A Survey of Analytical Tools for Explosion Investigation

K. R. Mniszewski

FX Engineering, Inc., Hinsdale, Illinois, USA

R. Pape

Engineering Systems Inc., Aurora, Illinois, USA

ABSTRACT

Practical analytical techniques that have been found to be useful in explosion investigation include: timeline analysis, experimental data comparisons, thermochemical code analysis, TNT and other air blast equivalency techniques, ground shock analysis, dynamic gas concentration estimates, simple fuel/air explosion codes, damage pattern analysis and system safety analysis methods. An example application of existing analytical tools to an explosion investigation is presented. Exotic analytical techniques are available but are not justified unless the loss is very large. Methodology is reviewed for completing a reasonable explosion investigation, including essential items from NFPA 921. Needs are addressed for desired technology advancements.

Keywords: explosion investigation, thermochemical equilibrium, blast equivalency, system safety analysis, ground shock

Introduction

The investigation of explosions can be an extremely complex task depending on the nature of the incident. Evidence is often destroyed by the forces involved or subsequent fires. The evidence may be spread out over an extremely large area. Fuels and oxidizers involved may or may not be easily identified. Pyrotechnic and explosive materials involved will generally be consumed in the event, and the materials that remain after and incident may be misleading. Fuel gases involved in a fuel-air explosion are often dissipated before any investigators are on the scene. The explosion origin can be difficult to pinpoint due to a lack of explosion seating (e.g., the absence of a crater). Propagation patterns may be lacking or conflicting in some cases. Ignition sources may be extremely difficult to identify, due to problems in establishing the origin, or perhaps in sorting out the source from a plethora of viable sources.

A basic knowledge of the chemistry and physics of explosions is necessary for an intelligent evaluation of an accident scene. Several specialized experts might necessarily be involved depending on the kind of answers that are desired. Typical questions that need answers are:

- Where was the origin of the explosion?
- What material exploded?
- How much material exploded?
- How was it initiated?
- What was the extent of damage/injury?
- How can it be prevented from recurring?

The best pathway to answering these questions is the scientific method. This paper is an overview of analytical tools that have proven to be useful in facilitating the scientific method in explosion investigations.

Conducting the Explosion Investigation

An explosion investigation and analysis is a complex endeavor that needs to be approached in a systematic manner using the scientific method. The initial steps will include securing the scene to prevent spoliation of evidence, assessment and documentation of the scene, and collection and preservation of evidence. This will be combined with other relevant data collection and interviews of witnesses. The data is then inductively analyzed and a hypothesis developed. The hypothesis is then deductively tested by comparing it to all known facts. If the hypothesis is inconsistent with the known facts, it should be discarded and another hypothesis examined. This may identify the need to collect additional data or perform other analyses.

Of course, the extent of an investigator's involvement may vary with his assignment and may only cover part of the overall investigation. In some cases an investigator's involvement may even occur several years after the incident.

Additional details of the investigation methodology are given in Chapters 2 and 13 of *NFPA 921, Guide for Fire and Explosion Investigation.*[1] The analytical tools described in this paper can be used to assist in both the development and testing of hypotheses, which is the essential element of the scientific method in explosion investigation.

Useful Analytical Tools

There are a wide variety of analytical tools for possible use in explosion investigation. These may range from simple fluid dynamic expressions for estimating leak rates, to complex three-dimensional computational fluid dynamic models for estimating explosive reaction propagation through a structure. Quite often design-basis tools are too conservative for use in evaluating explosions. That is because engineering design-basis tools are usually standardized to assume idealized phenomena and incorporate large safety factors to insure public safety. Although the typical accidental explosion is far from ideal, some design-basis explosion mitigation guides can be utilized in a reverse-engineering fashion to be useful to the investigator. Other tools borrowed from fire investigation techniques and systems safety science are extremely valuable.

Analytical tools that have proven especially useful in practice are listed below. Many of these tools may be incorporated in future editions of NFPA 921.

Timeline Analysis

A timeline is a graphical or narrative representation of the events related to the incident that are arranged in some chronological order. The events included in the timeline may occur before, during or after the incident. This valuable investigative tool can show relationships between events, identify gaps or inconsistencies in information and sources, assist in witness interviews, and otherwise assist in the analysis and investigation of the incident.

The value of the timeline is dependent on the accuracy of the information used to develop it and the interpretations of the person assembling it. One example of a complex timeline diagram is shown in Figure 1 from reference 2.

