

## 40

# The Science and Engineering of Explosions

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### 40.1

#### Introduction

The topic of “explosions” is extremely important in loss prevention engineering. The goal is to improve scientific and technical knowledge and understanding of explosions in general, and methods for their prevention and control. Topics covered in this chapter include: fundamentals of explosions, blast damage due to overpressurization, blast fragment missile damage, evolution of flammable material, dispersion and possible ignition of released material, plume and puff distribution, vapor cloud explosions (VCEs), and energy of mechanical explosions. The emphasis is on understanding and applying the technical ideas in real-world situations; the learning objectives are set out below. In the source release of material, the evolution and dispersion of liquids and gases being released under pressure is considered. They can be toxic or flammable or explosive in nature, and this is extremely dangerous. If the ensuing cloud comes in contact with an ignition source, and the fuel:air ratio is within flammability bounds, the resulting explosion and fire can often be devastating.

#### Learning Objectives

1. Develop an understanding of explosion phenomena, from fuel release, dispersion and possible ignition, and explosion, to the devastation produced and subsequent investigation.
2. Develop an appreciation of the safety and loss prevention issues involved in the occurrence of explosions, and methods that be used to prevent them, and/or that can mitigate the extent of damage.
3. Develop an ability to calculate useful information from empirical equations that describe the observed explosion phenomena, so permitting deductions to be made for other situations that are interpolated or extrapolated from a limited amount of experimental data.
4. Introduce mathematical modeling concepts related to the computer-based calculation procedures for simulating fuel release, dispersion, and possible ignition

Explosions, and the evolution, dispersion, and possible ignition of flammable fuel release into the atmosphere, are important safety topics in loss prevention engineering, and ASME (1973), Combustion Institute (1979), AGA (1988), Lilley (1990a,b, 1995a,b, 1996a,b, 2012), NFPA (2008), and SFPE (2008) list some of the basic properties of flammable liquids, gases, and solids. In the release and dispersion of flammable material, either particles of solids, liquid droplets of various sizes, or a vapor cloud are formed which spread and disperse as the released material mixes and is carried downstream in the atmosphere. See other references given in the extensive reference list. Solid and liquid droplet trajectories were discussed in detail by Lilley (2010).

If the initial breakage does not produce an immediate explosion and fire, the main problem with the released material is that it is important to know if a potential ignition source is located where the fuel concentration is within the flammable or explosive limits, these being the percentage (usually by volume) of a substance in air that will burn once ignited. Most substances have both an upper (rich) and a lower (lean) flammable (explosive) limit, called the upper explosive limit (UEL) and lower explosive limit (LEL), respectively. Either too much or too little fuel in the vapor–air mixture can prevent burning. There is a wide range of fuels with different flammable limits. Higher temperatures and/or higher pressures generally increase the range over which a given fuel–air mixture is capable of being ignited and burned. Lilley (2012) discussed the entire “fire dynamics” problem from ignition to investigation and beyond.

Chemical engineering problems of release and dispersion of toxic substances were discussed in detail in Lees (1980), Hanna and Drivas (1987), Crowl and Louvar (1990), EPA, NOAA and NSC (1992), Kletz (1994), LaGrega, Buckingham, and Evans (1994), DeNevers (1995), and Wark, Warner, and Davis (1998). Cote and Linville (1990) described many of the manufacturing processes used in industry, identified the fire hazards associated with those processes, and detailed the methods used to control and eliminate them. Litigation aspects associated with the reasons for the occurrence of fires and explosions – origin, cause, and responsibility – have been addressed in several texts, including Kennedy and Kennedy (1985, 1990), Berry (1989), and Patton (1994). Lilley (1995a,b, 1996a,b, 1997a–c, 1998a,b, 1999, 2003, 2004a, 2012) has listed some of the basic properties of flammable liquids, gases, and solids.

Many of the effects of explosions, release, and dispersion of material are presented in empirical equations, and programmed into Visual Basic for Applications (VBA) codes, behind the Excel spreadsheet, and results are automatically tabulated with 2D and 3D graphic illustrations. In the dispersion of the released material, in particular, the mass fraction, volumetric fraction, and parts per million at locations further downstream and to the side are calculated, and related to the possible ignition. A multitude of parameters affecting the situation can be changed to illustrate their influence on the calculations. Depending on the atmospheric stability conditions, wind speed, and amount of material released, the concentration levels of the released material at specific locations may or may not provide potential ignition from a competent ignition source.

