for making hydrodynamic energy available for an accelerating flame propagation is through the boundary conditions. Boundary effects are extremely complex, involving wave interactions and turbulent flame structures, and only the gross effects of simple boundary geometries have been successfully investigated.

Several general observations can be made on the effectiveness of the boundary conditions in providing hydrodynamic energy to an accelerating deflagration wave. The compression wave interactions are strongly influenced by boundary geometry. Coalescence of these reflections with the deflagration accelerates it, producing stronger pressure pulses which are again reflected, and so on. As the deflagration accelerates it becomes turbulent, and as the intensity of the turbulence increases, larger amounts of hydrodynamic energy become available at the deflagration. In general, the rate of acceleration is slow at the lower velocities and extremely rapid just prior to detonation.

It is possible for some of the energy released by the early deflagration to be coupled to the blast wave by the following mechanism. As the detonation moves through the unreacted but energetic gas, its strength increases above the normal detonation level thereby recapturing and making available some of the early energy release.

In the accident environment complex boundary effects are provided by structures and the ground. Thus, not only are complex wave interactions and turbulent deflagrations likely, but local volumetric explosions induced by radiative or shock focusing are a distinct possibility. Locally confined combustion can induce a detonation wave in the cloud provided that a propagating detonation wave is established during the partial confinement.

1.2.3 Topographical and Meteorological Conditions

Site specific factors of terrain and atmospheric conditions have a variety of effects on a vapor cloud explosion. Thus, the universal observation is made that if a particular accident had occurred at a different place or different time, it could have been either much worse or not as bad.

In addition to the boundary effects on the combustion process, the local terrain influences the vapor cloud formation since the cloud is heavier than air and tends to hug the ground. In the

case of the 1970 Franklin County, Missouri (11) pipeline rupture, the propane vapor cloud flowed downhill into a shallow valley and slowly filled it. The valley in effect formed a huge container for the vapor cloud although ignition was delayed 24 minutes until a source 1500 ft from the rupture was reached.

Atmospheric conditions have a profound influence on both the nature of the vapor cloud explosion and the resulting blast effects. Unfortunately, quantitative evaluation of the phenomena involved is subject to extremely large error at the present time. Burgess, et al (12) points out three basic difficulties in applying simple air pollution type dispersion models:

- Measurements of statistical correlation coefficients are made at low concentrations and far from the source.
- Dispersion models relate average concentrations over extended time periods.
- Vapor clouds are heavier than air thereby suppressing the vertical dispersion.

Other more general difficulties are:

- Gaussian type diffusion models are essentially space-time averaged curve-fitting techniques that do not account for the relative importance of the mechanisms involved.
- The dispersion is strongly influenced by site-specific factors, especially for negative buoyant clouds.
- The source conditions are not simple, either a very intense flow at the spill or a complex volume source of large size after the spill momentum becomes small.
- Deterministic dispersion models are not far enough advanced at the present time.

As an example of these observations, Burgess and Zabetakis (13) estimated the flammable material involvement for the previously mentioned pipeline rupture using a standard dispersion model. In this case, a relatively low flow rate, continuous source spilled liquid propane under known atmospheric conditions (a temperature inversion was present). Their results indicate that the dispersion model is capable of predicting the TNT equivalent yield to within about half the value obtained from knowledge of the explosion damage-distance data.

However, they assumed that the blast energy of the material involved equals the detonation energy release. This is not the case as will be shown later, and a better value is about 20% of the materials's heat of combustion. Using the correct value of blast energy, the dispersion model would predict blast effects an order of magnitude less, i.e., at only about 10% of the TNT equivalent yield established by the damage data.

Several common characteristics of vapor cloud explosions must be remembered when applying notions of atmospheric dispersion. The entire process from rupture to ignition is relatively fast, on the order of minutes, for such large quantities of material. Initial mixing by air entrainment and convection is capable of producing only slightly rich mixtures under favorable circumstances. The vapor cloud is heavier than air and, therefore, has its own flow properties.

Atmospheric diffusion mixing rates tend to decrease as the concentration decreases. Dispersion of an already jet mixed vapor is required over at least one order of magnitude of dilution before a large part of the cloud is below the lower flammable limit. For a time then, atmospheric dispersion would tend to favor the growth of a large material involvement.

Meteorological conditions tend to produce strong directional effects resulting from the vapor cloud geometry which tends to be elongated in the wind direction. This type of asymmetry is peculiar to vapor cloud explosions and is of major importance since it is a space effect. It should be noted that most large accidental vapor cloud explosions are asymmetric.

A second type of asymmetry, common to all explosions, is reflection of blast energy to the ground by atmospheric conditions, most notably a temperature inversion. This effect produces localized caustics where the blast damage can be an order of magnitude higher than the spatial propagation of energy would give.

1.3 Approach

The approach of the present study is to conduct a technical review of the literature pertinent to vapor cloud explosions and including accident reports, experimental data, and theoretical models to establish criteria and a methodology for estimating TNT equivalency.

TNT equivalency is widely used to related specific blast effects of specific energy source types. For vapor cloud explosions, a generalized concept of TNT equivalency is implied since specificity is lacking. Partly because of this and partly because of a lack of information, considerable disagreement presently exists in the application of TNT equivalency to the estimation of potential blast damage resulting from accidental vapor cloud explosions.

It has been suggested by the U.S. Nuclear Regulatory Commission that a TNT mass equivalency of 10% be used to determine safe stand-off distances from nuclear plants. The West German Reactor Safety Commission guideline uses a 50% TNT mass equivalency for gases liquified under pressure, 100% for hydrocarbons with carbon-to-carbon triple bonds or cumulated carbon-to-carbon double bonds (e.g., acetylene), and 100% for nonliquified gases.

Estimates of TNT equivalency by various investigators in this field vary even more widely. The Bureau of Mines (3) suggests the energy release is 10% of the calorific energy content of the material released in 30 seconds. Bulkley and Jacobs (3) suggest an equivalency for hydrogen of 10 pounds of TNT per pound of hydrogen while Bradford (3) reports a deliberate hydrogen explosion of 0.3 pounds of TNT per pound of hydrogen. Strehlow (14) implies that a 10% TNT energy equivalency is a more probable upper limit for accidental explosions. Kletz (6) suggests a TNT energy equivalency of 1% by arguing that a 10% energy yield of a 10% material involvement is a realistic scenario. Geiger (7) gives an equivalency

of 4 pounds of TNT per pound of hydrocarbons as the explosive potential of hydrocarbon vapor clouds which is widely quoted in the West German literature as by, for example, Jungclaus (15).

Lee (16) recently completed a study in which he computed the blast energy necessary to produce the same airblast as observed experimentally for hydrocarbon-air detonations. He found that the blast energy is about 20% of the calorific energy which translates directly into TNT energy equivalency. In general then, estimates of TNT equivalency range from a fraction of a percent to the theoretical energy content of the material.

The approach taken herein is to establish TNT equivalency at the 1 psi blast overpressure level for accidental vapor cloud explosions near nuclear plants. Geiger (7) presents results of structural response calculations for the blast loading of a specific wall of a reactor building, shown in Figure 3. At the 1 psi level, the structure is sensitive to diffraction loading and insensitive to impulsive loading. Although no general conclusions can be drawn, this case is assumed here to be representative of nuclear plants, and, therefore, the customary practice of calculating TNT equivalency with respect to overpressure will be followed.

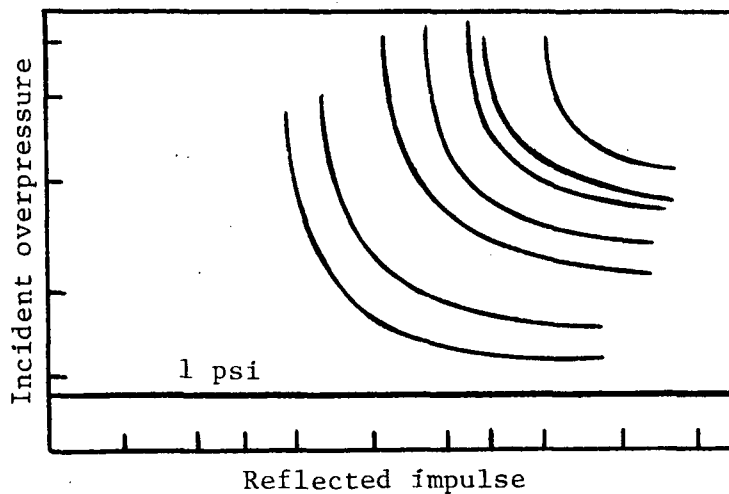


Figure 3 Loading response curves for a reactor building wall element as a function of peak overpressure and impulse (7)

2. CRITERIA AND METHODOLOGY OF TNT EQUIVALENCY

The generally accepted definition of TNT equivalency is that an arbitrary energy release is equivalent to a TNT explosion if the same specific blast effects are produced. This is not a universal concept but one that provides a parametric study of explosive effects in terms of known and well-understood, reproducible, and scalable explosions.

The converse of this statement, that is, predicting specific blast effects from knowledge of the TNT equivalency, depends upon the reproducibility and scalability of the explosion. Vapor cloud explosions are known to be among the least reproducible and scalable in accident and even controlled conditions. Therefore, a systematic exposition of the TNT equivalency of vapor cloud explosions must underlie its use in a safety and regulatory context.

2.1 Definition and General Criteria

TNT equivalency may be defined on either an energy or mass basis, the latter yielding an immediate and unambiguous physical interpretation. Energy equivalency is more basic in terms of the blast mechanisms involved thereby permitting a generalized formulation of the class of hydrocarbon-air vapor cloud explosions. Accordingly,

$$\alpha_e = \frac{e_{\text{TNT}} W_{\text{TNT}}}{e_{\text{HC}} W_{\text{HC}}} \quad (2.1)$$

where e_{TNT} and e_{HC} are the energies per unit mass of the explosives, W_{TNT} is the equivalent TNT weight, and W_{HC} is the weight of the actual or potential hydrocarbon material involvement. Mass equivalency is given by

$$\alpha_m = \frac{W_{\text{TNT}}}{W_{\text{HC}}} = \frac{e_{\text{HC}}}{e_{\text{TNT}}} \alpha_e \quad (2.2)$$

Equivalency is established by choosing the value of W_{TNT} on the basis of equal specific blast effects. In general, TNT equivalency can vary with distance, the type of blast effects used to establish equivalency, and among vapor cloud explosions depending on their reproducibility and scalability.

The interpretation of α_e depends on the values assigned to the specific energies. Thus, if e_{TNT} is the blast energy of TNT and e_{HC} the calorific energy content of the hydrocarbon fuel, α_e is a measure of the vapor cloud blast effectiveness for specific blast effects. If e_{HC} is defined as blast energy, then α_e provides a direct measure of the scalability of vapor cloud explosions.

It is reasonable to limit the type of blast effects to peak overpressure in calculating W_{TNT} , for the reason stated in Section 1.3, i.e., the loading response of typical targets at low overpressure. In addition, the uncertainty in using corresponding TNT impulse and dynamic effects is probably no greater than the uncertainty in calculating them for vapor cloud explosions. For certain types of deflagrations and at the higher overpressures such as the 3 psi level (used by the West Germans in determining safe standoff distances of nuclear plants), it may be necessary to include blast loading effects beyond the diffraction cutoff time.

In the present study, TNT blast effects are represented by the averaged peak overpressure-scaled distance data of Kingery, et al (17) for hemispherical surface bursts. These data are well-defined, extensive, and scale well with other results for condensed explosives such as the Keefer data presented in the Distant Plain report (18). Kingery does not provide corresponding energy data for his TNT, and, therefore, an exact physical interpretation of TNT equivalency is limited regardless of the choice of e_{TNT} .

Thus, the customary valuation of e_{TNT} as 1800 Btu per pound of TNT is adequate. Consistency is the only criterion which is satisfied if energy scaling of TNT blast effects is made with respect to this value. It should be noted that this value is the approximate blast energy of TNT which for condensed explosives is also nearly equal to the chemical energy release upon detonation (about 28% of the calorific energy content).

For a particular hydrocarbon-air explosion consistency in the choice of e_{HC} is also the major criterion. Obvious advantages in the estimation of TNT energy equivalencies result, however, if

hydrocarbon-air explosions can be treated as a class independent of the particular fuel through a suitable choice of e_{HC} for each fuel. Among the choices are the fuel's calorific heat of combustion, the energy release upon combustion, and the hydrodynamic energy of the explosion products.

Calculations of chemical energy releases and blast energies are exceedingly complex for air explosions and depend upon the fuel-air concentration. Combustion and subsequent products expansion occurs at temperatures, about 2500°F to 4500°F, to which dissociation processes are extremely sensitive. Furthermore, at these low energy densities, the coupling of the available hydrodynamic energy of the explosion products to the blast wave is complex. In general, making distinctions among different fuels on the basis of these calculations would be subject to error of the same order as the actual differences between the various fuels.

It is reasonable then to distinguish fuels on the basis of their calorific energy content alone. This implies calorific scaling of the energy partitioning of a vapor cloud explosion which can be expected to introduce insignificant error compared to the general scalability of these explosions. It has become customary practice to use the low or net value of the heat of combustion for this purpose since water vapor cannot condense at these temperatures; appropriate values are given in Table 1 for various combustible gases that have been involved in vapor cloud accidents.

2.2 Asymmetric Model

Spatially asymmetric blast effects are unique to and commonly observed in accidental vapor cloud explosions. Thus, the effective blast energy in one general direction from the explosion may be much greater than that in the opposite direction. It is presumed that this type of asymmetry is associated with the cloud geometry, location of the ignition source, and the nature of the explosive combustion.

TABLE 1. HEAT OF COMBUSTION OF COMBUSTIBLE GASES INVOLVED IN VAPOR CLOUD ACCIDENTS[†]

Material	Formula	Low Heat Value(Btu/lb) ^{††}	e _{HC} /e _{TNT}
Paraffins	(C _n H _{2n+2})	(18,857-21,502)	(10.48-11.95)
Methane	CH ₄	21,502	11.95
Ethane	C ₂ H ₆	20,416	11.34
Propane	C ₃ H ₈	19,929	11.07
n-Butane	C ₄ H ₁₀	19,665	10.93
Isobutane	C ₄ H ₁₀	19,614	10.90
Alkylbenzenes	(-)	(17,259-17,984)	(9.59-9.99)
Benzene	C ₆ H ₆	17,446	9.69
Alkylcyclohexanes	(C _n H _{2n})	(18,642-18,846)	(10.36-10.47)
Cyclohexane	C ₆ H ₁₂	18,846	10.47
Mono olefins	(C _n H _{2n})	(19,214-20,276)	(10.67-11.26)
Ethylene	C ₂ H ₄	20,276	11.26
Propylene	C ₃ H ₆	19,683	10.94
Isobutylene	C ₄ H ₈	19,367	10.76
Miscellaneous			
Hydrogen	H ₂	51,571	28.65
Ammonia	NH ₃	8,001	4.45
Ethylene Oxide	C ₂ H ₄ O	11,482	6.38
Vinyl Chloride	C ₂ H ₃ Cl	8,239	4.58
Ethyl Chloride	C ₂ H ₅ Cl	8,246	4.58
Chlorobenzene	C ₆ H ₅ Cl	11,754	6.53
Acrolein	C ₃ H ₄ O	11,830	6.57
Butadiene	C ₄ H ₆	20,200	11.22
HC Groups(est)	-	19,000	10.56

[†] Strehlow (2) and Davenport (1)

^{††} Chemical Engineers Handbook, 3rd edition, 1950; also Davenport (1)

A typical vapor cloud spatial blast pattern is shown in Figure 4 as an isodamage curve at the ground surface, represented by the peak overpressure, ΔP_s , equal to a constant. It is assumed that other isodamage curves would scale similarly. The equivalent TNT energy is found from the ΔP_s vs energy scaled distance, λ_e , curve for TNT at the given ΔP_s . Therefore, in terms of λ_e ,

$$\left. \begin{aligned} E_{TNT}^{(1)} &= (R_1/\lambda_e)^3 \\ E_{TNT}^{(2)} &= (R_2/\lambda_e)^3 \end{aligned} \right\} (2.3)$$

where R_1 and R_2 are the minimum and maximum isoblast radii, respectively. Letting $\beta = R_2/R_1$, the degree of asymmetry,

$$E_{TNT}^{(2)}/E_{TNT}^{(1)} = \beta^3 \quad (2.4)$$

These TNT equivalent energies are considered ideally to relate to separate hemispherical blasts. Assuming that the actual explosion is the net effect of the two blasts occurring in their respective half surface-spaces shown in Figure 5, then each contributes half of their hemispherical energies, and

$$E_{TNT} = \frac{1}{2}E_{TNT}^{(1)} + \frac{1}{2}E_{TNT}^{(2)} \quad (2.5)$$

Since $\alpha_e = E_{TNT}/E_{HC}$ for symmetric blast effects,

$$\alpha_e = \frac{1}{2}(\alpha_e^{(1)} + \alpha_e^{(2)}) \quad (2.6)$$

where the α_e 's are the TNT equivalencies for the respective equivalent symmetric blast.