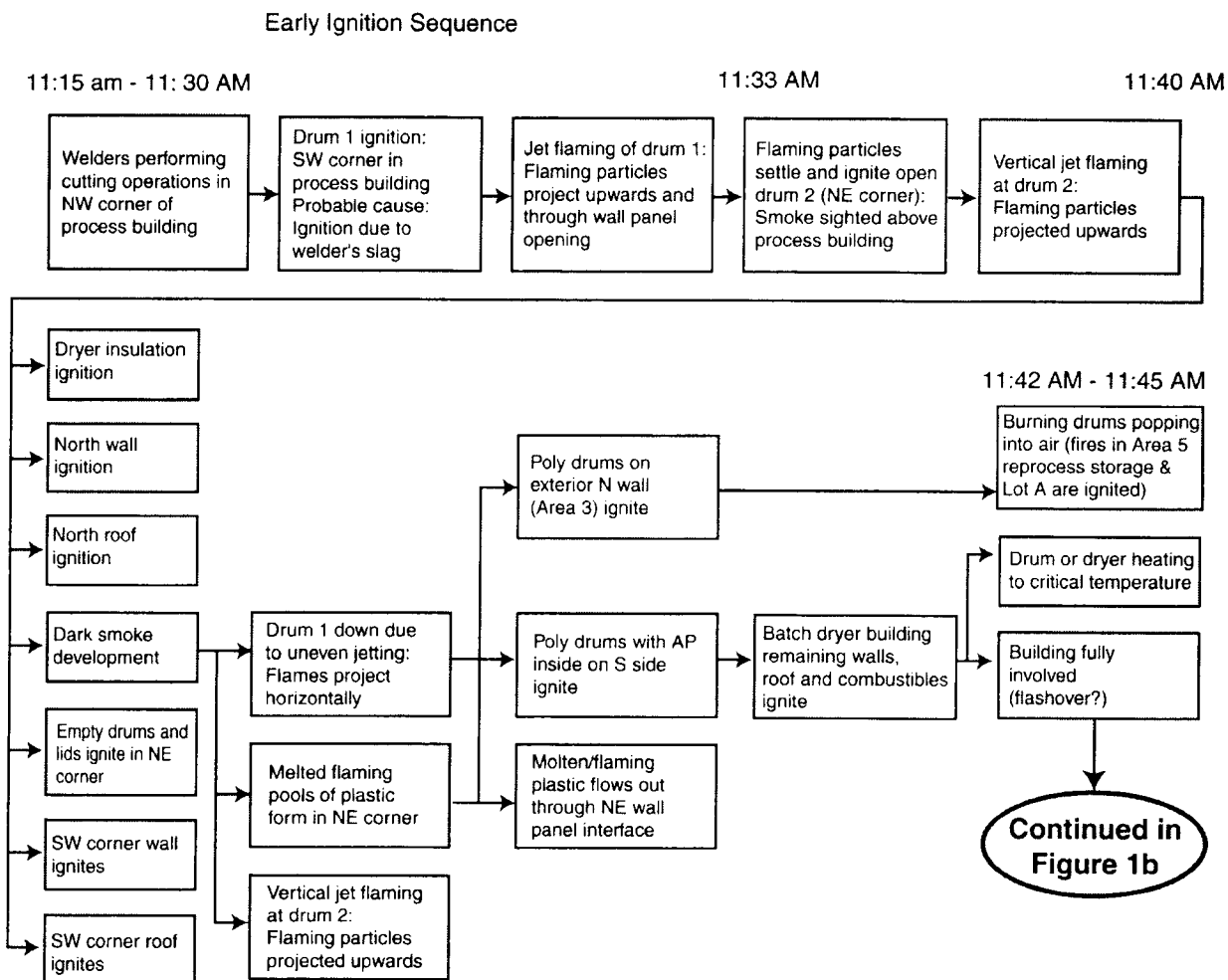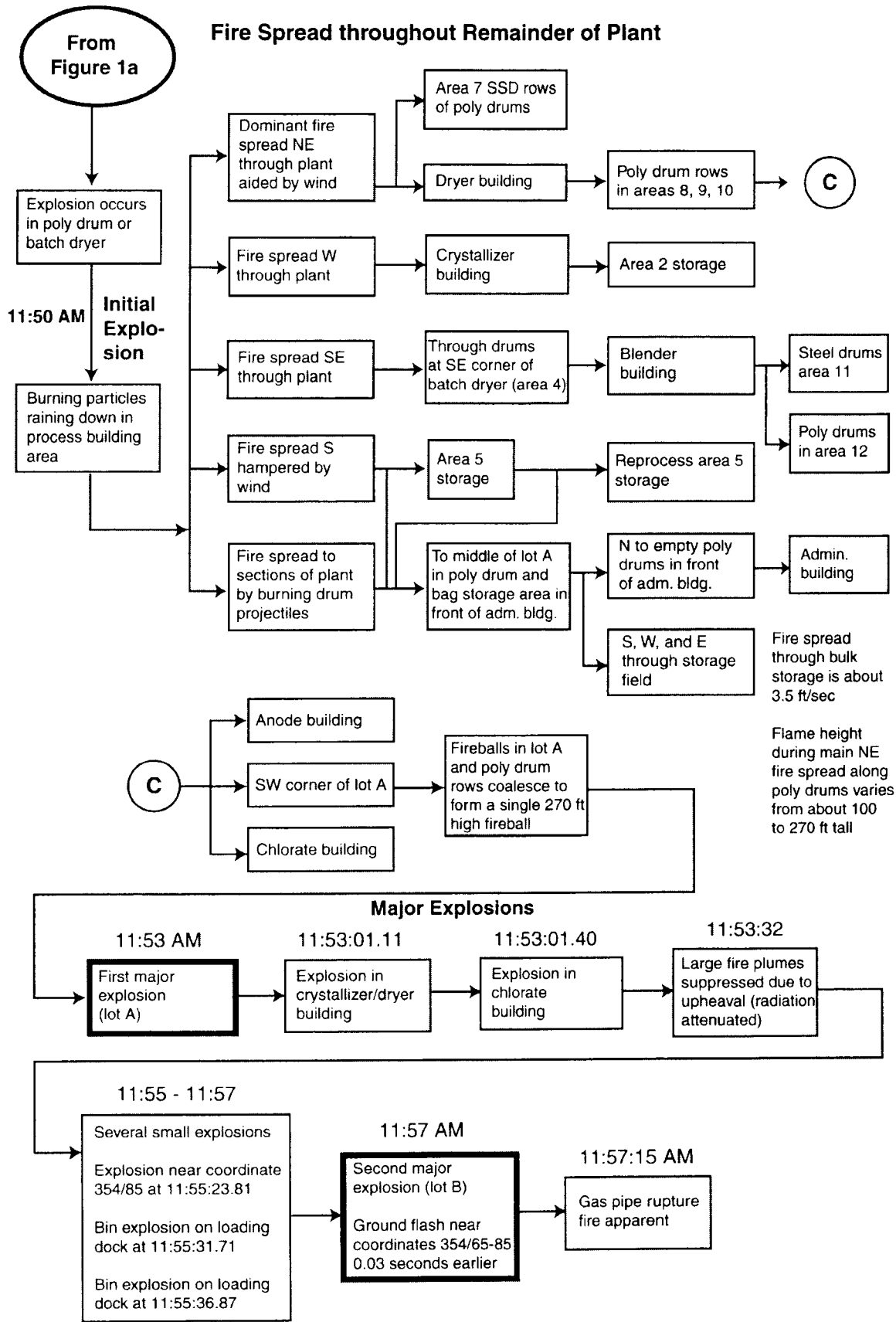## Early Fire Spread in Batch Dryer and Process Building

Early Ignition Sequence

11:15 am - 11:30 AM

11:33 AM

11:40 AM

Welders performing cutting operations in NW corner of process building

Drum 1 ignition: SW corner in process building Probable cause: Ignition due to welder's slag

Jet flaming of drum 1: Flaming particles project upwards and through wall panel opening

Flaming particles settle and ignite open drum 2 (NE corner): Smoke sighted above process building

Vertical jet flaming at drum 2: Flaming particles projected upwards

Dryer insulation ignition

North wall ignition

North roof ignition

Dark smoke development

Empty drums and lids ignite in NE corner

SW corner wall ignites

SW corner roof ignites

Drum 1 down due to uneven jetting: Flames project horizontally

Melted flaming pools of plastic form in NE corner

Vertical jet flaming at drum 2: Flaming particles projected upwards

Poly drums on exterior N wall (Area 3) ignite

Poly drums with AP inside on S side ignite

Molten/flaming plastic flows out through NE wall panel interface

Batch dryer building remaining walls, roof and combustibles ignite

11:42 AM - 11:45 AM

Burning drums popping into air (fires in Area 5 reprocess storage & Lot A are ignited)

Drum or dryer heating to critical temperature

Building fully involved (flashover?)