## 40.2

### Fundamentals of Explosions

#### 40.2.1

##### Basics

The National Fire Protection Association's *Guide to Fire and Explosion Investigation*, NFPA 921 (NFPA, 2011), simply and generally defines explosion as "The sudden conversion of potential energy (chemical or mechanical) into kinetic energy with the production and release of gases under pressure, or the release of gas under pressure. These high-pressure gases then do mechanical work such as moving, changing, or shattering nearby materials." Another general description considers an explosion to be the process of rapid release of energy involving spontaneous and vigorous reactions with rapid production of very large volumes of gases and heat fluxes, having destructive effects on nearby surroundings. Explosions are mostly classified into diffuse and concentrated types of explosions, with low-yield and high-yield explosives, and background familiarity with fires and explosions may be gleaned from Crowl and Louvar (1990) and Lees (1980). Further information about fires and explosions is available in short courses by Lilley (2003, 2004a) and a handbook chapter on fire dynamics (Lilley, 2012). Typical explosion characteristics are given in Table 40.1.

Cote and Linville (1990) aimed to describe many of the manufacturing processes used in industry, to identify the fire hazards associated with those processes, and to detail the methods used to control and eliminate them. They provide a basic reference book for those charged with protecting life and property in industry. They give a broad yet thorough introduction to the vast array of major industries and industrial processes, with emphasis on the fire hazards that accompany them. Information is presented about major industries and industrial processes, fire hazards associated with them were identified, and methods used to eliminate or control the hazards are explained. Litigation aspects associated with the reasons for the occurrence of fires – origin, cause, and responsibility – have been addressed in several texts, including Berry (1989) and Patton (1994).

Important technical fundamentals about chemical process safety, health, and loss prevention have been addressed in AIChE (1990), Crowl and Louvar (1990), NFPA (2008), and SFPE (2008). Identified are the many principles, guidelines, and calculations that are necessary for the safe design and operation of chemical plants, and analysis of failures. Numerous worked-out examples and exercises illustrate how the principles are applied in practice. The coverage includes the following:

- **Fires and explosions** – These can be prevented by the design of inerting, purging, and ventilation systems. Static electricity build-up (from flowing fluids) is computed.
- **Vessel overpressure protection** – Relief systems protect process vessels from runaway reactions, external fires, and so on. Two-phase flow relief sizing procedures are included.

**Table 40.1** Typical explosion characteristics<sup>a</sup>; see NFPA 921 (NFPA, 2011).

Typical characteristics	Lighter-than-air gases	Heavier-than-air gases	Liquid vapors	Dusts	Explosives	Backdrafts	BLEVEs <sup>b</sup>
Low-order damage	3	4	4	2	2	5	2
High-order damage	2	1	1	2	3	0	2
Secondary explosion	3	3	2	4	0	1	0
Gas/vapor/dust pocketing	3	2	2	2	0	0	0
Deflagration <sup>c</sup>	4	4	4	4	1	5	4 <sup>d</sup>
Detonation	1	1	1	1	4	0	1 <sup>d</sup>
Underground migration	2	2	2	0	0	0	0
BLEVEs	2	3	5	0	0	0	5
Post-explosion fires	3	3	4	3	1	5	3
Pre-explosion fires	2	2	2	3	2	5	4
Seated explosions	0 <sup>e</sup>	0 <sup>e</sup>	0 <sup>e</sup>	0	4 <sup>f</sup>	0	2
Minimum ignition energy (mJ) <sup>g</sup>	0.17–0.25	0.17–0.25	0.25	10–40	<sup>g</sup>	—	<sup>h</sup>

<sup>a</sup>0 = never 1 = seldom, 2 = sometimes, 3 = often, 4 = nearly always, 5 = always.

<sup>b</sup>BLEVE = boiling liquid expanding vapor explosion.

<sup>c</sup>Deflagrations may transition into detonations under certain conditions.