The maximum and minimum asymmetric TNT equivalencies and nominal symmetric TNT equivalency are related, in terms of the degree of asymmetry, by

$$\left. \begin{aligned} \alpha &= \frac{1}{2}(1+\beta^3)\alpha_{\min} \\ \alpha &= \frac{1}{2}(1+\beta^{-3})\alpha_{\max} \end{aligned} \right\} (2.7)$$

where α is either mass or energy TNT equivalency. Alternatively,

$$\alpha_{\max}/\alpha_{\min} = \beta^3 \quad (2.8)$$

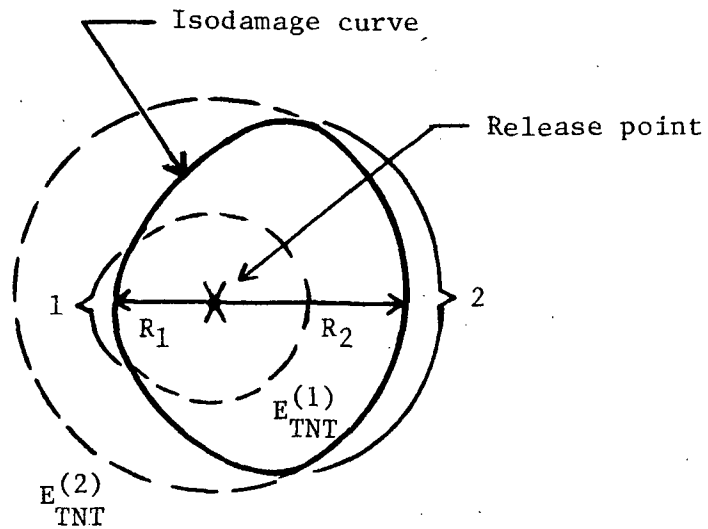


Figure 4 Asymmetric isodamage ($\Delta P_s = \text{constant}$) curve

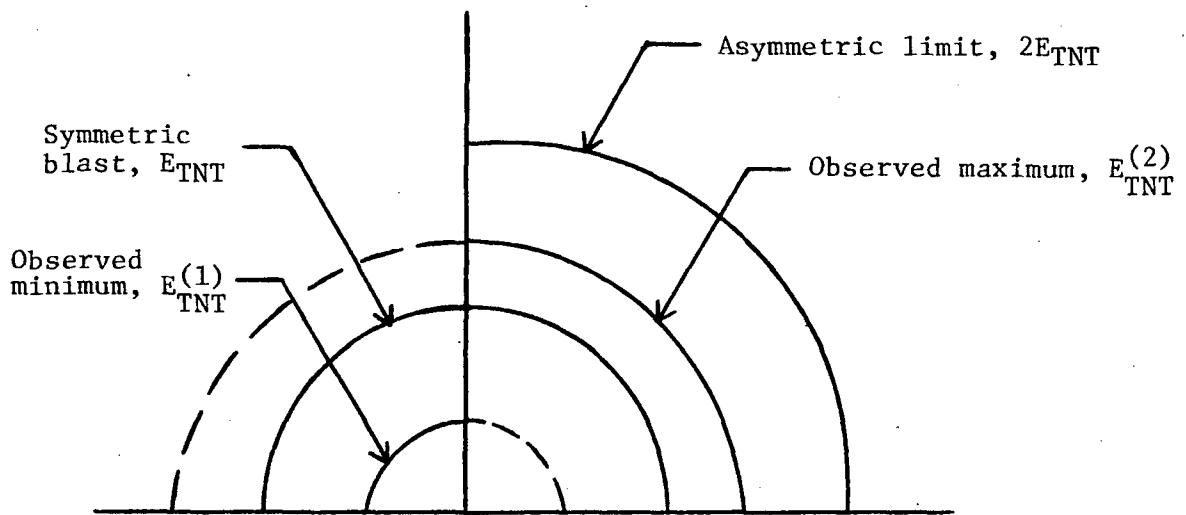


Figure 5 Half surface-space blast asymmetry model

3. TNT EQUIVALENCY OF CONTROLLED VAPOR PHASE EXPLOSIONS

The blast effects of controlled vapor phase explosions depend upon the total energy release, rate of release, and energy density. From theoretical analyses of ideal blasts, e.g., point source, uniform pressure, self-similar detonation, and piston-type deflagration, among others, the influence of varied energy source conditions on the blast wave can be computed.

A limited data base exists for these explosions but can be used to establish ideal TNT equivalencies of hydrocarbon-air mixtures. The experiments consist of centrally ignited balloons of various geometries having diameters from 1.5 to 62.5 feet.

3.1 Detonation Experiments

Blast data are obtained for tangent sphere, elevated sphere, and hemispherical source geometries. In order to ascertain the TNT equivalencies of these explosions, it is necessary to properly scale the data with respect to energy.

Kogarko, Adushkin, and Lyarmin (9) conducted tangent sphere experiments and found that the overpressure-distance data of various stoichiometric mixtures fall into a fuel-oxygen or fuel-air class of blast effects when scaled by the low value of their heats of combustion. They empirically represent this result by the following equations:

$$\left. \begin{aligned} \Delta P_s &= A/\lambda + B/\lambda^2 + C/\lambda^3, \quad \lambda = R/E^{1/3} > \lambda_h \\ \Delta P_s &= D/\lambda^{1.7}, \quad \lambda_o < \lambda < \lambda_h \end{aligned} \right\} (3.1)$$

where ΔP_s is in psi and λ in ft/Btu^{1/3}; the constants are given in the table below:

Constant	Fuel-Air	Fuel-Oxygen
A	1.7685	1.9748
B	0.8552	1.0384
C	0.3165	0.4431
D	2.5527	3.3381
λ_o	0.166	0.104
λ_h	0.62	0.62

Measurements made within five balloon radii were at elevated locations and thereby represent free air or spherical blast effects with no surface reflections; at larger distances, surface measurements were made and therefore represent hemispherical effects.

Solving Equations 3.1 at $\Delta P_s = 1.0$ psi gives $\lambda(\text{air}) = 2.21 \text{ ft/Btu}^{1/3}$ and $\lambda(\text{oxygen}) = 2.46 \text{ ft/Btu}^{1/3}$. Thus, fuel-air detonations are represented as 27.5% less efficient in generating low overpressure blast effects than fuel-oxygen detonations.

Balcerzak, Johnson, and Kurz (18) detonated 10 ft and 13.5 ft diameter tangent spheres and a 32 ft diameter sphere at a 25 ft height-of-burst. The experimental and scaled results of these blasts are summarized in Table 2. It should be noted that the overpressures are calculated from time-of-arrival data and, therefore, subject to basic errors of this procedure.

A 125 ft diameter hemisphere containing a 3.5 to 1 oxygen to propane mole ratio was detonated as part of Operation Distant Plain. Reisler's (19) results for this event are summarized in Table 3. Since the mole ratio was not stoichiometric, it is necessary to determine the proper calorific energy scaling. If the chemical reaction goes to completion, then the energy content is represented by simple stoichiometry calculations. However, rich mixtures can yield a larger chemical energy release than stoichiometric mixtures as shown by hydrodynamic detonation calculations including the effects of dissociation. Thus, the calorific energy as used here is the value associated with the total fuel mass to compensate for these effects (the same approach is used for the Balcerzak, et al data). A more detailed analysis of the effect of stoichiometry on energy scaling is provided in Section 3.3.

TABLE 2. SPHERICAL DETONATIONS OF METHANE-OXYGEN (18)

Gas mixtures: 1.5:1 and 2.0:1 O₂-CH₄ mole ratios
 Ambient pressure: 13.4 psi
 Experimental configurations:

Test	Diam(ft)	H.O.B. (ft)	Mole ratio	Est. mass of CH ₄ (lb)	Sach's scale factor(Btu ^{-1/3})
A	10	tangent	1.5:1	8.0	1.746(10 ⁻²)
B	10	tangent	2.0:1	6.6	1.856(10 ⁻²)
C	13.5	tangent	1.5:1	19.6	1.293(10 ⁻²)
D	32	25	1.5:1	260.9	5.456(10 ⁻³)

	ΔP _s (psi)	R(ft)	λ _e [*]		ΔP _s (psi)	R(ft)	λ _e [*]
A	76.1	9	0.157	C	86.9	12	0.155
	57.1	12	0.210		55.4	16	0.207
	35.9	16	0.279		37.6	20	0.259
	23.5	20	0.349		20.0	28	0.362
	12.2	28	0.489		12.5	36	0.465
	7.2	36	0.629				
B	62.3	12	0.223	D	59.0	40.3	0.220
	34.0	16	0.297		48.9	45.0	0.246
	22.0	20	0.371		40.0	50.4	0.275
	12.2	23	0.520		34.0	55.2	0.301
	8.6	36	0.668		29.3	60.0	0.327
					21.4	70.4	0.384
			11.4	100.0	0.546		
			3.4	201.1	1.097		

* λ_e - (ft/Btu^{1/3})

TABLE 3. HEMISPHERICAL DETONATION OF PROPANE-OXYGEN (19)

Gas mixture: 3.5:1 O₂-C₃H₈ mole ratio
 Ambient pressure: 13.71 psi
 Balloon: 125 ft diameter hemisphere
 Est. mass of C₃H₈: 12,000 lb
 Sach's scale factor: 1.56(10⁻³) Btu-1/3

ΔP_s (psi)	R(ft)	λ_e (ft/Btu ^{1/3})
178	71	0.111
47	116	0.181
35	156	0.243
36	156.3 (10)*	0.244
35	160.8 (30)	0.251
22	201	0.314
23.2	202.2 (22)	0.315
22.5	213.4 (52)	0.333
16.5	250	0.390
15.6	250	0.390
11.7	295	0.460
7.2	382	0.596
4.0	564	0.880
3.1	678	1.058
1.8	998	1.557
0.36	4190	6.536

* Instrument elevation (ft)

The data of Woolfolk and Ablow (20) for spherical detonations of hydrogen-oxygen-nitrogen balloons is summarized in Table 4. Two balloon diameters, 3.0 ft and 5.25 ft, were used for 0%, 10% and 20% nitrogen dilutions; the effect of these dilution levels on detonation overpressures is small.

Figure 6 is the overpressure-energy scaled distance plot of this experimental data. Also shown is the energy scaled TNT data of Kingery for $e_{\text{TNT}}=1800$ Btu/pound of TNT. Superimposed on the fuel-oxygen data are the hemispherical and corresponding spherical TNT curves translated to fit the Kogarko fuel-oxygen curve at the lower overpressures. Two important results are immediately seen from this figure. The first is that the only fuel-air data are that of Kogarko, and the second being the excellent general agreement of the fuel-oxygen vapor phase data with the translated TNT data.

With respect to the latter result, the following observations are made: (1) at the lower overpressures, below about 10 psi, the spherical and hemispherical vapor phase and condensed phase explosions produce the same shock decay consistent with the point made by Brinkley (21) and others that the details of the source conditions become unimportant at large distances; (2) the tangent sphere data lie between the two limiting cases at the higher overpressures and approach the hemisphere case as distance increases (except for the elevated sphere where the Mach stem region is seen); and (3) close-in, the data do not follow the TNT decay shape; in this region source conditions are important and scaling by total energy is not valid except as a parametric reference of blast effects.

3.2 Empirical Calculation of TNT Equivalency

The TNT energy equivalency of vapor phase explosions can be computed from the experimental data. Note that the only hydrocarbon-air data are that of Kogarko, et al for small balloons. Although α_e is approximately constant with distance at the low overpressures,

TABLE 4. SPHERICAL DETONATIONS OF HYDROGEN-OXYGEN-NITROGEN (20)

Gas mixtures: stoichiometric H₂-O₂ with 0%, 10%, 20% N₂ dilutions
 Ambient pressure: 14.37 psi
 Experimental configurations:

Shot	Radius(ft)	N ₂ (%)	ΔH_{LC} (Btu/lb mixture)	Sach's scale factor(Btu ^{-1/3})
26	1.493	0	5775	0.0732
27	1.483	10	4568	0.0761
31	1.503	20	3659	0.0789
36	2.625	0	5781	0.0401
35	2.592	10	4593	0.0415

ΔP_s (psi)	R(ft)	λ_e^*	ΔP_s (psi)	R(ft)	λ_e^*
26	-	4.63	36	20.5	7.19
	5.9	9.19		15.4	8.92
	6.3	9.29		10.1	11.75
	2.0	15.72		2.1	26.67
	0.94	26.94		1.7	29.66
	0.81	29.86		1.2	35.53
27	19.1	4.63	35	21.5	7.19
	6.0	9.19		16.9	8.92
	6.0	9.29		11.6	11.75
	1.9	15.72		2.2	26.67
	0.96	26.94		2.0	29.66
	0.82	29.86		1.2	35.53
31	20.8	4.63			
	5.9	9.19			
	5.9	9.29			
	2.0	15.72			
	0.99	26.94			
	0.75	29.86			