Continued in Figure 1b

Figure 1a. Pepcon fire spread diagram.

Fire Spread throughout Remainder of Plant

From Figure 1a

Explosion occurs in poly drum or batch dryer

11:50 AM **Initial Explo- sion**

Burning particles raining down in process building area

Dominant fire spread NE through plant aided by wind

Area 7 SSD rows of poly drums

Dryer building → Poly drum rows in areas 8, 9, 10 → **C**

Fire spread W through plant → Crystallizer building → Area 2 storage

Fire spread SE through plant → Through drums at SE corner of batch dryer (area 4) → Blender building → Steel drums area 11

Poly drums in area 12

Fire spread S hampered by wind → Area 5 storage → Reprocess area 5 storage

Fire spread to sections of plant by burning drum projectiles → To middle of lot A in poly drum and bag storage area in front of adm. bldg. → N to empty poly drums in front of adm. bldg. → Admin. building

S, W, and E through storage field

Fire spread through bulk storage is about 3.5 ft/sec

C → Anode building

SW corner of lot A → Fireballs in lot A and poly drum rows coalesce to form a single 270 ft high fireball

Chlorate building

Flame height during main NE fire spread along poly drums varies from about 100 to 270 ft tall

Major Explosions

11:53 AM
First major explosion (lot A)

11:53:01.11
Explosion in crystallizer/dryer building

11:53:01.40
Explosion in chlorate building

11:53:32
Large fire plumes suppressed due to upheaval (radiation attenuated)

11:55 - 11:57
Several small explosions

Explosion near coordinate 354/85 at 11:55:23.81

Bin explosion on loading dock at 11:55:31.71

Bin explosion on loading dock at 11:55:36.87

11:57 AM
Second major explosion (lot B)

Ground flash near coordinates 354/65-85 0.03 seconds earlier

11:57:15 AM
Gas pipe rupture fire apparent

Figure 1b. Pepcon fire spread diagram (continued).

Experimental Data Comparisons

Useful experimental data for explosion investigation covers a broad range of topics. These can include data on minimum ignition energy of dust clouds, maximum explosion pressure of a mixture of gases, maximum explosion pressure under specified vented conditions, explosion limits of fuel gases, critical diameters of solid explosives, explosion air blast or TNT equivalency, etc. Each investigation is unique and requires data sources unique to the relevant issues. Sources of such data are much too numerous to list here, but some useful tabulations are found in references 1, and 3–7.

An important point regarding the use of such data sources is that much of the tabulated data is derived from standard tests, and caution should be exercised in their use. These data sources are usually developed to result in conservative values so that their use will always err on the side of safety. Often times these data do not adequately fit the accident scenario of interest.

For example, the high and low strength enclosure venting data models in NFPA 68[3] are too conservative for many cases where less than the worst-case scenario is evident. Thus, it is usually quite difficult to use NFPA 68 venting guides to help in the analysis of an accidental building explosion. This is because the strength of the structure and explosion vent parameters is often unknown. In addition, information on the fuel-gas mixture content and concentration generally are lacking.

The use of ASTM E 1226[8] test data involving maximum pressure development for dusts is another example where the source data do not adequately fit the scenario. The standard test requires sieving the dust sample to 200 mesh. This gives conservative results in most cases, even though the fines are more easily lofted than coarse particles, they generally dominate the explosion effects. Due to the sieving, the test does not consider the agglomeration of particles with, for example, wood dusts in high humidity or plastic dusts in low humidity (due to electrostatic forces).

Fuel/Air Explosion Models

There are simplified methodologies for predicting maximum pressure development in a vented enclosure as well as flame speed and shape. However, these quasi-empirical methods require input such as burning velocity, turbulence factors, enclosure geometry, and physical vent parameters. Some of these methods are summarized in reference 9 or listed in NFPA 68.[3]

It should be noted that the present state-of-the-art in explosion science does not allow one to reliably predict diffuse fuel explosion pressure development within an enclosure, using any methodology. Computational Fluid Dynamics (CFD) is beginning to provide major improvements in the analytical prediction of the effects of volumetric explosions (i.e., gas, dust and hybrid explosive systems). A range of CFD computer codes exist, and many of these codes are commercially available, some examples are the commercial FLUENT code, the KIVA code[10] and the IIT code.[11,12] These codes clearly demonstrate that CFD technology is very close to providing a valuable tool for explosion investigation, but at least three problems remain before this analysis tool can be practical. First, to represent realistic configurations the geometry is generally complex. In some cases two-dimensional analysis may be sufficient, but many times three-dimensional computations are appropriate. In addition, the analysis probably requires a fine numerical grid in at least some locations, and as a consequence a full evaluation generally requires substantial computer running time. Often a simplified configuration is adequate and can go a long way toward making the analysis more practical. Second, for explosion analysis the numerical method must have the ability to resolve shock waves. This requires special numerical schemes such as Godunov, Van Leer, Flux Corrected Transport (FCT), Total Variation Decreasing (TVD), and others.[13–25] Third, the reaction kinetics must be represented realistically. One approach, given in references 11 and 12, uses the reaction kinetics in Arrhenius form. Generally major simplifications in the kinetics scheme are made in analyses of this type.