<sup>d</sup>The strength of the confining vessel may allow the pressure wave at failure to be supersonic.

<sup>e</sup>Gases and vapors may produce seats if confined in small vessels, and if the materials on which they explode can be sufficiently compressed or shattered.

<sup>f</sup>All high explosives and some low explosives will produce seated explosions if the materials on which they explode can be sufficiently compressed or shattered.

<sup>g</sup>Ignition energies vary widely. Most modern high explosives are designed to be insensitive to ignition. Energies for detonations are nine orders of magnitude larger than the minimum ignition energies.

<sup>h</sup>BLEVEs are not combustion explosions and do not require ignitions.

- **Hazards identification and risk assessment** – These are carried out by HAZOP, fault trees, event trees, and other techniques. Accident probability is calculated.
- **Source models** – These are described quantitatively. Various spill scenarios from accidents are formulated.
- **Dispersion modeling** – Calculations for areas affected by the accidental release of process materials are given.

Information is provided about latest process safety techniques so as to aid in the prevention and mitigation of catastrophic incidents. Table 40.2 states the means of measuring and controlling fire hazards of materials and these will be of special interest. Materials may be solids, liquids, and gases and the table includes ignition, spread and growth, and fire impact. Some key points about fire hazards of gases and dusts are that gases and dusts burn rapidly once ignited, the principal measurement tool is determination of flammability limits, and there is a possibility of reducing the likelihood of ignition of gas or dust by adding chemical inhibitors

**Table 40.2** Means of measuring and controlling fire hazards of materials; see NFPA (2008).

Hazard component	Ignition		Spread and growth		Fire impact	
	Measurement	Ignition control	Measurement	Control of spread and growth	Measurement	Control of fire impact
<i>Gases</i>	Ignitability limits	Storage and handling safeguards Inerting of atmospheres	Flammability limits, density, diffusion coefficient	Tank venting procedures	Placarding, NFPA Hazardous materials identifiers	Emergency response and evacuation Placarding, NFPA hazardous materials identifiers
<i>Liquids</i>	Flash point	Handling safeguards Hazard classification systems	Volatility	Ventilation and flame arrest Storage and tank separation	Placarding, NFPA Hazardous materials identifiers	Emergency response and evacuation Placarding, NFPA hazardous materials identifiers
<i>Solids</i>						
Textiles, cushioning materials	Ease of ignition tests and small-scale flame spread tests	Flame-resistive materials and treatments Protective layers	Supported flame spread Rate of heat release	Material selection and assembly Detection and suppression	Toxicity of combustion products (under development) Smoke generation	Breathing apparatus for firefighters Smoke control systems
Structural materials, building components and finishes	Ease of ignition tests and small-scale flame spread tests	Flame-resistive materials and treatments Protective layers	Flame spread Rate-of-heat release	Fire resistivity Low combustibility Fire-resistive coatings Detraction and suppression	Fire endurance (stability, integrity, insulation) Smoke and toxic combustion products	Breathing apparatus for firefighters Smoke control systems Construction design, compartmentation, separation

to raise the lower flammability limit (LFL). Key points about liquids are that most hazardous combustibles have high vapor pressure, or high volatility, or low flash point. Note that the flash point is defined as the temperature at which a liquid gives off vapors which can be ignited and flash a flame momentarily over the surface under specified laboratory conditions. Concerning solids, unless these materials are present as dusts, or in other forms that present high surface areas, their fire hazards are similar to those of liquids. Solid material may be flexible (as in textiles and cushioning) or structured (as in steel, concrete, wood, and plastic foams).

#### 40.2.2

##### Explosion Characterization

Explosions are either detonations or deflagrations; the difference depends on the speed of the shock wave emanating from the explosion. It is known that the maximum pressure achieved and the maximum rate of pressure increase are important in characterizing the effect of an explosion. Experimental data are used in modeling simulations of the characteristics of explosions. The limits of flammability or explosivity are used to determine the safe concentrations for operation or the quantity of inert required to control the concentration within safe regions. The maximum rate of pressure rise is indicative of the robustness of an explosion. Hence the explosive behavior of different materials can be compared on a relative basis. Parameters that affect the behavior of explosions are the following:

- ambient temperature
- ambient pressure
- composition of explosive material
- physical properties of explosive material
- nature of ignition source: type, energy, and duration
- geometry of surroundings: confined or unconfined
- amount of combustible material
- turbulence of combustible material
- time before ignition
- rate at which the combustible is released.