* $\lambda_e - (\text{ft/Btu}^{1/3})$

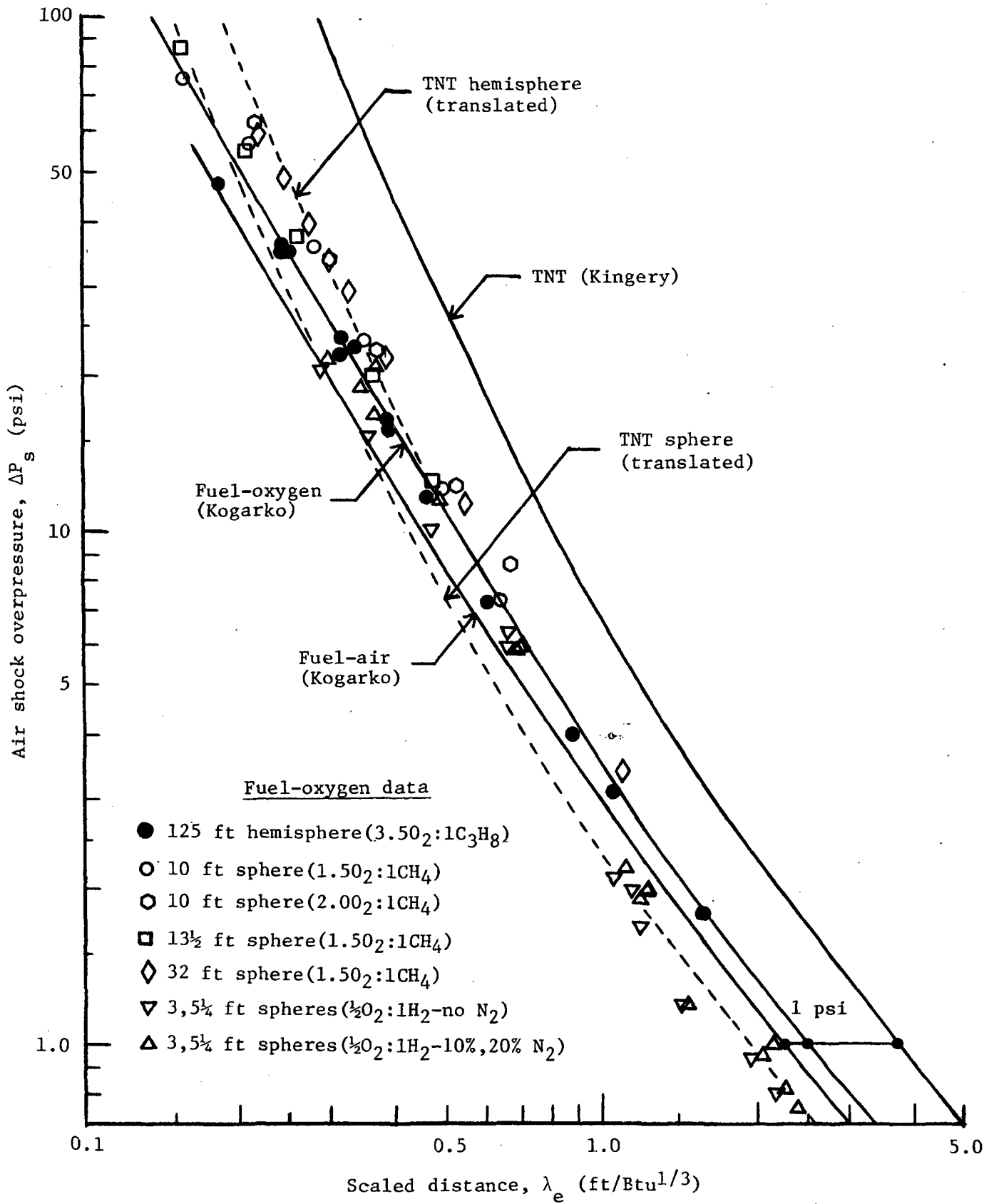


Figure 6 Peak overpressure-energy scaled distance for vapor phase and TNT detonations

the computation will be made specifically at the 1 psi peak over-pressure level. Thus, at $\Delta P_s = 1.0$ psi,

$$\begin{aligned}\lambda_e(\text{fuel-oxygen}) &= 2.46 \text{ ft/Btu}^{1/3} \text{ (Kogarko)} \\ \lambda_e(\text{fuel-air}) &= 2.21 \text{ ft/Btu}^{1/3} \text{ (Kogarko)} \\ \lambda_e(\text{TNT}) &= 3.74 \text{ ft/Btu}^{1/3} \text{ (Kingery)}\end{aligned}$$

From Equation 2.1 and the definition of λ_e ,

$$\alpha_e = (\lambda_{\text{HC}}/\lambda_{\text{TNT}})^3 \quad (3.2)$$

and, therefore,

$$\begin{aligned}\alpha_e(\text{fuel-oxygen}) &= 28.5\% \\ \alpha_e(\text{fuel-air}) &= 20.6\%\end{aligned} \quad (3.3)$$

These results are consistent with the previously defined criteria of TNT equivalency and, in particular, the use of the low value of the heat of combustion since Kogarko's data is based on this.

Applying this result to Equation 2.2 yields the TNT mass equivalency for hydrocarbon-air vapor phase explosions,

$$\alpha_m(\text{fuel-air}) = 0.206 \frac{e_{\text{HC}}}{e_{\text{TNT}}} \quad (3.4)$$

and a value representative of methane and propane is

$$\bar{\alpha}_m = 2.4 \text{ (240\%)}$$

In general,

$$\alpha_m = 1.144(10^{-4})\Delta H_{\text{LC}} \quad (3.5)$$

where ΔH_{LC} is the low calorific heat in Btu per pound of fuel from Table 1. Some valuations of interest are given:

Material	TNT mass equivalency (%)
Methane	246
Propane	228
Propylene	225
Isobutane	224
Ethylene	232
Butadiene	231

As an example, 1 pound of propane is equivalent to 2.28 pounds of TNT for the same low overpressure symmetric blast effects. Using the 1972 East St. Louis, Illinois rail tank car accident as an example of asymmetric effects, $\beta = 2.25$, and for a detonative average equivalency of 228%, the maximum and minimum mass equivalencies would be

$$\alpha_{\min} = 0.37 \text{ lb TNT/lb C}_3\text{H}_8$$

$$\alpha_{\max} = 4.19 \text{ lb TNT/lb C}_3\text{H}_8$$

A degree of asymmetry of $\beta = 1.5$ would give

$$\alpha_{\min} = 1.04 \text{ lb TNT/lb C}_3\text{H}_8$$

$$\alpha_{\max} = 3.52 \text{ lb TNT/lb C}_3\text{H}_8$$

Thus, the maximum TNT equivalency is quite sensitive to asymmetric detonations of vapor phase mixtures.

The general applicability of overpressure TNT equivalency to waveform effects can be seen from the overpressure impulse data of Kogarko and Kingery, shown in Figure 7. Taking $\lambda_e = 2.5 \text{ ft/Btu}^{1/3}$ as typical of the 1 psi overpressure region, the corresponding vapor phase impulses can be scaled to their TNT equivalents from

$$\left. \begin{aligned} \lambda_{\text{TNT}} &= \lambda / \alpha_e^{1/3} \\ I^\circ_{\text{TNT}} &= I^\circ / \alpha_e^{1/3} \end{aligned} \right\} (3.6)$$

where α_e and I° are 0.206 and 0.079 psi-msec/Btu^{1/3} for air and 0.285 and 0.079 psi-msec/Btu^{1/3} for oxygen. The resulting general agreement is apparent from Figure 7.

3.3 General Considerations of Vapor Phase Detonations

Limited theoretical considerations of vapor phase detonations are of interest to put the empirical information of the preceding sections in a better perspective. In particular, the partitioning of energy, the effect of mixture composition, and the very important effects of source energy density and deposition rate will be discussed.

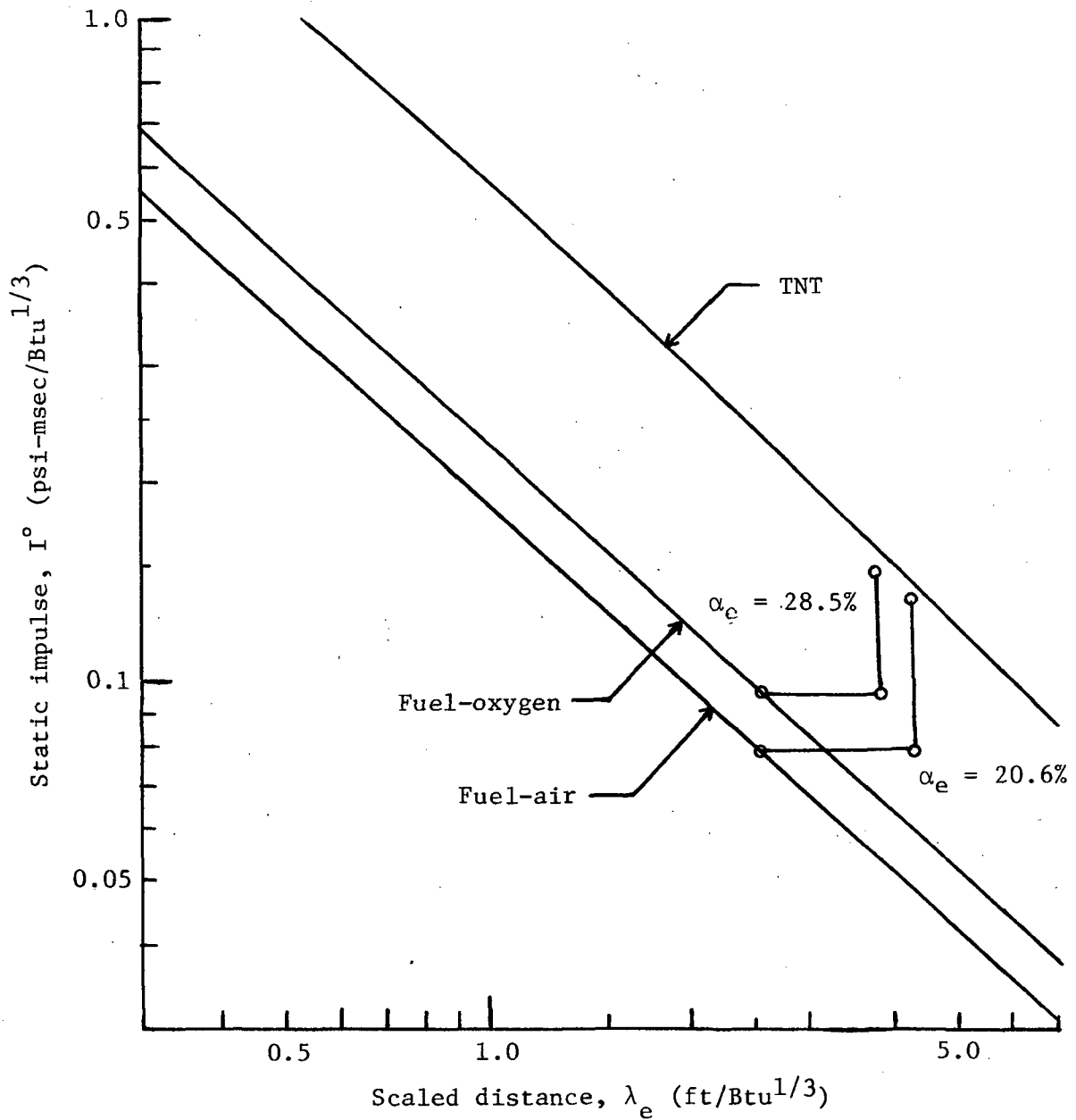


Figure 7 Energy scaled static impulse-distance for Kogarko vapor phase and TNT detonations

The calorific energy content of a fuel is released only if the reaction goes to completion, i.e., water vapor and carbon dioxide as the final combustion products. At the reaction temperatures of detonation, the chemical kinetics of dissociation must be included in the hydrodynamic theory. The actual energy release will, therefore, be some fraction of the calorific value depending principally on the carbon monoxide formed (the heat of formation of CO is 28% of that for CO₂).

The available hydrodynamic energy per unit mass of mixture can be computed as

$$E_H = W + E_{KE} - E_D \quad (3.7)$$

where

$$\left. \begin{aligned} W &= \int_{v_{cj}}^{v_f} P dv = \text{expansion energy} \\ E_{KE} &= \frac{1}{2} u_{cj}^2 = \text{kinetic energy} \\ E_D &= \frac{1}{2} (P_{cj} + P_o) (v_o - v_{cj}) = \text{detonation compression energy} \end{aligned} \right\} (3.8)$$

and the subscript cj indicates the Chapman-Jouget detonation conditions. This formulation is useful because it does not depend on empirical data such as final cloud size and can be readily computed since the detonation state does not vary as it propagates. Assuming perfect gas behavior of the explosion products and an isentropic expansion,

$$P = P_{cj} (v_{cj}/v)^{\bar{\gamma}} \quad (3.9)$$

and, therefore,

$$W = \frac{P_{cj} v_{cj}}{\bar{\gamma} - 1} \left[1 - \left(\frac{P_o}{P_{cj}} \right)^{(\bar{\gamma} - 1)/\bar{\gamma}} \right] \quad (3.10)$$

Using the theoretical results of Johnson (18) for the detonation of various mixtures of methane and oxygen and a value of $\bar{\gamma} = 1.24$, the following results are obtained as a function of the oxygen to methane concentration ratio, ξ (all energies are written as Btu per pound of gas mixtures):

ξ	ΔH_{LC}	Released Energy	E_H	$\frac{E_H}{\Delta H_{LC}}$ (%)
1.0	3593	2466	1497	41.7
1.2	3805	2848	1578	41.5
1.5	4043	2790	1500	37.1
2.0	4313	2556	1323	30.7
2.5	3594	2350	1189	33.1
3.0	3081	2180	1084	35.2

Figure 8 is a plot of these data. Computing λ_e at $\Delta P_s = 1.8$ psi for the Distant Plain results in Table 3 in terms of the calorific energy yields $\alpha_e = 41.8\%$. Interpreting the ratio $E_H/\Delta H_{LC}$ as the effective blast energy, and similarly interpreting α_e , excellent general agreement is obtained. (It should be remembered that α_e is for propane-oxygen.)

Thus, for stoichiometric fuel-oxygen vapor phase mixtures, about 60% of the fuel's calorific energy content is released and about 50% of that is available as blast energy. About half of the released energy remains in the products as residual heat. From the theoretical values of detonation pressure and propagation velocity computed by Kogarko, et al, values of $E_H/\Delta H_{LC}$ equal to 28.6% for methane-oxygen and 29.3% for propane-oxygen are obtained.