The work presented in references 11 and 12 was in support of experimental detonation tube studies of a wide variety of pyrotechnic formulations being evaluated for landmine neutralization and other applications for the Army. Formulations evaluated included particulate explosives (e.g., TNT and RDX), particulate ammonium perchlorate (AP), atomized and flaked aluminum, and other constituents dispersed in air and nitrogen (e.g., reference 26). Although the work was not directly in support of process accident investigation, the results of both the analytical and experimental investigations are potentially useful in understanding explosion effects from a dispersed pyrotechnic in a process accident.

Usually an analysis involving major effort, such as a detailed CFD model is only justified in cases of very large losses. Although the accuracy might not be improved by such an analysis (e.g., overpressure prediction), the insight into the physics involved might be greatly enhanced. For these reasons, there is still a strong reliance on measurements from large-scale experiments. Although large-scale experiments are costly, these experimental results are more easily accepted than are predictions based upon analysis.

TNT Equivalency and Other Equivalency Methods

TNT equivalency or other equivalency methods are particularly useful for the analysis of large-scale accidents with high overpressures at the origin (e.g., vapor cloud, condensed explosive, and some pyrotechnic material accidents). In TNT equivalency methods, the available explosion energy in the accident is converted to the equivalent mass of TNT. Thus, explosion effects, particularly overpressure as a function of distance, are then basically a function of the TNT equivalent mass. Explosion effects for TNT are well known and available in various references (e.g., see references 5 and 27–30).

The TNT equivalency approach is discussed in the context of chemical process explosions in Perry's *Chemical Engineer's Handbook*.[31] Pyrotechnics manufacturing operations are in fact chemical process plants, with specialized aspects due to the reactive nature of the final products and many of the in-process material

forms. Of particular concern in the general chemical process industry are chemical reactor runaway reactions, inert pressure vessel explosions, and pressure vessel explosions involving flash vaporizing liquids. For pressure vessel explosions involving compressed gas, the equivalent mass of TNT is computed by assuming isentropic expansion of the gas from the initial vessel pressure to ambient pressure and dividing by the detonation energy of TNT. The resultant energy is partitioned into 30% for blast, 40% for fragments, and 30% for other dissipative mechanisms. For diffuse fuels such as flammable vapor clouds, a yield factor is typically applied to the calculation to account for inefficiencies in explosive combustion, mainly due to inhomogeneities in fuel-air mixing. This factor usually ranges from 1 to 40% depending on the circumstances. TNT equivalency methods are generally thought to be satisfactory as long as the far-field potential is the major concern. In the near field, where there can be significant distortion of the blast, then either numerical modeling or simulation experiments must be conducted.

Other equivalency methods have evolved in recent years for systems such as flammable vapor clouds. The multi-energy method has received wide acceptance for use with unconfined vapor cloud explosions. In this method, potential sources of strong blast are identified, energies are computed, and the relative blast strength is estimated. Strong blast sources generally correspond to locations where there is partial confinement or where the cloud is congested with obstacles that produce turbulence. Sachs-scaled blast parameters are utilized to determine blast variables of interest as a function of distance. Blast variables generally include peak over-pressure, positive phase impulse, time of arrival, positive phase duration, and shock velocity. A good compilation and discussion of these methods is listed in reference 32.

Ground Shock Analysis

After an accidental explosion occurs, there are generally numerous reports of damage to surrounding property. This damage is many times attributed to air blast or ground shock. For

air blast damage, the TNT equivalency methods described above can be used to evaluate which of these claims are credible. An extension of the air blast methods can be employed to evaluate ground shock damage, as well. Ground shock analysis methods have been used for the design of structures to resist accidental explosions in pyrotechnics manufacturing and storage facilities, and to design structures to resist weapons effects in military applications. Ground shock can be evaluated as having two contributing parts: the air blast induced ground shock and the direct induced ground shock. The air blast induced ground shock is (as the name implies) the ground shock disturbance that follows the air shock as it propagates outward from the explosion center. The direct induced ground shock is the disturbance that passes from the explosion directly into the ground medium. This component depends on the coupling of the explosion to the ground at the source. Many times the explosion is not in direct contact with the ground surface, and the resulting direct induced ground shock is substantially diminished because of this poor coupling. To conduct a ground shock analysis, the characteristics of the soil medium (e.g., seismic velocity and density) and characteristics of an underlayer such as the water table or a rock layer must be known.

Sources of information on this subject can be found in references 28–30. These are each in a workbook form, which aid in their application by a knowledgeable practitioner. Each of the references were developed for different specific purposes, and their domains of applicability must be considered by the user. The Pantex Manual[28] concentrates on buried explosions, either in direct ground contact or within an underground cavity. Since the explosions are buried, no air blast induced ground shock is considered. TM 5-1300[29] is concerned with designing structures against accidental explosions. It considers both air blast induced ground shock and direct induced ground shock. These methods do not directly include an underlayer. TM 5-855-1[30] is concerned with designing structures against conventional weapons. To use this approach for an above ground accidental explosion, an equivalent TNT hemisphere is assumed to sit on the ground surface. The height of the burst is not automatically taken into account for

ground shock. An underlayer can be considered. These references provide the procedures to conduct a good assessment of the effects of ground shock on structures, based on predicted maximum displacement, velocity and acceleration. A criterion used frequently for the threshold of damage is a maximum velocity of 2 inches (51 mm) per second. A more comprehensive approach is to conduct a structural analysis for a specific structure, given the predicted ground shock characteristics.

Dynamic Fuel Concentration Modeling

The analysis of flammable gas concentrations has been used to evaluate whether a gas leak could have been responsible for a fire/explosion incident and to assist in determining the source of the gas. These models can be used to calculate the gas concentration as related to time and elevation in the space, and they can be correlated with explosion damage. Models may range from simple exponential mixing calculations in a control volume, to detailed computational fluid dynamic (CFD) models incorporating diffusion, turbulence and gravity effects.

Flammable gas concentration modeling, combined with an evaluation of explosion/fire damage and the location of possible ignition sources, can be used to establish whether or not a suspected or alleged leak could have been the cause of an explosion/fire and to determine what source(s) of gas or fuel vapor was consistent with the explosion/fire scenario, damage, and possible ignition sources. Useful sources of information on this topic include references 9, 33, and 34.