A plot of the logarithm of the maximum pressure slope versus the logarithm of the vessel volume frequently produces a straight line of slope  $-1/3$ . This relationship is called the “cubic law,” with

$$\left(\frac{dP}{dt}\right)_{\max} V^{\frac{1}{3}} = \text{constant} = K_g \quad (40.1)$$

$$\left(\frac{dP}{dt}\right)_{\max} V^{\frac{1}{3}} = K_{St} \quad (40.2)$$

where  $K_g$  and  $K_{St}$  are the deflagration indices for gas and dust, respectively. As the robustness of an explosion increases, the deflagration indices  $K_g$  and  $K_{St}$  increase. Typical values are given in Table 40.3; see Bartnecht (1981). The consequences of an explosion in a confined space lead to

**Table 40.3** Average values of deflagration indices for selected gases and dusts; see Bartnecht (1981).

Gas	$K_g$ (bar m s <sup>-1</sup> )	
Methane	55	
Propane	75	
Hydrogen	550	

Dust	$P_{\max}$ (bar)	$K_{St}$ (bar m s <sup>-1</sup> )
PVC <sup>a</sup>	6.7–8.5	27–98
Milk powder	8.1–9.7	58–130
Polyethylene	7.4–8.8	54–131
Sugar	8.2–9.4	59–165
Resin dust	7.8–8.9	108–174
Brown coal	8.1–10.0	93–176
Wood dusts	7.7–10.5	83–211
Cellulose	8.0–9.8	56–229
Pigments	6.5–10.7	28–344
Aluminum	5.4–12.9	16–750

<sup>a</sup>PVC = poly(vinyl chloride).

$$\left[ \left( \frac{dP}{dt} \right)_{\max} V^{\frac{1}{3}} \right]_{\text{vessel}} = \left[ \left( \frac{dP}{dt} \right)_{\max} V^{\frac{1}{3}} \right]_{\text{laboratory}} \quad (40.3)$$

where the subscript “vessel” is for the reactor or building and the subscript “laboratory” applies to data determined in the laboratory using either the vapor or dust explosion apparatus. This equation allows the scale-up of experimental explosive behavior to real situations. The constants  $K_g$  and  $K_{St}$  are fixed for a particular material, but they depend on the situation: the composition of the mixture, the mixing within the vessel, the shape of the reaction vessel, and the energy of the ignition source.

#### 40.2.3

##### Vapor Cloud Explosions

VCEs are extremely dangerous and destructive. They can occur following a fracture or breakage of a vessel or piping, containing a superheated and/or pressurized liquid or gas, especially so if the liquid being released changes to vapor form as it is released and enters the lower atmospheric pressure. Liquefied petroleum gas (LPG) is an example of this, since it is only because of the high pressure in the tank that it is in liquid form. There is now either a sudden release (called a “puff” release) of a large quantity of flammable material (vapor of liquid droplets) or a continuous release (called a “plume” release) of flammable vapor. Then, the cloud

is carried downstream in the wind and mixes with air and reduces in concentration as dispersion of the vapor occurs. Details and sample calculations are given in Lilley (2008) for both puff and plume vapor cloud dispersion, where a simple VBA code behind the Excel spreadsheet is used for making calculations, which are then immediately portrayed in tabular and graphic form on the Excel spreadsheet. Finally, ignition of the resulting vapor cloud may occur if a suitable ignition source presents itself at a location in the vapor cloud where the fuel–air mixture is within the flammability limits.

### 40.3

#### Types of Explosions

##### 40.3.1

##### Diffuse Explosions

With stoichiometric or fuel-lean fuel–air mixtures, great amounts of heat are liberated in a very short time, and items will be readily affected. Clothing may be set on fire but other items such as furniture are less affected. There is no great potential hazard for an ensuing fire unless from easily ignitable elements such as clothing, curtains, and so on, which can themselves burn more and then ignite other items. These types of explosion result from having a mixture of fuel in the form of gas or vapor mixed with the right amount of air or more than enough air to allow complete combustion of all the fuel throughout the entire space at the same moment.