Similar calculations for air mixtures of methane, propane, and acetylene can be made from Kogarko's values at the C-J state. The resulting values of $E_H/\Delta H_{LC}$ are about 50% for hydrocarbon-air mixtures, considerably higher than for oxygen mixtures. This is not surprising since more chemical energy will be released at the lower detonation temperatures. Using

$$\eta_{th} = 1 - \left(\frac{P_o}{P_{cj}} \right)^{(\bar{\gamma}-1)/\bar{\gamma}} \quad (3.11)$$

as an approximate measure of thermal efficiency, then

$$\eta_{th} = \begin{cases} 48.5\% \text{ for } CH_4-O_2 \\ 42.2\% \text{ for } CH_4\text{-air} \end{cases}$$

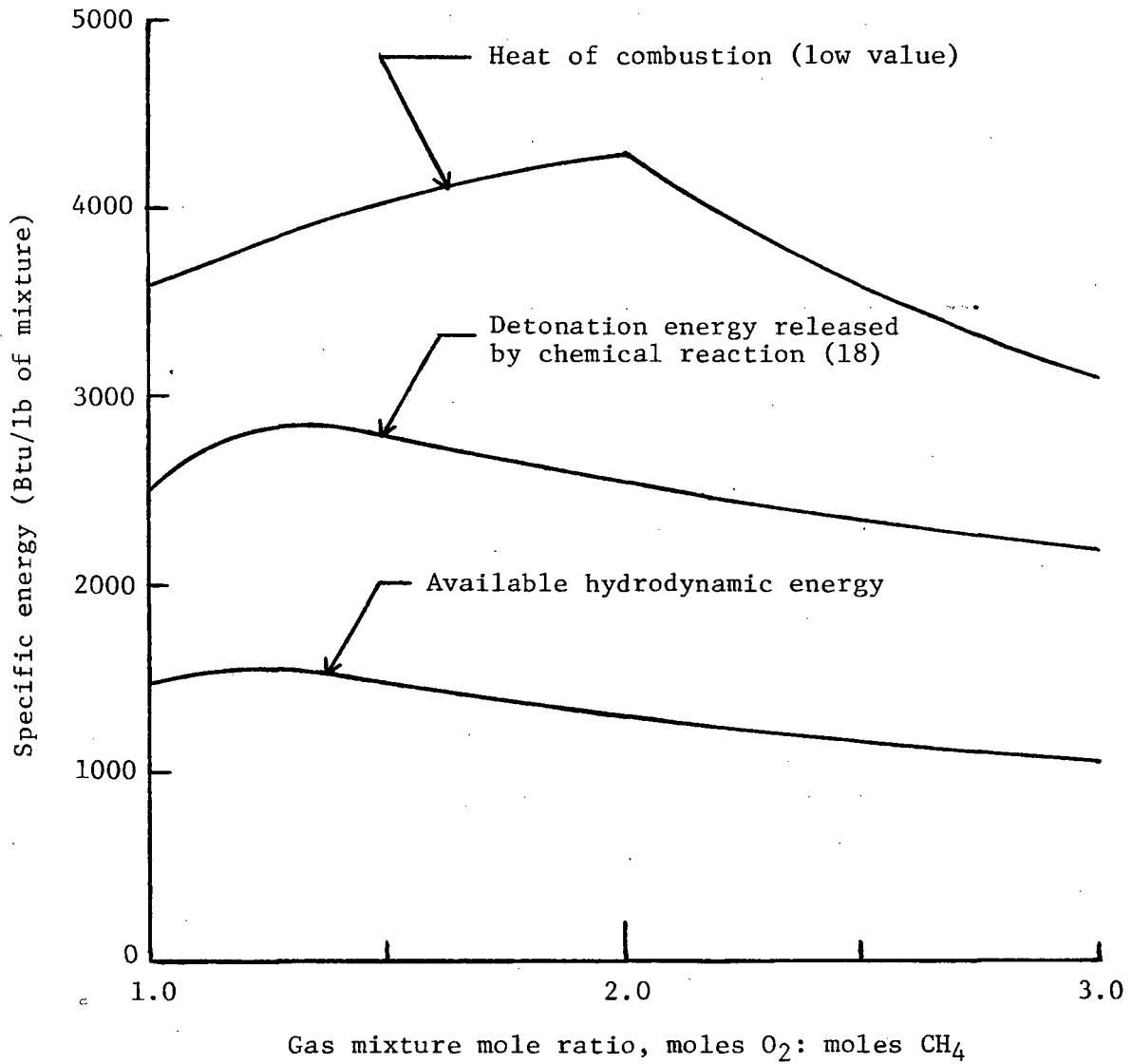


Figure 8 Theoretical energy partitioning of fuel-oxygen explosions (methane)

Thus, consistent with the second law of thermodynamics, fuel-air detonations make available a smaller proportion of their total energy release as hydrodynamic energy, about 13% less, than fuel-oxygen detonations. Evaluating E_H from equations 3.7 to 3.10 and using the values of η_{th} given above, approximate values of the chemical energy released upon detonation can be computed.

$$(\text{energy released}) = \begin{cases} 63.3\% \text{ for } \text{CH}_4\text{-O}_2 \\ 87.4\% \text{ for } \text{CH}_4\text{-air} \end{cases}$$

Therefore, fuel-air detonations release about 38% more chemical energy than fuel-oxygen detonations, consistent with the chemical kinetics of detonation combustion.

What is surprising is that less than half of the theoretically available hydrodynamic energy appears as energy driving the air shock based on the empirical calculations of α_e . Kogarko, et al relate the blast inefficiency of fuel-air compared to fuel-oxygen detonations to their three to four difference in energy density. Since, however, the energy deposition rate does not scale directly with energy, it is possible that cloud size may be a factor through the detonation velocity or some other mechanism.

It should be mentioned that Lee (16) has computed the effective blast energy as about 20% for fuel-air and 25% for fuel-oxygen detonations. But his approach was to simply fit the Kogarko data to the airblast calculation theory of Brinkley (21) by varying the initial condition on the blast energy. Thus, this agreement sheds no additional light on the efficiency of fuel-air explosions.

As mentioned in Sections 2.1 and 3.1, it is difficult to assign an explosion scaling quantity on an a priori basis, especially for estimating accident conditions. In principal, a measure of blast energy relative to specific blast effects would seem to be the more universal concept of a scale factor.

This energy concept can be approximated by the available hydrodynamic energy for the purpose of computing relative effects of known explosions. Thus, it is possible to directly compare the hemispherical detonations of the propane-rich oxygen mixtures used

in Distant Plain with the stoichiometric TNT equivalency of accidental explosions and, in particular, with the stoichiometric data of Kogarko, et al.

Since the stoichiometries of the gas mixtures are known, and theoretical Chapman-Jouget detonation states including dissociation have been computed by Johnson (33), Equations 3.7 to 3.10 can be evaluated for the actual gas mixture (A) and a stoichiometric gas mixture at the same ambient conditions (B). Using the hemisphere test data for Event 2a, a 125 ft diameter balloon, and Shots 2 and 6, 17 ft diameter balloons, for which C-J data are available, the following results are obtained (for $\bar{\gamma}=1.24$):

Shot	Diam. (ft)	Mole Ratio	$\frac{P_{cj}^{(A)}}{P_o}$	$E_H^{(A)}$	$E_H^{(B)}$
2a	125	3.5	40.0	1409	1202
2	17	3.24	40.9	1418	1183
6	17	3.12	41.3	1450	1199

$E_H^{(A)}$ - Btu/lb of actual mixture

$E_H^{(B)}$ - Btu/lb of blast equivalent stoichiometric mixture

where $P_{cj}/P_o=34.5$ for a stoichiometric mixture. Thus, in order for a stoichiometric mixture to have the same blast effects as a test mixture, a quantity equal to the ratio of $E_H^{(B)}$ to $E_H^{(A)}$ would have to be detonated. These stoichiometric blast equivalencies are summarized below:

Shot	2a	2	6
Pounds of stoichiometric mixture to 1 pound of test mixture	1.172	1.2	1.21
Decrease in scale factor (%)	5.4	6.2	6.6

Table 5 contains the relevant experimental data of these shots scaled to the theoretical blast equivalent stoichiometric mixtures. The overpressure-equivalent scaled distance data are plotted in Figure 9 from Table 5 and Equation 3.1 for the Kogarko data where the constants have been adjusted to a mass basis through the cube root of 2400 kcal/kg of mixture. Excellent agreement of the data

TABLE 5. HEMISPHERICAL DETONATIONS OF PROPANE-OXYGEN (19,33)

Shot	Hemisphere diam(ft)	P _o (psi)	T _o (°R)	ρ _o (lb/ft ³)
Event 2a	125	13.71	534	0.08310
2	17	11.8	495	0.07753
6	17	11.8	525	0.07327

Shot	Moles O ₂ to moles C ₃ H ₈	Est. total mass(lb)	Sach's scale factor(lb ^{-1/3})
Event 2a	3.4	42,490.0	0.02656
2	3.24	99.7	0.18867
6	3.12	94.2	0.19166

ΔP _s (psi)	R(ft)	λ _m [*]	ΔP _s (psi)	R(ft)	λ _m [*]
2a 178	71	1.9	2 157	10	1.9
47	116	3.1	88.5	14	2.64
35	156	4.14	55	18	3.4
36	156.3	4.15	36.8	22	4.15
35	160.8	4.3	23.1	28	5.3
22	201	5.34	13.2	38	7.2
23.2	202.2	5.4	7.7	52	9.8
22.5	213.4	5.7	4.5	73	13.8
16.5	250	6.64	2.9	100	18.9
15.6	250	6.64	1.75	145	27.4
11.7	295	7.8	6 121.4	10	1.9
7.2	382	10.15	74.3	14	2.7
4.0	564	15.0	47.9	18	3.45
3.1	678	18.0	20.5	28	5.4
1.8	998	26.5	11.5	38	7.3
0.36	4190	111.3	7.9	52	10.0
			4.53	73	14.0
			2.74	100	19.2
			1.5	145	27.8

* λ_m - distance scaled by mass of blast equivalent stoichiometric mixture, (ft/lb^{1/3})

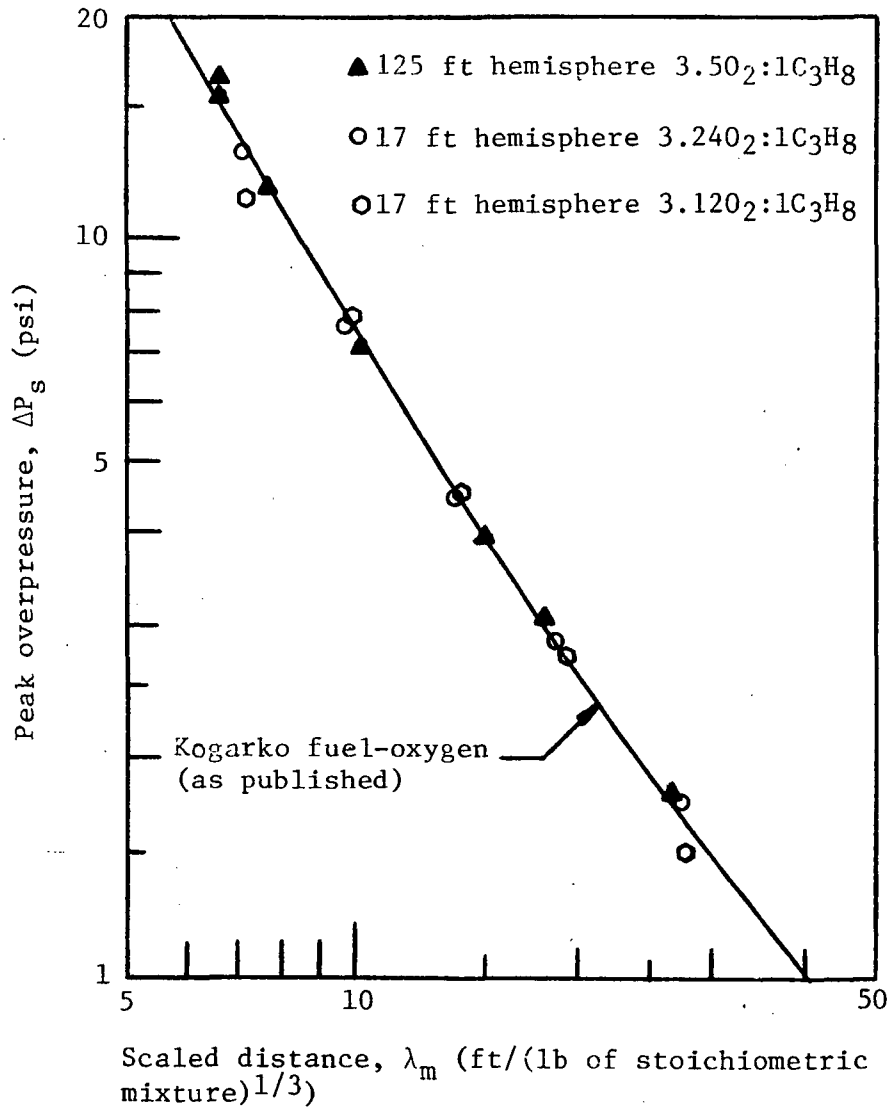


Figure 9 Overpressure-distance of fuel-oxygen hemisphere detonations scaled by mass of blast equivalent stoichiometric mixture

is obtained thereby substantiating the choice of the Kogarko curve in Section 3.2 to establish the TNT equivalency of hemispherical detonations.

3.4 Deflagration Explosions

As pointed out in the introduction, a vapor cloud explosion resulting from sufficiently rapid deflagration is a likely accident scenario. The TNT equivalency of a general vapor cloud explosion would be expected to vary with the mode of energy release, distance, and specific blast effects. Before considering actual accident data, it is the purpose of this section to examine the more general applicability and order of magnitude of TNT equivalency just developed.

Experimental data of Kogarko, et al (9) and Woolfolk and Ablow (20) exist for combustion initiation of fuel-oxygen mixtures. These data have been energy scaled and plotted in Figure 10 along with the detonation curve of Kogarko. The Woolfolk data are for stoichiometric mixtures of hydrogen and oxygen with 0%, 10%, and 20% nitrogen dilutions and two balloon sizes, 3.0 ft and 5.25 ft diameters. Noting that the spatial flame speeds are observed to be proportional to a power of time, the kinematics of the combustion can be computed and are presented in Figure 11.

These figures clearly show the pronounced effects of balloon size, spatial flame speed, and nitrogen dilution on the deflagration process. Taking volumetric expansion of the burning gases into account, the relative burning velocities are of the order of the critical turbulent flame speeds of Lee (10). In fact, the transition to detonation might have occurred for the large balloon of pure hydrogen and oxygen, rather than a crossover of deflagration-detonation blast strength as reported by the authors. With either interpretation, it appears that the energy deposition rates control the airblast which is very sensitive to the magnitude of the flame speed.