Thermodynamic Chemical Equilibrium Analysis

Fires and explosions that are suspected of being caused by reactions of known or suspected chemical mixtures can be investigated by a thermodynamic analysis of the probable chemical mixtures and potential contaminants. This type of analysis can be used to help answer causal investigative questions such as: What reaction(s) could have caused the fire/explosion? Was the reaction spontaneous or did it require an outside source of energy? Was

there an improper mixture of chemicals or a contamination? Did a chemical or chemical mixture overheat? Was there a vapor release followed by an outside ignition?

Thermodynamic reaction equilibrium analysis requires tedious hand calculations or the use of a complex computer code. Several of these thermodynamic codes that are available are reviewed in reference 35. These computer programs usually require the input of material and the material's properties that include the chemical formula, density, mass, entropy and heat of formation. Sources for this information include the JANAF tables,[36] Chemical and Chemical Engineering Handbooks, published papers, material safety data sheets, and the NIST Chemistry WebBook.[37]

The state of the art of equilibrium thermochemical codes for explosion analysis is represented by the CHEETAH Code.[38] This code was developed by Lawrence Livermore Laboratory. It is an improved version of the TIGER Code.[39] The Code is quite easy to use—it is user friendly. However, this code is currently available only to the government and government contractors working on government projects. To use the code properly, the user should have a reasonable understanding of how equilibrium thermochemical codes work. For example, there are several options for equation of state and species libraries, each of which has certain domains of applicability. There are a number of state characterizations to choose from. The primary application of this code is for the characterization of condensed explosive and pyrotechnic propellant formulations, but diffuse fuel-air applications are easily handled. Because of the limited availability of this code, other codes such as NASA-Lewis and others (see reference 35) should be employed where necessary.

Damage Pattern Analysis

Damage pattern analysis usually includes analysis of debris and structural damage. Often, it is very useful to prepare diagrams showing relative damage patterns. Debris patterns often can show the direction and relative force of the explosion. However, different drag or lift forces of various fragment shapes will tend to favor some shapes continuing on further trajectories. These factors must be considered in relative force comparisons. Quite often, investigators erroneously assume that the fragments that have gone the furthest are representative of the strongest force and direction of the explosion. References 27 and 32 aid in this type of analysis.

Structural damage analysis usually involves the estimation of overpressures and sometimes the impulse necessary to produce the damage. Several generalized overpressure damage listings are compiled in the literature (see references 1, 9, 27, 31, and 32). These are quite useful for making quick estimates. These lists are usually derived from data where explosive impulse is very high at a given overpressure, where the overpressure approximates a static application. Thus, such data can be quite useful for applications involving fuel, gas or dust explosions, where such an approximation is usually valid.

If needed, various structural computer programs can be used, however, sometimes a structural damage expert will be necessary. Some examples of practical computer programs are listed in reference 40.

Systems Safety Analysis

Systems Safety Analysis (SSA) techniques are particularly useful for explosion investigations. They can help identify potential causes of an explosion, and they can indicate where further analysis should be directed. A formalized SSA is generally most useful in a large and/or complex incident. It can be very effective in identifying all factors, both physical and human, which did or could have contributed to the cause of the explosion. Similarly, it can be helpful in eliminating potential causes of an explosion.

These techniques include Failure Modes and Effects Analysis (FMEA), Fault Tree Analysis, HAZOP Analysis, What-If Analysis, etc. In general, these tools provide a systematic method for analyzing large complicated systems to determine hazards or faults. The tools can utilize either qualitative or quantitative formats. Hazard probabilities or failure rates can be factored in when using quantitative for-
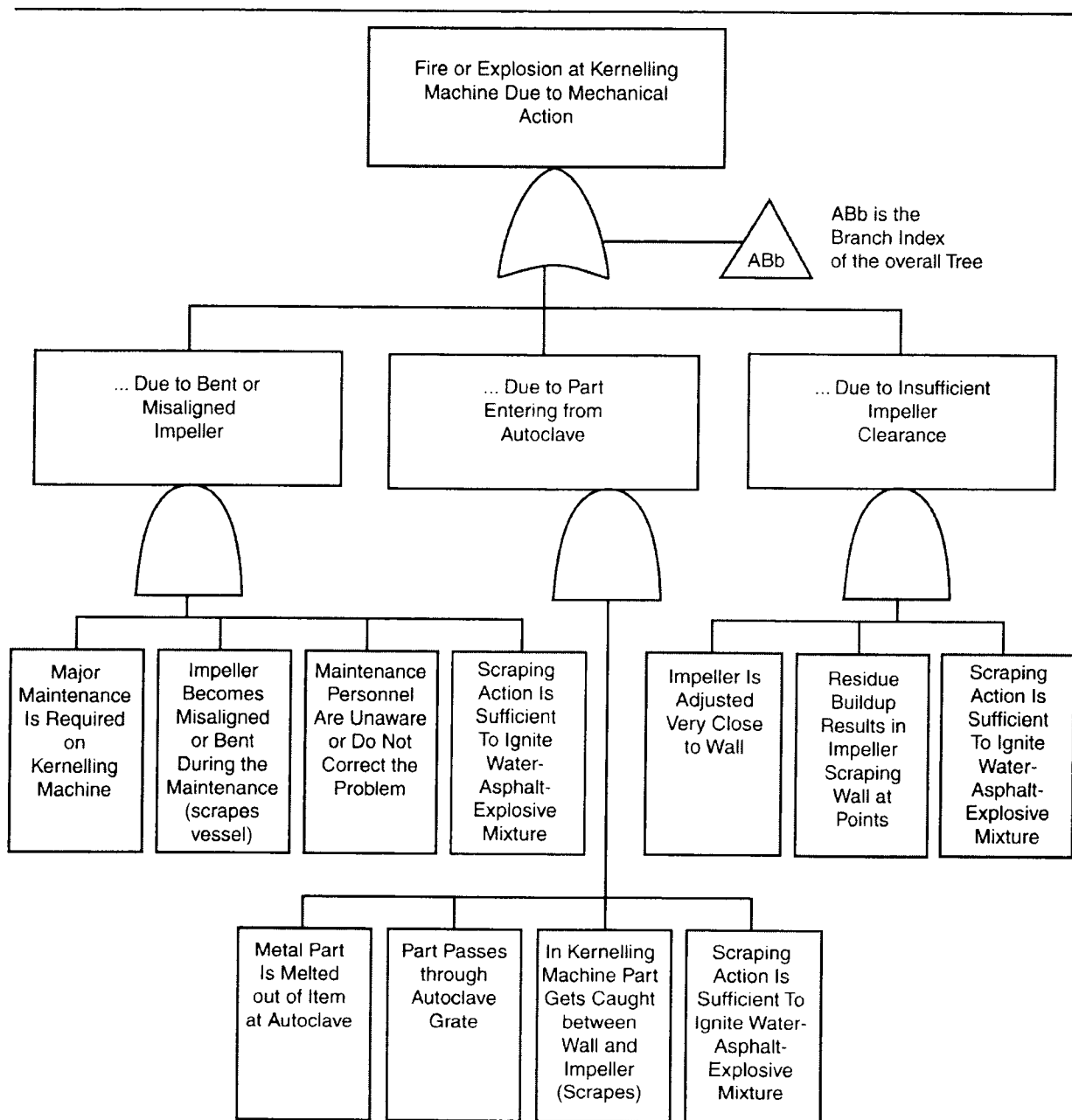
Figure 2. Fault Tree Example.