On the other hand, diffuse explosions with fuel-rich mixtures have an insufficient amount of air, resulting in incomplete combustion with fuel left over. Chemical reaction has not been completed. The sudden cooling and contraction of the heated gas/air sucks cooler air from the surroundings for further combustion with the unburned fuel, and a rolling fire occurs. A typical witness comment is “I heard a swoosh and saw a fire.”

##### 40.3.2

##### Concentrated Explosions

Concentrated explosions are from combustion of a material that carries along with fuel an internal oxidant, being independent of the surrounding oxygen that is in the air. Alternatively, the material may contain a very unstable material capable of rearranging its structure when detonated. These explosions are generally accompanied by high-velocity projectiles and/or fragmentation. Common concentrated or high-yield explosives include the following:

- **Aromatic Nitro Compounds** – These aromatic hydrocarbons are readily nitrated with strong nitric acids (e.g., toluene and benzene) to form trinitro compounds [e.g., trinitrotoluene (TNT) and trinitrobenzene (TNB)].



- **Dynamites** – These are nitroglycerine absorbed in dope compounds of combustible absorbent wood pulp and an extra oxidizing material, such as sodium nitrate.
- **Others** – These include picric acid, mercury fulminate mixed with potassium chlorate, tetryl, plastic explosives, and so on.

The properties of concentrated explosives include that all explosives have very high mechanical and thermal sensitivity, most explosives are subject to detonation, that is, mechanical effects that cause explosion, and surrounding temperatures and heat fluxes can alter the rate of the explosion.

#### 40.3.3

##### **Differences Between Concentrated and Diffuse Explosions**

The differences between diffuse and concentrated explosions lie in the reaction rate and reaction volume. Diffuse explosions require more time for total reaction. Concentrated explosions are concentrated in space, such as the explosion of dynamite. This is in contrast to a room filled with a combustible fuel vapor–air mixture which would generate a diffuse explosion. The total forces produced may be comparable but, because of differences in reaction rates and reaction volume, damage in the near vicinity of concentrated explosions is greater than that of the diffuse type. The potential for fire hazards is minimal with concentrated explosions compared with diffuse-type explosions, especially if the diffuse explosion is with a fuel-rich mixture. Concentrated explosions do not depend on surrounding oxygen for the combustion explosion to take place.

#### 40.3.4

##### **Effects of an Explosion**

An explosion includes the rapid release of high-pressure gas into the environment. The effects depend on the following factors:

- rate of release
- pressure at release
- quantity of gas released
- direction of release
- mechanical effects coincident with the release
- temperature of released gas.

If the rate of release is greater than the speed of sound, energy is dissipated in a shock wave. Its strength decreases with distance away from the source. Deflagration explosion is the name given when the propagation reaction rate is subsonic. On the other hand, detonation explosion is the name given when the propagation reaction rate is supersonic.

The vessel in which the explosion takes place might rupture if the internal pressure builds up to a high enough level. This is the sudden and rapid destructive

release of energy (mostly mechanical) as the enclosed internal pressure exceeds the capability of the vessel walls to withstand it. The rupture is accompanied by noise.

Steam explosions occur by the sudden contact between very hot and cold liquids resulting in violent explosions. An example is the rapid vaporization of water from the liquid to the vapor state because of rapid heat transfer rates. This could occur, for example, when water is added to a pan of hot oil, when the hot oil is still liquid at a temperature well above the boiling point of water.