The major result of interest is that as the nitrogen concentration approaches that of air, the blast effects will depend on

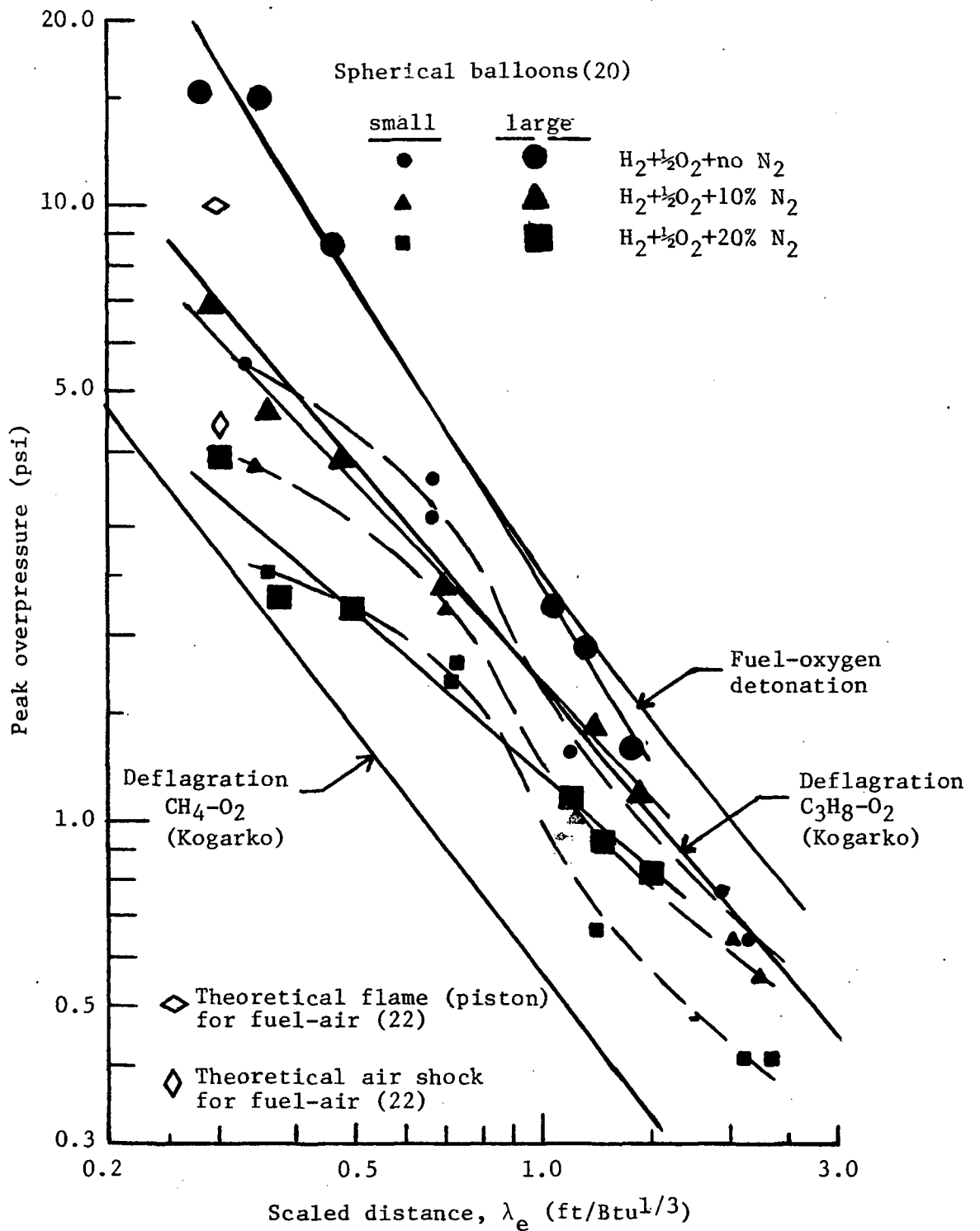


Figure 10 Spherical blast effects of deflagrations in fuel-oxygen mixtures

$R=Ct^m$		
$H_2+\frac{1}{2}O_2$	m	C
no N ₂	1.36	7.71
10% N ₂	1.43	5.62
20% N ₂	1.49	3.97

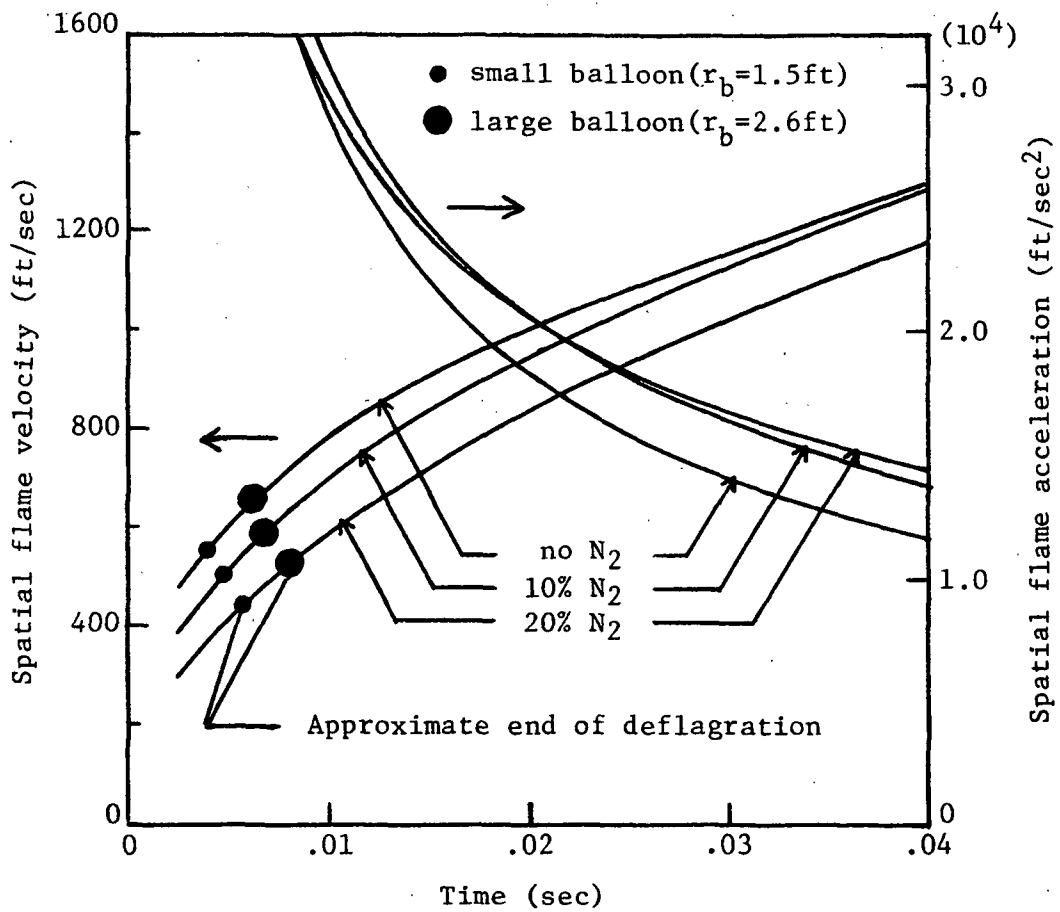


Figure 11 Deflagration kinematics for Woolfolk and Ablow combustion tests

the vapor cloud size provided acceleration mechanisms are present. As pointed out by Lee, the corresponding critical flame speeds will also increase due to the decreasing energy density.

Numerous theoretical models of deflagration have been constructed with a major emphasis on the piston representation of the flame. The significant results of this work show the strong dependence of blast on deposition rate. Lee (16) calculates that a minimum spatial flame speed of about 400 fps must be attained to produce a propagating shock front. A parametric study by Williams and presented in the Lind report (23) has recently yielded the significant result that there exists "a limiting shock strength which depends on the efficiency of the wave pattern in the noncombustible gas." For hemispherical deflagrations of methane in air, he suggests an upper limit of $P_s/P_o < 3$ for the shock intensity, i.e., maximum overpressures of 30 psi.

Calculations were made by Munday and Cave (22) for air deflagrations using an accelerating piston model which attains a constant speed of two-thirds the acoustic value, approximately the critical turbulent flame speed of Lee. Although results are not shown for the 1 psi overpressure level, about 16 cloud radii, computed overpressures at 2.25 cloud radii are about 10 psi at the flame and 4.5 psi at the shock (see Figure 10). Since the flame extinguishes at about the same time, it is not clear whether this represents the maximum shock pressure attainable.

Thus, the assumption that a detonation represents an upper limit to the general far field blast effects of a vapor cloud explosion is not unreasonable based on the available information. It should be noted that the actual material involvement will tend to be larger in a deflagration explosion.

3.5 Summary of Controlled Experimental Results

The analysis of controlled vapor phase explosion data contributes to the evaluation and calibration of potential vapor cloud blast effects. The principal results are:

1. Kogarko's published results (9) must be viewed as hemispherical in the far field, i.e., instrument readings, to be consistent with other hemispherical and spherical balloon tests. We note that many publications, e.g., West German papers, base TNT equivalency on sphericity of Kogarko's work and are, therefore, too high by a factor of two.
2. It appears that fuel-air mixtures yield a higher net fraction of available hydrodynamic energy than fuel-oxygen mixtures even though the corresponding airblast is less according to presently available experimental data.
3. Blast effects of rapid deflagrations are extremely sensitive to the spatial flame velocity; thus, cloud size can be expected to be a critical parameter of accidental vapor cloud explosions even if detonation is not achieved.
4. The mixture's stoichiometry significantly influences the production of hydrodynamic energy (for fuel-oxygen mixtures) and, therefore, possibly affects the flame acceleration mechanisms; it is also possible that, for a time, this effect of rich mixtures offsets a portion of the dispersed material losses.

4. TNT EQUIVALENCY OF ACCIDENTAL VAPOR CLOUD EXPLOSIONS

The nature of an accident inherently precludes its use in the development of a rigorous methodology of vapor cloud explosions. The objective of this section is, therefore, to determine if the criteria and methodology of TNT equivalency developed in this study are reasonable with respect to an accident environment.

After general considerations of the transportation accident history, a detailed analysis of five major vapor cloud explosions will be presented. Three of these are rail tank car incidents, and the other two, one industrial and one pipeline, are included because of their importance and identifiability with potential bulk transportation accidents.

4.1 History

Napadensky (24) lists a recent average of 8,234 train accidents per year. From Pierson (25), data collected by the Office of Hazardous Materials Operations, DOT indicate that about 4.5% of these involve hazardous materials of all types. According to Napadensky (26), over a period from 1964 to 1974 there were 117 train accidents involving fire and/or explosions, 43 having both, 65 fire only, and 9 explosions only.

During this same period there were 120 rail accidents involving tank cars. From these data an accident will involve one, two, or three tank cars 63% of the time with almost equal probability for each, four through nine tank cars 33% of the time and again with equal probability, and 10 or more cars less than 5% of the time. There have been accidents with fire involvement and secondary explosions of more than one tank car as the data would suggest.

However, there is no known transportation accident in which the contents of more than one storage tank contributed to the material involvement of a vapor cloud explosion. The criteria of applying TNT equivalency to potential accidents can, therefore, include the mass limitation equal to the contents of the largest storage vessel under most conditions.

Davenport (1) lists a total of seven railroad and three truck transportation accidents involving vapor cloud explosions. In view of this and the general accident data, the probability of such an explosion near a specific site is obviously extremely small.

4.2 Flixborough, England Industrial Process Accident

In 1974, a pipe failed releasing about 60 tons of hot cyclohexane under 136 psi pressure; ignition occurred in less than a minute. Although this is an industrial accident, the quantity of material involved and high pressure release mechanism are representative of tank car accidents. A detailed survey of the extensive blast damage was conducted by the Safety in Mines Research Establishment. Results presented by Munday and Cave (22) are analyzed here to yield the TNT equivalency and its sensitivity to damage data.

The overpressure-distance damage data are shown in Figures 12 and 13; the latter log-log plot clearly shows the sensitivity of TNT equivalency to blast damage data. At each damage point,

$$\alpha_e = \frac{W_{\text{TNT}} E_{\text{TNT}}}{(W\Delta H_{\text{LC}})_{\text{C}_6\text{H}_{12}}} = 7.96(10^{-7})W_{\text{TNT}} \quad (4.1)$$

where the equivalent TNT weight is computed from

$$W_{\text{TNT}} = (R_{\text{data}}/\lambda_{\text{TNT}})^3 \quad (4.2)$$

the λ_{TNT} found corresponding to each overpressure.

The calculated values of α_e for the 39 damage points range from 0.4% to 73.2% having an average value of 11.4% and standard deviation of 12.4%. Assuming a symmetric explosion and, therefore, eliminating the four data points with $\alpha_e > 20.6\%$ as unreasonably high (from Equation 3.3) yields

$$\bar{\alpha}_e = 7.8\% \text{ (5.7\% standard deviation)}$$

$$\bar{\alpha}_m = 81.7\%$$

This estimate of TNT equivalency is about 56% higher than most estimates in the literature and corresponds to a TNT equivalent

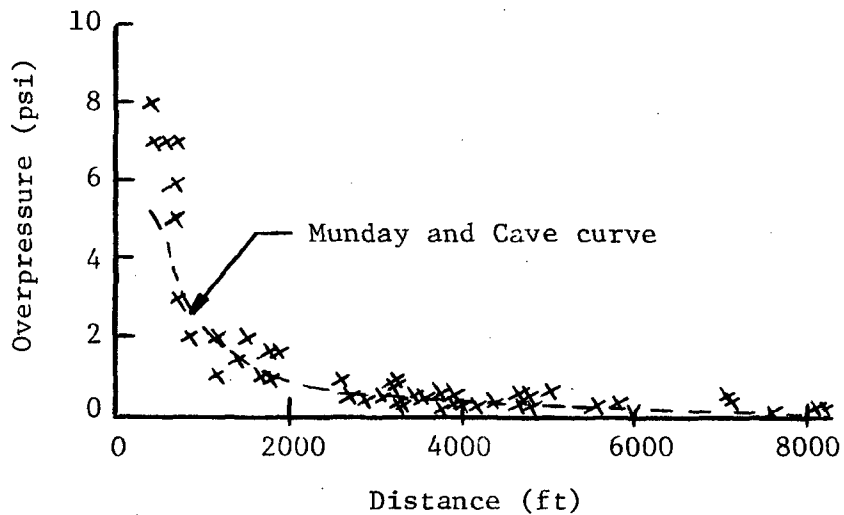


Figure 12 Flixborough damage data points (22)
 (estimated graphical interpolation
 error of 0.05 psi and 20 ft)

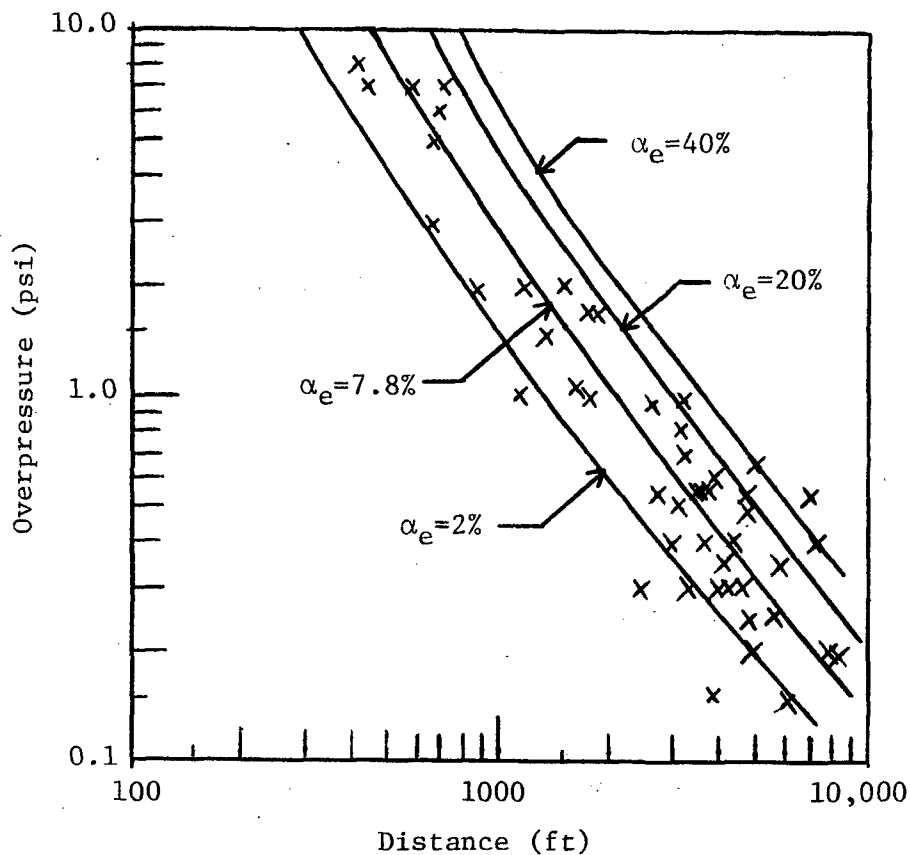


Figure 13 Flixborough data points and range of TNT
 energy equivalency on log-log plot

weight of 49 tons. It should be noted that the eliminated data all have less than 1 psi overpressure.