mats. Some of the more common techniques—failure mode and effects analysis and fault tree analysis—are described below.

Failure Modes and Effects Analysis

A FMEA is a relatively simple and straight-forward technique to identify basic sources of failure within a system and to follow the consequences of these failures in a systematic fashion. In fire/explosion investigations, the purpose of the FMEA is a systematic evaluation of all equipment and/or actions that could have contributed to the cause of the incident. A FMEA is prepared by filling in a table with row headings such as those shown in the example in Table 1. The row headings and format of the table are flexible, but at least three items are common: the item (or action) being analyzed, the basic fault (failure) or error that created the hazard, and the consequence of the failure. Additional rows are added by the investigator as needed for

Table 1. Example Failure Mode and Effects Analysis.

Item No.	Part Name	Operating Mode	Failure Mode	Est. Prob.	Failure Effects	Hazard Description	Haz. Cat.	Recommended Controls	Remarks
301	Cellulose hoppers (not enclosed)	Normal abnormal	Conveyor control failure, hopper overfills	Low	Fire or dust explosion if initiation source present	Flammable cellulose material present in unwanted areas due to hopper overfill	II	• Level sensor in hopper interlocked with conveyor power • Sprinkler system • TV surveillance • Consider dust collection system at conveyor transfer point • Inspection ports	Cellulose fire is likely to be a smoldering type
			ESD at hopper discharge	High	Fire or dust explosion if ESD is sufficient	Cellulose discharge process generates ESD	II	• Design unit to minimize problem using conductive materials and proper grounding and bonding	
			Severe friction in hopper auger	Low	Fire in cellulose; possible spread to other parts of the process	Cellulose in presence of frictional heat source	II	• Design unit to minimize problem • TV surveillance	
302	Weigh conveyor (enclosed)	Normal abnormal	Mechanical or control failure, overfills nitrator	Low	Fire or dust explosion if initiation source present; or denitration/fire/explosion if cellulose not wetted properly in nitrator causes hot spots	Flammable cellulose material spilled in unwanted areas due to nitrator overfill, and improper wetting of cellulose in nitrator	II	• Consider non-water fire suppression system • TV surveillance • See recommended controls for nitrator	Minimize possibility of water introduction into nitrator

the particular investigation at hand. An assessment of the likelihood of each individual failure mode is frequently included. Also, it is sometimes helpful to assess the severity of a given failure. Also, it is sometimes helpful to assess the severity of a given failure relative to the fire/explosion. FMEA tables can also be catalogued by item and serve as reference material for further investigations.

When filling out the table, the investigator should consider for each item/action the range of environmental conditions and the process status (i.e., normal operation, shutdown, startup, etc.). Qualitative or quantitative values can be assigned as probabilities of occurrence. Then, when a sequence of failures is required for an incident to occur, the probabilities can be combined to assess the likelihood that any given sequence of events led to the incident.

The usefulness of FMEA is limited by the ability of the investigator to identify all system components (or human actions) that may have contributed to the incident. Furthermore, the evaluation of the likelihood that a given sequence of events caused the incident is only as good as the ability of the investigator to assign accurate probabilities to each of the individual failure modes that contributed to the sequence.

Fault Tree Analysis

A fault tree is a diagram used to analyze an undesired event. The undesired event is placed at the top of the diagram, and all the causes that can lead to the event are grouped below. This approach is repeated for each cause and continues until the desired level of detail is reached or the root causes of the event are determined. The diagram takes the form of an inverted tree. The relationships between the events leading to the undesired event are described by the use of "AND" and "OR" gates at the junction(s) leading to the next level of the event. An example diagram is shown in Figure 2.

Once a complete fault-tree is developed for an undesired event, an investigator can look at each of the root causes of the undesired event and all of the steps necessary for the event to happen. If any of the necessary steps did not occur, the root cause associated with that particular path can be eliminated.

It is possible to assign values associated with the probability of occurrence to the root causes and other independent aspects of the fault-tree. The probability of each path leading to the undesired event can then be evaluated. The investigator will find that information on the probability of the occurrence of causes is difficult to find or not available. In most cases the assignment of a probability of occurrence will be based on experience, engineering judgment, tests, incident reports, models or published data. Any time probabilities are assumed, the sensitivity of the outcome to the assumed value should be determined by reevaluating the outcome with slightly modified values.

Reference 41 provides additional guidelines for conducting these and other types of systems safety analyses.

Example Application

The use of some of these tools is illustrated for the Pepcon explosion investigation.[2] This incident originated as a fire in a large ammonium perchlorate (AP) plant located in Henderson, Nevada. The fire quickly spread through most of the facility by means of thermal radiation, firebrands, a continuous (linear) source of fuel, and some natural self-propelled missiles. Two large explosions occurred during the fire, each equivalent in energy to a few hundred tons of TNT. The explosions claimed two lives, injured 372 people and damaged plant buildings and nearby residential buildings. Some of the tools used in the analysis are illustrated below, in limited detail.

A videotape of the event from a nearby mountaintop permitted advanced reconstructive techniques, such as superimposing CAD outlines of the plant on video records. This, together with witness accounts, greatly aided in constructing a detailed timeline of events from ignition, through various modes of flame spread through the plant, to the two large explosions (see Figure 1). The size and shape of the extremely large fire plumes advancing through the plant were determined. Graphical plot plan diagrams of the fire/explosion progress were prepared for different time slices (one example is shown in Figure 3).
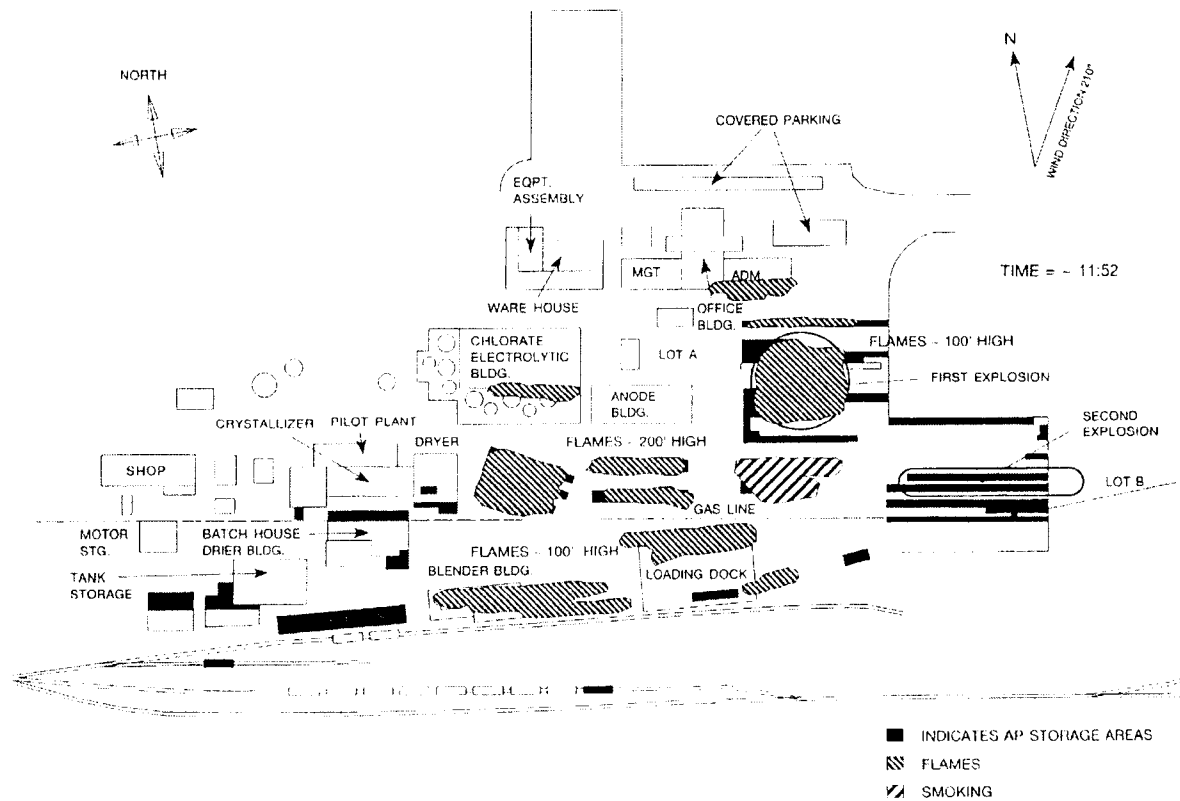
Figure 3. Pepcon Fire Progress at 11:52 AM

Thermal radiation heat transfer calculations aided in the determination and confirmation of the flame-spread theories. A radiant heating model was constructed that showed that significant preheating of drums/bins of AP in storage lots near the huge fire plumes had occurred before initiation of the detonation. The model consisted of a marching/growing radiant plume model coupled with a one-dimensional conduction heat transfer model of a bin. Due to the large size of the bins and their orientation with respect to the immense fire plumes, an assumption of modeling the bin as a semi-infinite solid was appropriate. This analysis was very useful in predicting that pyrolysis of AP in strongly preheated bins would cause them to burst and disperse some of their contents onto nearby fuels, providing a more-easily initiated explosion layer, which could serve as an explosive booster to the drums and bins.

Explosion dynamics estimates aided in determining the locations of the initial small explosions and in estimating the amount of prod-

uct involved in the large explosions as sympathetic detonations. Experimental data on AP and AP/fuel explosion characteristics provided guidance for possible modes of explosion initiation and propagation. A thermodynamic equilibrium analysis was done to determine the energy release from AP and different fuels at the plant. Structural damage data helped assess the overpressures experienced in the area.

Possible causes of the initial fire were ascertained, and the most probable was related to welding sparks coming into contact with contamination-sensitized AP. The official cause remains undetermined. Conclusions were formulated regarding major factors involved in the ignition, the extreme rate of fire spread, and the explosion initiation and propagation.

Summary

Currently the engineer investigator has a range of practical analytical tools for effective investigation of explosions. These "tools" can be applied to the investigation of incidents in pyrotechnics manufacturing facilities. Most of the tools require that accurate data from the incident be available. Thus, data gathering activities are crucial to a successful investigation.

Although many analytical methods are available, desirable advancements in the area of explosion science to aid in such investigations include: verified field modeling of vented explosions in enclosures, a wider range of data and models for estimating vented explosion external pressures, more refined models for gas mixing, additional experimental investigation and modeling for estimating cascade fuel/air explosion overpressures in successive compartments, and verified field modeling of explosions in highly elongated geometries.

References

1) NFPA 921, *Guide for Fire and Explosion Investigations*, National Fire Protection Association (1998 ed.).

2) K. R. Mniszewski, "The Pepcon Plant Fire/Explosion: A Rare Opportunity in Fire/Explosion Investigation", *J. Fire Protection Engineering*, Vol. 6, No. 2 (1994).

3) NFPA 68, *Guide for Venting of Deflagrations*, National Fire Protection Association (1998 ed.).

4) R. K. Eckhoff, *Dust Explosions in the Process Industries*, Butterworth-Heinmann (1991).

5) CPIA, *Hazards of Rocket Propellants*, Vol. 1–3, Chemical Propulsion Information Agency, CPIA Publication 394 (1985).