At $\alpha_e = 7.8\%$, half of the data points lie above and half below the average curve both close-in and far-out; for $\Delta P \geq 5$ psi, four of the six points are above the curve. The average α_e of the 10 points with $\Delta P \geq 2$ psi is only slightly higher than the overall average. This is a significant result since there has been wide acceptance of the point made by Brasie and Simpson (3) that maximum damage effects generally result in minimum TNT equivalencies and vice-versa.

In their damage assessments, Brasie and Simpson used impulse loading calculations for some of the damage data. Impulse values are generally subject to wide variations and must be considered unreliable at the present time. Eliminating that data move the Brasie and Simpson results in closer agreement with the above observation of Flixborough data. Thus, added confidence is given to adequate damage data in the low overpressure region of damage effects.

Strehlow (27) provides the following formula for the TNT equivalent weight at low overpressures:

$$W_{TNT} = \left(\frac{\text{radius of 50\% glass}}{200} \right)^3$$

where the scaled distance of 200 represents about 0.15 psi overpressure. A 50% variation in ΔP from 0.15 psi results in a 100% variation in W_{TNT} from this formula and, therefore, α_e .

A general examination of the sensitivity of TNT equivalency is provided by the Flixborough data. Representing the peak overpressure-distance decay as linear in logarithmic coordinates below about 10 psi gives the following sensitivity equation:

$$\frac{\Delta \alpha}{\alpha} = 3 \left(\frac{\Delta R}{R} + \frac{5}{7} \frac{\Delta P}{P} \right) \quad (4.3)$$

where P is the overpressure and the decay exponent is taken as 1.4 for the Kingery TNT data. The ΔR error reflects ambiguities in defining an origin of the vapor cloud explosion and is less important

at large distances; the ΔP error relates to the estimation of a structure's response to blast loading.

Overpressure sensitivity can be examined by assuming $\Delta R=0$ which is probably not too severe for the Flixborough data. Thus,

$$\frac{\Delta P}{P} = \frac{7}{15} \left(1 - \frac{\alpha}{\alpha_e}\right) \quad (4.4)$$

at each data point. Performing the calculations yields

$$\overline{\left(\frac{\Delta P}{P}\right)} = 28\%$$

which yields the overall sensitivity of the TNT equivalency to overpressure as

$$\overline{\left(\frac{\Delta \alpha}{\alpha}\right)} = 60\%$$

or $3.1\% < \alpha_e < 12.5\%$ on the average. Only nine data points had values of $\Delta P/P > 50\%$, four of which were eliminated for reasons stated earlier.

Using the experimental data of Wiehle (28) in which known structures were subjected to known blast environments, the following empirical table for $\Delta P/P$ was constructed (representing the uncertainty of overpressure to within one standard deviation of the average under known conditions):

P (psig)	$\frac{\Delta P}{P}$ (fachwork walls)	P (psig)	$\frac{\Delta P}{P}$ (masonry cavity walls)
3.00	23%	2.75	11%
5.85	16%	5.15	8%

For the six data points having $P \geq 5$ psig, $\overline{\Delta P/P} = 22\%$ and for the four points having $P = 2, 3$ psig, $\overline{\Delta P/P} = 27\%$. Thus, the Flixborough data are in general qualitative agreement with the above table.

Another useful way to view the data is to assume its accuracy but that it represents asymmetry in the blast pattern. Then using $\alpha_e = 7.8\%$ as the average symmetric yield and $\alpha_{\min} = 2\%$, the degree

of asymmetry would have been $\beta = 1.89$ and $\alpha_{\max} = 13.6\%$, consistent with the nominal standard deviation of the data. The importance of this viewpoint, as well as the statistical approach, is that the TNT equivalency should be associated with a reasonable upper limit of accident data and not an average for purposes of estimating safe standoff distances.

One final computation yields a distance of 2100 ft at which 1 psi overpressure occurs for $\alpha_e = 7.8\%$; at that distance, $\alpha_e = 2\%$ gives 0.6 psi overpressure, and $\alpha_e = 13\%$ gives 1.3 psi overpressure.

4.3 Franklin County, Missouri Pipeline Rupture

In December 1970 an underground pipeline ruptured releasing about 31,750 gallons of pressurized liquid propane over a 24 minute period until an ignition source was found some 1500 ft from the rupture (11). As mentioned in Section 1.2.3, this accident shows the significance of adverse topographical and meteorological conditions. It represents a potential transportation accident of a rail tank car having a relatively small puncture.

Applying the TNT equivalency methodology developed in this study to the damage data of Burgess and Zabetakis (13) yields

$$\bar{\alpha}_e = 8.7\%$$

$$\bar{\alpha}_m = 96\%$$

compared with their estimation of 7.5% equivalency. The atmospheric dispersion calculations were eliminated here for reasons stated in Section 1.2.3; also, the glass damage statistical estimate was eliminated as unreliable and so was one structural damage data point which clearly was too high for spatial blast effects. The corresponding TNT equivalent weight computed is 62 tons.

4.4 East St. Louis, Illinois Rail Tank Car Accident

In January 1972 a tank car containing 28,289 gallons of propylene (94%) and propane (6%) was punctured (8). A vapor cloud formed while the car was still moving. The subsequent explosion injured 230 people and caused extensive structural damage; from 870 to 1000

homes and buildings were estimated to have suffered damage. Non-railroad damage was estimated at about \$6.3 million. Figure 14 shows the damage occurring in the immediate vicinity of the explosion area.

The blast was highly asymmetric and caustics occurred as shown by the damage map in Figure 15. Serious structural damage occurred in areas 1 and 5 and broken glass in area 6. From the loading conditions, about 122,7700 pounds of material were being transported and taking 19,700 Btu per pound of fuel mixture as the heat of combustion gives for the TNT energy equivalency

$$\alpha_e = 7.4424(10^{-7}) \left[\frac{R_{\text{damage}}}{\lambda_{\text{TNT}}} \right]^3$$

and assuming an asymmetry of $\beta = 2.25$ gives

$$\alpha_{\text{min}} = 0.1614\bar{\alpha}$$

$$\alpha_{\text{max}} = 1.8386\bar{\alpha}$$

The damage data are interpreted in the direction of maximum blast output, since this area is larger and includes more structures, and is listed below:

Region	Damage Description	R_{max} (ft)
1	heavy structural	1500
2	light structural-heavy cosmetic	2650
3	light cosmetic-glass	4200
4	light glass	5750

Since isolated damage points are not being used, values of α_{max} will be selected and the resulting overpressures computed from λ_{TNT} .

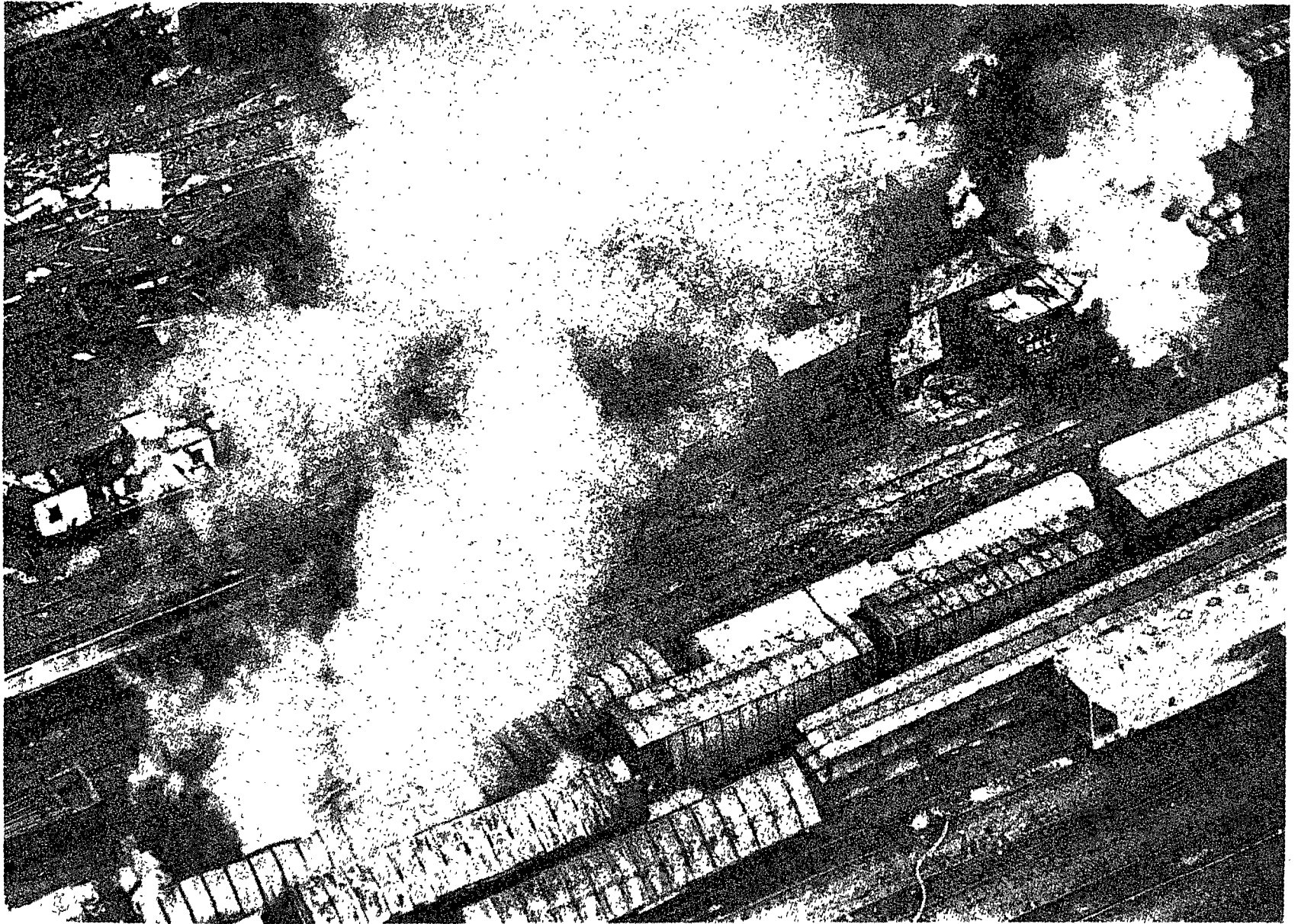


Figure 14 Explosion area at East St. Louis accident (29)

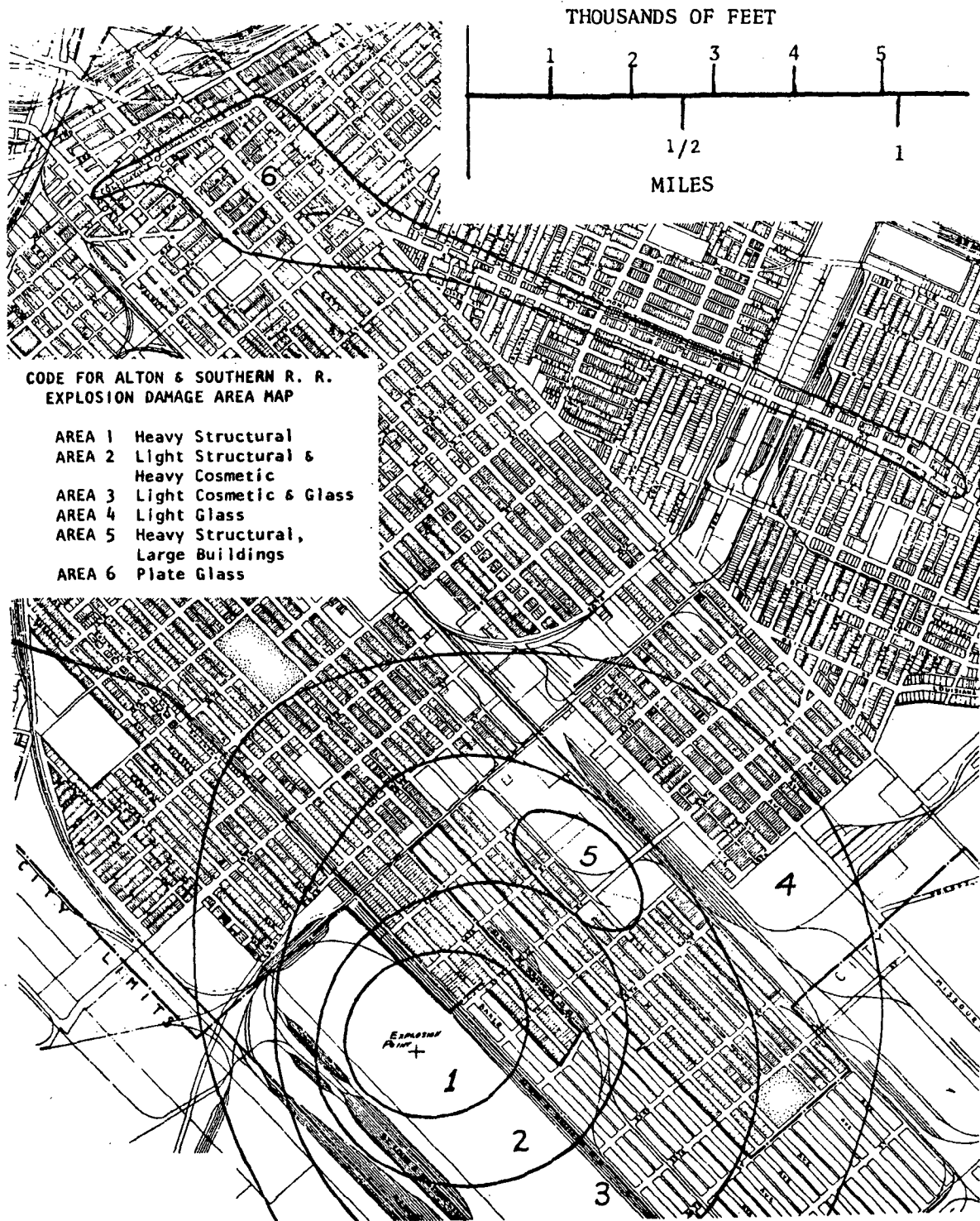


Figure 15 East St. Louis isodamage map (14)

Region	$\alpha_{\max} =$	Overpressure(psi)			Blast effects range of ΔP^\dagger
		10%	20%	30%	
1		1.76	2.41	2.92	2-5
2		0.85	1.14	1.36	1-3
3		0.49	0.63	0.75	0.25-1.5
4		0.34	0.44	0.50	0.1-1.0
$\bar{\alpha}_e =$		5.4%	10.9%	16.3%	

† These values represent a best judgment using several sources of blast effects data.

Inspection of the above table clearly indicates that $\alpha_{\max} = 10\%$ is unreasonably low while even $\alpha_{\max} = 30\%$ is not too high. The corresponding values of $\bar{\alpha}$ are given as the last line of this table.

Thus, interpreting the possible average TNT equivalency of this accident as a 10% yield is certainly reasonable. This should be compared with Strehlow's (29) estimate of from 0.1% to 0.3% on an energy basis. The TNT equivalent weight for $\alpha_e = 10\%$ is 67 tons for a mass equivalency of 109%. It should be noted that this particular asymmetry effectively doubles the average blast output in one general direction.

4.5 Decatur, Illinois Rail Tank Car Accident

In July 1974 a jumbo tank car was punctured releasing about 31,366 gallons of isobutane (30). A vapor cloud formed from an estimated spill rate of 5000 gallons per minute. An unknown ignition source was found some 8 to 10 minutes later.

The damage pattern was highly asymmetric with the following results: 7 killed-356 injured; 283 freight cars demolished-312 others damaged; 700 residences damaged-67 buildings uninhabitable due to collapsed roofs and walls; structural damage to 1 mile-broken glass to 3 miles. Commercial damage was estimated at \$4.9 million and residential damage at \$2.5 million. Figure 16 shows the damage to a newly constructed school building.

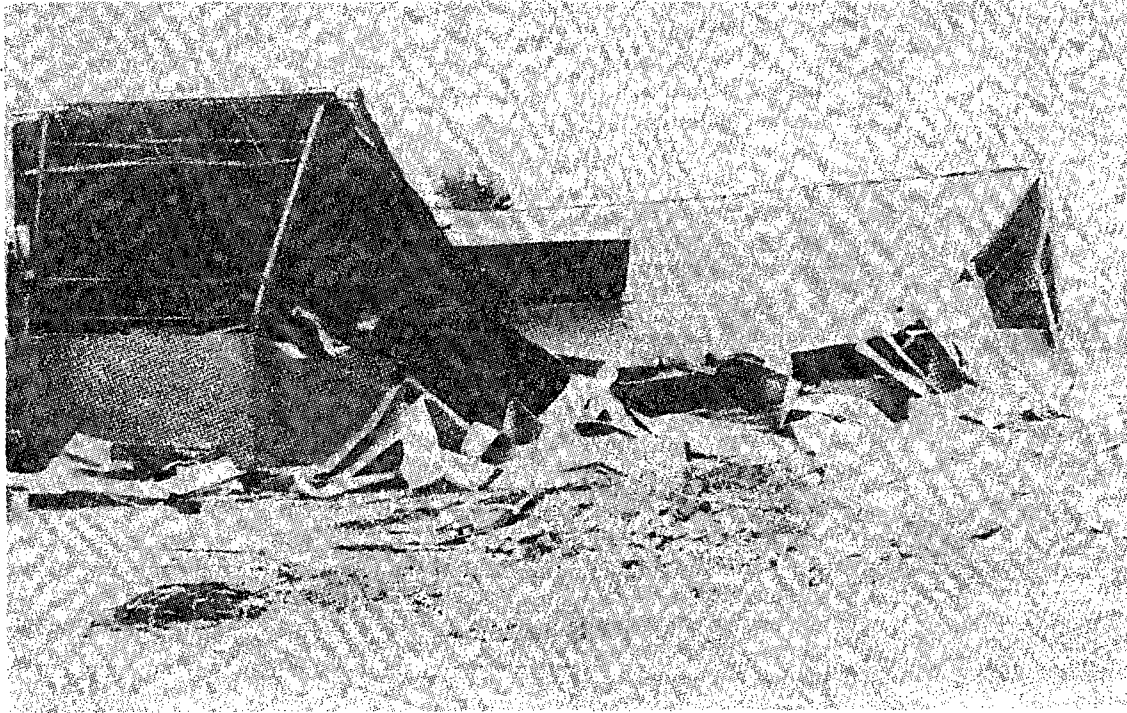


Figure 16 NTSB Report NTSB-RAR-75-4 damage to Lake View School, Decatur, Illinois (30)

Strehlow (14) computed a weighted average TNT energy equivalency of from 0.5% to 2% corresponding to 5 to 10 tons of TNT. Using 152,375 pounds of isobutane as the material involvement, the TNT equivalency can be grossly estimated using the methods of this study. Davenport (private communication) gives the distance of the pictured school building as 1100 ft and estimating the incident diffraction loading as 2 to 3 psi yields

$$\alpha_e = 4.3\% \text{ to } 10.2\%$$

$$\alpha_m = 47\% \text{ to } 111\%$$

and corresponding TNT weights of 35 to 84 tons. This estimate is also consistent with the statement of structural damage to 1 mile.

4.6 Houston, Texas Rail Tank Car Accident

In September 1974 a jumbo tank car was punctured releasing 33,864 gallons of butadiene which formed a vapor cloud in an 11 mph wind, igniting 2 to 3 minutes later (31). Figure 17 is a picture of the damage in the immediate area; 231 railroad cars were destroyed and 282 others damaged. There was major structural damage in the surrounding area with nonrailroad damage (including liability) estimated at \$5.5 million.

Damage data were not available for the present study, but Davenport (1) cites 2 to 3 psi overpressure at 1000 ft from the puncture. This corresponds to 53,000 to 127,000 pounds of TNT and implies an equivalency of

$$\alpha_e = 3\% \text{ to } 7\%$$

$$\alpha_m = 34\% \text{ to } 79\%$$

4.7 Summary of Accident Analysis Results

The analysis of accidental vapor cloud explosion information was based on the methodology developed in this report. The principal results are summarized below:

1. Accidental vapor cloud explosions have occurred for massive releases of pressurized hydrocarbon combustibles. The resulting damage-distance patterns are representative, in general, of airblast phenomena indicating either an extremely fast deflagration or detonation.
2. Accident data analysis has inherent weaknesses associated with it such that even the most exhaustive damage study can be expected to pin down the magnitude of the explosion by only a factor of two relative to a specific blast loading. The available data do, however, indicate large explosive involvement and, therefore, a considerable explosion hazard of vapor clouds of the type that can occur in transportation accidents.
3. The five major accidental vapor cloud explosions reported herein had TNT energy equivalencies of about 13.6% (7.8% average), 8.7%, possibly over 30% (10% average), up to 10.2%, and up to 7%, using the available data. These values represent hazards significantly larger than generally reported in the literature, as for example, Strehlow and Baker (32).

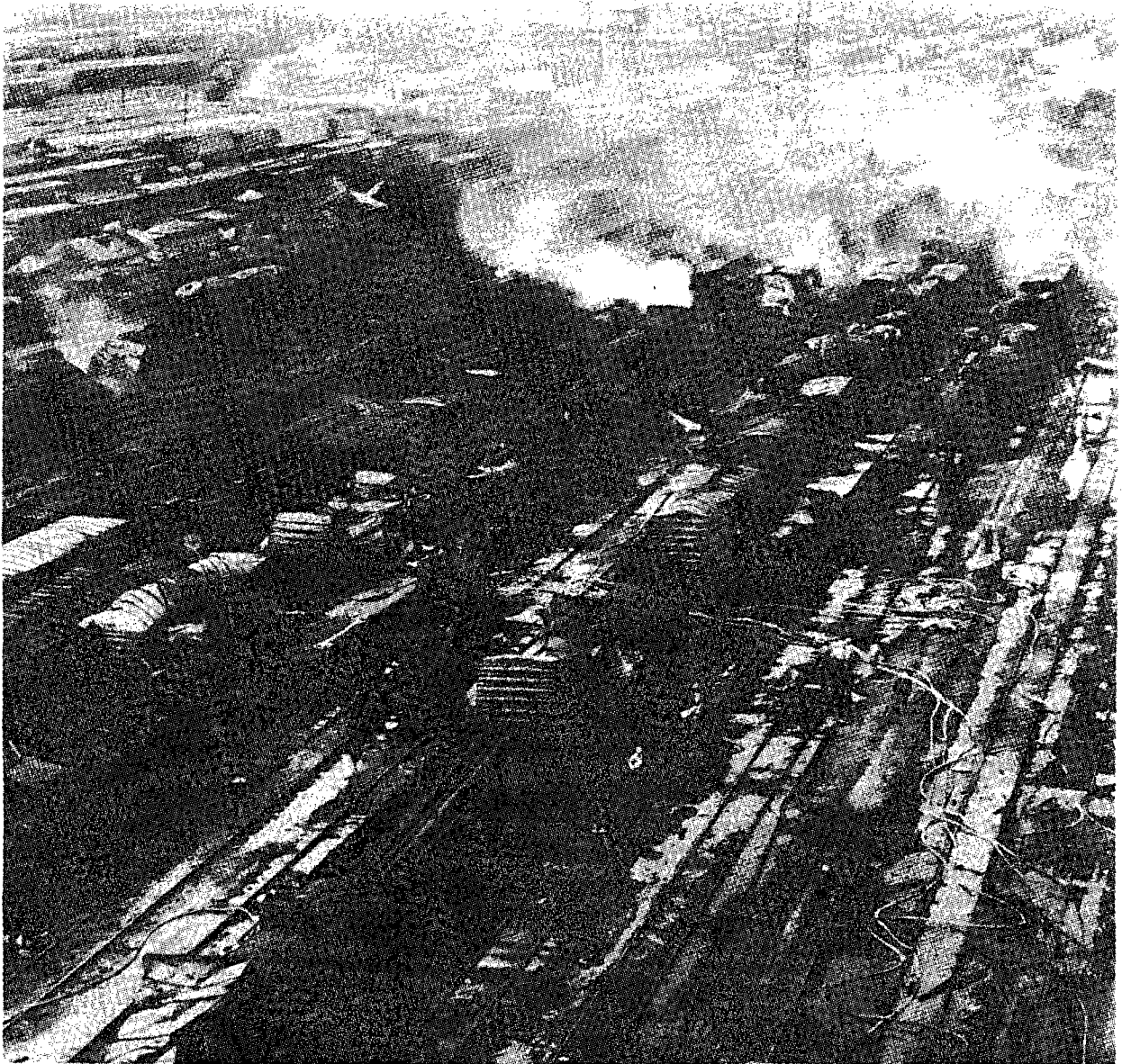


Figure 17 Explosion area of Houston accident (31)

5. CONCLUSIONS AND RECOMMENDATIONS

5.1 Conclusions

We conclude that the concept of TNT equivalency applied to accidental vapor cloud explosions is a useful technique in evaluating their potential blast damage at the lower overpressures. A quantitative methodology has been formulated in this study for estimating the TNT equivalency of detonating vapor clouds based upon the existing experimental and accident data. In addition, a study of the general physics of the vapor cloud phenomenon has yielded valuable insight into the various mechanisms that influence the explosion event.

Although the probability of occurrence of a vapor cloud explosion can be defined statistically, an expected value of the blast effects cannot be because (1) they occur infrequently, (2) post-accident data are inherently inadequate, and (3) too many critical parameters are involved. Therefore, we conclude that estimates of potential blast damage should be based on the total range of values that is established by the state of the physics at the appropriate time.

An accidental vapor cloud TNT mass equivalency of 10% (energy equivalency of 0.8%) has been suggested, in the absence of test data by the NRC staff in Working Paper B of Regulatory Guide 1.91 (Revision 1) and entitled "Evaluations of Explosions Postulated to Occur on Transportation Routes Near Nuclear Plants". We conclude that this a priori judgment is unrealistic when compared to the existing body of knowledge and actual accidents.

Similarly, we conclude that the TNT equivalencies appearing in the West German Safety Codes and Guides and presumably based on a moderate deflagrative explosion in the immediate vicinity of a nuclear plant are nonconservative. Specifically, a TNT mass equivalency of 100% (energy equivalency of 8.4%) for hydrocarbons with carbon-to-carbon triple bonds or cumulated carbon-to-carbon double bonds, 100% (8.4%) for nonliquified gases, 50% (4.2%) for gases liquified under pressure are all judged by us to be nonconservative when compared with the results of this study.

The TNT equivalencies of gases liquified at low temperature (cryogenic) cannot be specifically estimated from this report. It should be noted that the vapor evolution from cryogenics is determined by external heat transfer mechanisms which are generally much slower than those occurring during pressure expansion and air entrainment. Therefore, beneficial effects of a longer time frame are generally realized.

In general, we conclude that the probability of occurrence of a vapor cloud explosion at a specific site is extremely low, but the potential destructive magnitude of an actual event, should it occur, must be recognized. Additional conclusions of the present study are made as follows:

1. Energetic materials of interest can be represented with few exceptions as a class of hydrocarbon-air explosions distinguished by their low value of heat of combustion. Other differences such as transition to detonation amplification factors and flammability or detonability limits should, at the present time, be incorporated into appropriate probability models. In general, a distinction must be drawn between probability considerations and the tractable physics of the phenomena.
2. The principal factors controlling the blast energy release are material involvement, combustion process, and topographical and meteorological conditions. Present theoretical and empirical knowledge is too limited to quantitatively evaluate realistic accidental vapor cloud explosion scenarios. However, each factor can contribute, at certain stages of the event, in the direction of producing maximum blast effects. In particular, point of ignition, terrain, and atmospheric conditions can create highly directional blast energy coupling to the surroundings resulting in asymmetric damage patterns. A priori limitations of these factors as made, for example, by Jungclaus (15) are not considered realistic in this study.
3. Asymmetric spatial effects are unique to and commonly observed in vapor cloud explosions. An important product of the current research is a model for treating these effects on a TNT equivalency basis. As a result we conclude that asymmetry of the blast yield can increase the effective TNT equivalency by up to a factor of two over the symmetric estimate.

4. In terms of the presently available data, the maximum expected TNT equivalencies of symmetric vapor cloud explosions is about 20% on an energy basis and 240% on a mass basis; for an asymmetric allowance, up to a maximum of twice these values should be definitely considered. The value of 20% energy equivalency is based upon the assumed validity of Kogarko's experiments; it should be noted that the corresponding theoretical value computed herein is about 37%, but this discrepancy cannot be resolved within the scope of the present study.

5.2 Recommendations

At the present time we recommend that safety standards for determining reasonable standoff distances of nuclear plants near potentially hazardous transportation routes be based on TNT energy equivalencies of from 20% to 40% for all pressurized hydrocarbon combustibles. The appropriate standoff distance formula is

$$R_s = \lambda_{TNT} \left[\frac{\alpha_e W_{HC} \Delta H_{LC}}{e_{TNT}} \right]^{1/3} \quad (5.1)$$

where R_s = standoff distance (ft)

λ_{TNT} = TNT scaled distance corresponding to design or other incident overpressure level (ft/lb-TNT^{1/3})

α_e = TNT energy equivalency

W_{HC} = weight of hydrocarbon in largest single pressurized storage tank being transported (lb)

ΔH_{LC} = low value of hydrocarbon's heat of combustion (Btu/lb-HC)

e_{TNT} = 1800 Btu/lb-TNT

At 1 psi incident overpressure, $\lambda_{TNT} = 45.5 \text{ ft/lb}^{1/3}$; assuming a typical value of ΔH_{LC} to be 20,000 Btu/lb of fuel,

$$R_s (1 \text{ psi}) = 101.5 (\alpha_e W_{HC})^{1/3} \quad (5.2)$$

Referring to Figure 18, we therefore recommend selecting the stand-off distance as a value between the $\alpha_e=20\%$ (nominal $\alpha_m=240\%$) and $\alpha_e=40\%$ (nominal $\alpha_m=480\%$) curves at the appropriate material weight. A precise value within these limits must be guided by judgment at the present time.

In view of the significant hazards posed by accidental vapor cloud explosions, we recommend that further investigations be pursued.

In particular, more results must be obtained regarding the hydrodynamic and blast aspects of violent fuel-air deflagrations, cloud generation and mixing mechanisms associated with pressurized fluids, and the asymmetric blast coupling of vapor cloud explosions.