6) J. M. Kuchta, *Investigation of Fire and Explosion Accidents in the Chemical, Mining, and Fuel-Related Industries—A Manual*, Bureau of Mines, Bulletin 680 (1985).

7) Zalosh, R. G., "Explosion Protection" Chapter, *Fire Protection Engineering*, Society of Fire Protection Engineers, 2nd ed. (1995).

8) ASTM E 1226-88, *Standard Test Method for Pressure and Rate of Pressure Rise for Combustible Dusts* (1988).

9) R. J. Harris, *The Investigation and Control of Gas Explosions in Buildings and Heating Plant*, E&FN Spoon Ltd. (1983).

10) A. A. Amsden, J. D. Ramshaw, P. J. O'Rourke and J. K. Dukowicz, "KIVA: A Computer Program for Two- and Three-Dimensional Fluid Flows with Chemical Reactions and Fuel Sprays", Los Alamos National Lab, NM, LA-10245-MS (1985).

11) R. Pape, D. Gidaspow and S. Wu, "Multiphase Flow in Slurry Bubble Column Reactors and Solid Propellant Rockets", *Second International Symposium on Numerical Methods for Multiphase Flows*, ASME Fluids Engineering Division, San Diego, CA (July 1996).

12) R. Pape and D. Gidaspow, "Numerical Simulation of Intense Reaction Propagation in Multiphase Systems", *AIChE Journal*, Vol. 44, No. 2 (February 1998).

13) G. C. Zha and F. Bilgen, "Numerical Solutions of Euler Equations by Using a New Flux Vector Splitting Scheme", *International Journal for Numerical Methods in Fluids*, Vol. 17 (1993) pp 115–144.

14) B. Van Leer, "Towards the Ultimate Conservation Difference Scheme V. A. Second-Order Sequel to Godunov's Method", *Journal of Computational Physics*, Vol. 32 (1979) pp 101–136.

15) S. K. Godunov, A. V. Zabrodin and G. P. Prokopov, "A Computational Scheme for Two-Dimensional Non Stationary Problems of Gas Dynamics and Calculation of the Flow From a Shock Wave Approaching a Stationery State", *Zh. vych. mat.*, Vol. 1, No. 6 (1961) pp 1020–1050.

16) B. A. Finlayson, *Numerical Methods for Problems with Moving Fronts*, Ravenna Park Publishing, Inc., Seattle, WA (1992).

17) M. R. Baer and R. J. Gross, "A Two-Dimensional Flux-Corrected Transport Solver for Convectively Dominated Flows", *Sandia Report SAND85-0613*, Reprinted (February 1989).

18) M. R. Book and M. A. Fry, "Airblast Simulations Using Flux-Corrected Transport Codes", *Naval Research Laboratory Memorandum Report 5334*, AD-A142 820 (May 1984).

19) D. L. Book, Ed., "Flux Corrected Transport", *Finite-Difference Techniques for Vectorized Fluid Dynamics Calculations*, Chapter 3, Springer-Verlag, New York (1981).

20) J. P. Boris and D. L. Book, "Flux-Corrected Transport III Minimal-Error FCT Algorithms", *Journal of Computational Physics*, Vol. 20 (1976) pp 397–431.

21) R. J. Gross and M. R. Baer, "ETBFCT-A Solver for One-Dimensional Transport Equations", *Sandia Report SAND85-1273* (October 1985).

22) S. R. Chakravarthy, K. Y. Szema, U. C. Goldbert and J. J. Gorski, "Applications of a New Class of High Accuracy TVD Schemes to the Navier-Stokes Equations", AIAA Paper 85-0165, American Institute of Aeronautics and Astronautics, *Twenty Third Aerospace Sciences Meeting*, Reno, NV (January 1985).

23) S. R. Chakravarthy and S. Osher, "A New Class of High Accuracy TVD Schemes for Hyperbolic Conservation Laws", AIAA Paper 85-0363, American Institute of Aeronautics and Astronautics, *Twenty Third Aerospace Sciences Meeting*, Reno, NV (January 1985).

24) H. C. Yee, "Linearized Form of Implicit TVD Schemes for the Multidimensional Euler and Navier-Stokes Equations", *Computers & Mathematics with Applications*, Vol. 12A, No. 4/5 (1985) pp 413–432.

25) H. C. Yee, "Construction of Explicit and Implicit Symmetric TVD Schemes and Their Applications", *Journal of Computational Physics*, Vol. 68, No. 1 (1997).

26) A. J. Tulis et al., "Phenomenological Aspects in Explosive Powder/Gas Two-Phase Detonations," *Int. Symposium on Combustion*, Combustion Institute, University of California, Irvine, CA (1994) p 79.

27) E. W Baker, et al., *Explosion Hazards and Evaluation*, Elsvier Publishing (1983).

28) U.S. Department of Energy DOE/TIC-11268, *A Manual for the Prediction of Blast and Fragment Loading on Structures*, (Pantex Manual) (1980).

29) U.S. Army TM 5-1300, *Structures to Resist the Effects of Accidental Explosions* (1990).

30) U.S. Army TM 5-855-1, *Fundamentals of Protective Design for Conventional Weapons* (November 1986).

31) R. H. Perry and D.W. Green, *Perry's Chemical Engineer's Handbook*, McGraw Hill (1999).

32) AICHE, *Guidelines for Evaluating the Characteristics of Vapor Cloud Explosions, Flash Fires and BLEVEs*, AICHE, Center for Chemical Process Safety, 1st ed. (1994).

33) R. H. Valentine, et al, "The Transient Mixing of Propane in a Column of Stable Air to Produce a Flammable but Undetected Mixture", *Winter Annual Meeting*, American Society of Mechanical Engineers (November 1974).

34) V. A. Rabinkov, "The Distribution of Flammable Gas Concentrations in Rooms", *Fire Safety Journal*, Vol. 13, Nos. 2 & 3 (May 1988).

35) K R. Mniszewski, "The Use of Computerized Thermodynamic Tools in Fire/Explosion Investigation", *J. of Fire Protection Engineering*, Vol. 3, No. 3 (1991).

36) D. R. Stull and H. Prophet, *JANAF Thermochemical Tables*, 2nd ed., Office of Standard Reference Data, National Bureau of Standards, Washington, DC (1971).

37) NIST Chemistry WebBook, on the internet at http://webbook.nist.gov