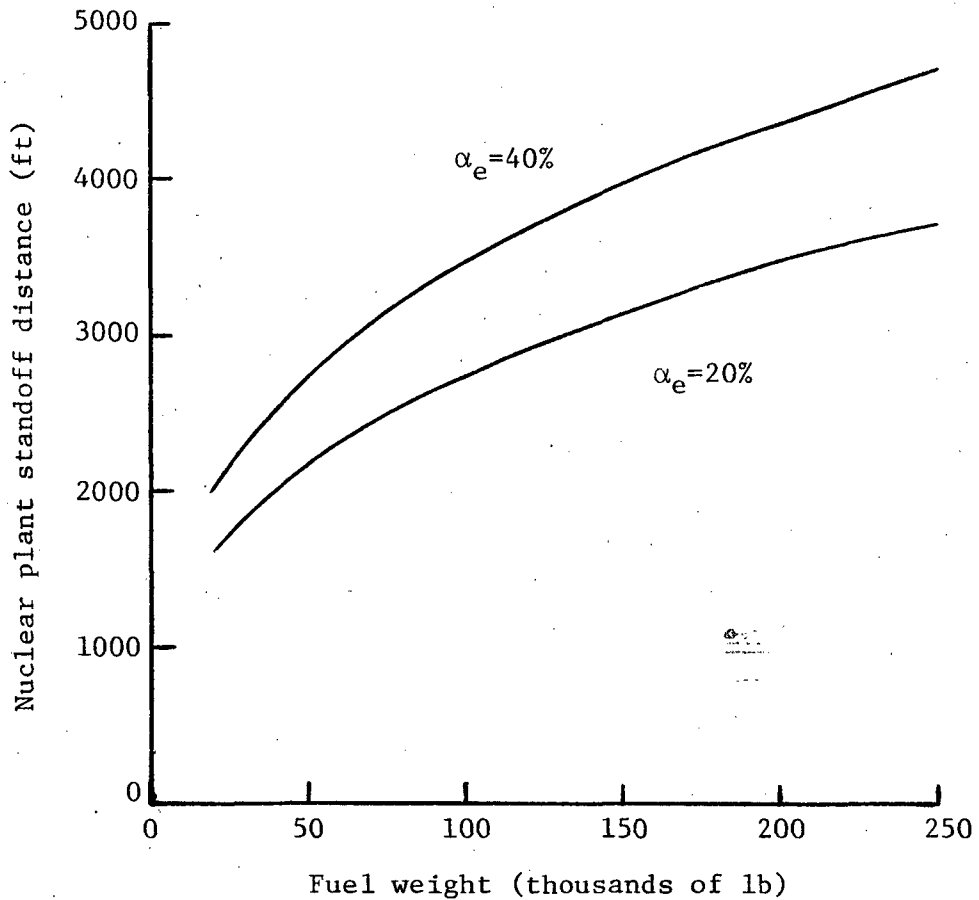


Figure 18 Estimated standoff distance of nuclear plant as function of potential combustible material involvement for 1 psi blast overpressure (heat of combustion of 20,000 Btu/lb of fuel assumed)

CITED REFERENCES

- 1 Davenport, J. A.; A Study of Vapor Cloud Incidents, Industrial Risk Insurers, Hartford, Connecticut, Presented to 83rd National Meeting of American Institute of Chemical Engineers, Houston, Texas, Paper 24a (to be published)
- 2 Strehlow, R. A.; Unconfined Vapor-Cloud Explosions - An Overview, Department of Aeronautical and Astronautical Engineering, University of Illinois, Urbana, Illinois, 14th Symposium (International) on Combustion, The Combustion Institute, 1189-1200, 1973
- 3 Brasie, W. C.; Simpson, D. W.; Guidelines for Estimating Damage Explosion, Dow Chemical Co., Midland, Michigan, Loss Prevention, Vol. 2, 91-102, February 1968
- 4 Hardee, H. C.; Lee, D. L.; Expansion of Clouds from Pressurized Liquids, Criteria and Heat Transfer Division, Sandia Laboratories, Albuquerque, New Mexico, SAND74-5210, September 10, 1974
- 5 Brasie, W. C.; Guidelines for Estimating the Hazard Potential of Chemicals, Dow Chemical Co., Midland, Michigan, Presented to 81st National Loss Prevention Symposium, AIChE, Kansas City, Missouri, April 1976
- 6 Kletz, T. A.; Unconfined Vapour Cloud Explosions - An Attempt to Quantify Some of the Factors Involved, Presented to 83rd National Meeting of American Institute of Chemical Engineers, Houston, Texas, (to be published)
- 7 Geiger, W.; Generation and Propagation of Pressure Waves Due to Unconfined Chemical Explosions and Their Impact on Nuclear Power Plant Structures, Nuclear Engineering and Design, 27 No. 2, 189-198, May 1974
- 8 Railroad Accident Report, Hazardous Materials Railroad Accident in the Alton and Southern Gateway Yard in East St. Louis, Illinois, January 22, 1972, National Transportation Safety Board, Washington, D. C., NTSB-RAR-73-1, January 1973
- 9 Kogarko, S. M.; Adushkin, V. V.; Lyamin, A. G.; An Investigation of Spherical Detonations of Gas Mixtures, International Chemical Engineering, Vol. 6, No. 3, July 1966
- 10 Lee, J. H. S.; Initiation of Gaseous Detonation, Department of Mechanical Engineering, McGill University, Montreal, Canada, Annual Review of Physical Chemistry, Vol. 28, (to be published)

- 11 Pipeline Accident Report, Phillips Pipeline Company, Propane Gas Explosion, Franklin County, Missouri, December 9, 1970, National Transportation Safety Board, Washington, D. C., NTSB-PAR-72-1, March 1972
- 12 Burgess, D. S.; Murphy, J. N.; Zabetakis, M. G.; Perlee, H. E.; Volume of Flammable Mixture Resulting from the Atmospheric Dispersion of a Leak or Spill, Pittsburgh Mining and Safety Research Center, Bureau of Mines, 15th Symposium (International) on Combustion, The Combustion Institute, Paper No. 29, 1975
- 13 Burgess, D. S.; Zabetakis, M. G.; Detonation of a Flammable Cloud Following a Propane Pipeline Break, Pittsburgh Mining and Safety Research Center, Bureau of Mines, Pittsburgh, Pennsylvania, RI-7752, 1973
- 14 Strehlow, R. A.; Personal Communication to Mr. Ludwig Benner, National Transportation Safety Board, May 1975
- 15 Jungclaus, D.; Basic Ideas of a Philosophy to Protect Nuclear Plants Against Shock Waves Related to Chemical Reactions, Nuclear Engineering and Design, 41 No. 1, March 1977
- 16 Lee, J. H.; Guirao, C. M.; Chiu, K. W.; Bach, G. G.; Blast Effects from Vapor Cloud Explosions, Department of Mechanical Engineering, McGill University, Montreal, Canada, Presented to 83rd National Meeting of American Institute of Chemical Engineers, Houston, Texas, (to be published)
- 17 Kingery, C. N.; Airblast Parameters versus Distance for Hemispherical TNT Surface Bursts, U. S. Material Command, Ballistic Research Laboratories, Aberdeen Proving Ground, Maryland, BRL Report 1344, September 1966
- 18 Balcerzak, M. H.; Johnson, M. R.; Kurz, F. R.; Nuclear Blast Simulation - Part I - Detonable Gas Explosion, General American Research Division, Niles, Illinois Final Report DASA 1972-I, July 1966
- 19 Reisler, R. E.; Ethridge, N. H.; LeFevre, D. P.; Giglio-Tos, L.; Airblast Measurements from the Detonation of an Explosive Gas Contained in a Hemispherical Balloon (Operation Distant Plain, Event 2a), Ballistic Research Laboratories, Aberdeen Proving Ground, Maryland, BRL Memorandum Report 2108, July 1971
- 20 Woolfolk, R. W.; Ablow, C. M.; Blast Waves for Non-ideal Explosions, Presented at the Conference on the Mechanism of Explosions and Blast Waves, Naval Weapons Station, Yorktown, Virginia, November 13-15, 1973

- 21 Brinkley, S. R.; Determination of Explosion Yields, Combustion and Explosives Research, Inc., Pittsburgh, Pennsylvania, CEP Technical Manual, Loss Prevention, Vol. 3, 1969
- 22 Munday, G.; Cave, L.; Evaluation of Blast Wave Damage from Very Large Unconfined Vapour Cloud Explosions, International Atomic Energy Agency, Vienna, 1975
- 23 Lind, C. D.; Explosion Hazards Associated with Spills of Large Quantities of Hazardous Materials - Phase I, Department of the Navy, Naval Weapons Center, China Lake, California, Interim Report CG-D-30-75, October 1974
- 24 Napadensky, H.; Pape, R.; Unione, A.; An Evaluation of the Sensitivity of TNT and the Probability of a TNT Explosion on the GM&O Railroad Line Past the Braidwood Reactor Site, IIT Research Institute, for Sargent and Lundy Engineers, March 1975
- 25 Pierson, K. L.; Hazardous Materials Incident Analysis as Related to Emergency Response, Transportation of Hazardous Materials Committee A3E06, Transportation Research Board, Washington, D. C., January 26, 1977
- 26 Napadensky, H. S.; Takata, A. N.; Potential Danger of Fixed Propane-Isobutane Storage Tanks in a Residential Area, IIT Research Institute Report V6141-J19, March 5, 1976
- 27 Strehlow, R. A.; A First Estimate of TNT Equivalence for Accidental Explosions, Department of Aeronautical and Astronautical Engineering, University of Illinois, Urbana, Illinois, July 1975
- 28 Wiehle, C. K.; Collateral Air Blast Damage, Stanford Research Institute, for Defense Nuclear Agency, Strategic Structures Division, Biennial Review Conference, February 1977
- 29 Strehlow, R. A.; Equivalent Explosive Yield of the Explosion in the Alton and Southern Gateway Yard, East St. Louis, Illinois, January 22, 1972, University of Illinois, Urbana, Illinois, AAEE-TR73-3, UILU-ENG-73-05-03, June 1973
- 30 Railroad Accident Report, Hazardous Materials Accident in the Railroad Yard of the Norfolk and Western Railway at Decatur, Illinois, July 19, 1974, National Transportation Safety Board, Washington, D. C., NTSB-RAR-75-4, April 1975
- 31 Railroad Accident Report, Hazardous Materials Accident at the Southern Pacific Transportation Company's Englewood Yard in Houston, Texas, September 21, 1974, National Transportation Safety Board, Washington, D. C., NTSB-RAR-75-7, May 1975

- 32 Strehlow, R. A.; Baker, W. E.; The Characterization and Evaluation of Accidental Explosions, Aeronautical and Astronautical Engineering Department, University of Illinois, Urbana, Illinois, Technical Report AAE75-3, UILU-Eng 75-0503, June 1975
- 33 Balcerzak, M. J.; Johnson, M. R.; Lucole, S. W.; Nuclear Blast Simulation - Detonable Gas Explosion Operation Distant Plain, General American Research Division, Niles, Illinois, for Defense Atomic Support Agency, Washington, D. C., Final Report DASA-1945, April 1967

OTHER REFERENCES

Kletz, T. A.; Some Questions Raised by Flixborough, Imperial Chemical Industries, Ltd., Petrochemicals Division, England, Presented at the AIChE Loss Prevention Symposium, Houston, Texas, March 1975

Covert, K.; Groothuizen, Th. M.; Pasman, H. J.; Trense, R. W.; Fuel-Air Explosives, Technological Laboratory TNO, Rijswijk, TDCK65977, January 24, 1975

Iotti, R. C.; Krotiuk, W. J.; Deboisblanc, D. R.; Hazards to Nuclear Plants from On (or Near) Site Gaseous Explosions, Ebosco Services, Inc., New York, N.Y., Presented to Topical Meeting on Water-Reactor Safety, American Nuclear Society, March 1973

Anthony, E. J.; Some Aspects of Unconfined Gas and Vapour Cloud Explosions, Journal of Hazardous Material, 1 (1975/77) 289-301, August 1976

Sutton, S. B.; McCauley, E. W.; An Assessment of Hazards Resulting from Atmospheric Propane Explosions at LLL, Lawrence Livermore Laboratory, University of California, UCID-16720, February 1975

Koch, C.; Bokemeier, V.; Phenomenology of Explosions of Hydrocarbon Gas-Air Mixtures in the Atmosphere, Nuclear Engineering and Design, 41 No. 1, March 1977

Pfortner, H.; Gas Cloud Explosions and Resulting Blast Effects, Nuclear Engineering and Design, 41 No. 1, March 1977

Nicholls, J. A.; Sichel, M.; Babrijel, Z.; Oza, R.; Fundamental Aspects of Unconfined Explosions: Phase II, Department of Aerospace Engineering, The University of Michigan, Ann Arbor, Michigan, Final Report AFATL-TR-76-78, July 1976

Guirao, C. M.; Bach, G. G.; Lee, J. H.; Pressure Waves Generated by Spherical Flames, Combustion and Flame, 27, 341-351, 1976

Kuhl, A. L.; Kamel, M. M.; Oppenheim, A. K.; On Flame Generated Self-Similar Blast Waves, Presented to 14th Symposium (International) on Combustion, The Combustion Institute, 1201-1214, 1973

Shchelkin, K. I.; The Theory of Combustion and Detonation, Foreign Technology Division, Wright-Patterson Air Force Base, Ohio, FTD-MT-24-324-73, AD-767985, September 12, 1973

Parsons, G. H.; Vanta, E. B.; Collins, P. M.; Bearly, J.; Techniques for Investigation of Unconfined Fuel-Air Detonations, Air Force Armament Laboratory, Elgin Air Force Base, Florida, Technical Report AFATL-TR-73-230, November 1973

Knystautas, R.; Lee, J. H.; On the Effective Energy for Direct Initiation of Gaseous Detonation, Combustion and Flame, 27, 221-228, 1976

Sternberg, H. M.; Hurwitz, H.; Calculated Spherical Shock Waves Produced by Condensed Explosives in Air and Water, Naval Surface Weapons Center, White Oak, Silver Spring, Maryland, Presented to 6th Symposium (International) on Detonation, San Diego, California, August 1976

Analysis of Risk in the Water Transportation of Hazardous Materials, Report of the Risk Analysis and Hazard Evaluation Panel, Committee on Hazardous Materials, National Academy of Sciences, Washington, D. C., 1976

D CPA Attack Environment Manual, Research Directorate, Defense Civil Preparedness Agency, June 1972

Custard, G. H.; Thayer, J. R.; Target Response to Explosive Blast, Falcon Research and Development Company, Denver, Colorado, Prepared for Armed Services Explosives Safety Board, September 1970

Proceedings of the First Fuel-Air Explosives Conference, Air Force Armament Laboratory, Elgin Air Force Base, Florida, Technical Report AFATL-TR-71-171, Vol. 1, Book 1, December 1971

Proceedings of the Conference on Mechanisms of Explosion and Blast Waves, The Joint Technical Coordinating Group for Air Launched Non-nuclear Ordnance Working Party for Explosives, Naval Weapons Station, Yorktown, Virginia, November 1973

Proceedings of Operation Distant Plain Symposium, Vol. 1,
DASA Information and Analysis Center, Santa Barbara,
California, DASIAC Special Report 60, DASA 1947-1,
September 1967

Baker, W. E.; Explosions in Air, Southwest Research Insti-
tute, University of Texas Press, Austin and London, 1973

Lewis, B.; von Elbe, G.; Combustion, Flames and Explosions
of Gases, Academic Press, Inc., 2nd Edition, 1961