#### 40.4

#### Combustion and Chemistry of Explosions

##### 40.4.1

##### Combustion

Inherent in the desire to reduce and even prevent fire and explosion accidents, one is concerned with the fire and explosion properties of materials, the nature of the prospective fire and explosion process, and the possibility of knowing and using procedures to reduce fire and explosion hazards. The essential elements for combustion to take place, and a fire or explosion to result, are embodied in what is called the fire triangle. It consists of three sides to a triangle representing fuel, oxidizer, and an ignition source. For a fire situation, we attach a fourth side and talk about a fire quadrilateral. The fourth side represents an uninhibited chain reaction. Both the fuel and oxidizer parts may be in solid, liquid, or gaseous form, and examples are as follows:

- **Fuels**
  - **Solids** – Wood, coal, charcoal briquettes, grain, magnesium, plastics
  - **Liquids** – Gasoline, diesel, kerosene, acetone, diethyl ether, pentane, hydrazine
  - **Gases** – Natural gas, methane, propane, acetylene, carbon monoxide, hydrogen.
- **Oxidizers**
  - **Solids** – Ammonium nitrate, ammonium perchlorate, potassium perchlorate, metallic peroxides, chlorates, perchlorates, nitrates, chromates, permanganates
  - **Liquids** – Nitrous oxide, nitric acid, chromic acid, sulfuric acid, hydrogen peroxide, perchloric acid
  - **Gases** – Air, oxygen, fluorine, chlorine, nitric oxide, nitrogen dioxide.

A competent ignition source is one which has enough temperature, size, and duration to initiate combustion, leading to a fire or an explosion. To initiate the combustion, for the third side of the triangle, the ignition source may take any of several forms:

- **Sparks** – Mechanical, electrical
- **Flames** – Standing pilots, accidental, deliberate, welding, cutting
- **Static electricity** – Fluid flow, dry atmosphere
- **Heat** – Equipment overheating, bearings wearing out, friction.

**Table 40.4** Examples of flammable ranges.

Fuel	Lower limit (%)	Upper limit (%)
Gasoline vapor	1.4	7.6
Methane (natural gas)	5.0	15
Propane	2.2	9.6
Butane	1.9	8.5
Hydrogen	4.0	75
Acetylene	2.5	81
Carbon monoxide	12.5	74

Data from well-known sources; see Lilley (2004a).

The major distinction between fires and explosions is the rate of energy release. Fires release energy relatively slowly, whereas explosions release energy very rapidly, typically on the order of microseconds. Fire can also result from explosions and explosions can result from fires.

#### 40.4.2

##### **Explosions, Lower and Upper Flammability Limits, and Mixtures of Gases**

Moving on now to explosions in vessels, note that the pressure reached in a closed vessel after an internal chemical reaction can be calculated from knowledge of the chemical reaction. The proportions of the reactants determine the species and temperature of the products, and from the mean mixture molecular mass (also called the mean mixture molecular weight) of the products, one can determine the pressure. Reactions that are close to stoichiometric produce the highest temperatures and pressures and, for example, a typical hydrocarbon–air reaction would generate a sevenfold increase in absolute temperature and absolute pressure. The percentage by volume of a gaseous fuel in air (also called the volumetric concentration) is important in determining whether ignition of the fuel–air mixture is possible. When there is a too low or too high fuel concentration, ignition is not possible.

It is important to know if a potential ignition source is located within the flammable or explosive limits, these being the percentage (usually by volume) of an in-air substance that will burn once ignited. Most substances have both a lower (lean) and an upper (rich) flammable (explosive) limit, called the lower flammable limit (LFL) and upper flammable limit (UFL), respectively (or LEL and UEL, respectively). Some typical values for several fuels are given in Table 40.4, for fuel-in-air mixtures on a volume percentage basis. Either too much or too little fuel in the vapor–air mixture can prevent burning. However, at the edge of a fuel-rich vapor cloud will be a region with other more flammable fuel:air ratios, so that, as such a cloud approaches, ignition is certainly possible from an igniting source. There is a wide range of fuels with different flammable limits. Higher temperatures

and/or higher pressures generally increase the range over which a given fuel–air mixture is capable of being ignited and burned. Babrauskas (2003) provides a wealth of information about the ignition problem. Data for LFL and UFL for many fuels are readily available; see, for example, Babrauskas (2003) and NFPA (2008, 2011).

Let  $y_i$  be the molar concentrations (same as volumetric concentrations if the species are gaseous) of species  $i$  in a mixture of fuels, each with  $\text{LFL}_i$  and  $\text{UFL}_i$  in air, respectively. The well-known Le Chatelier's law gives expressions for calculating the LFL and UFL of the gaseous mixture in air:

$$\text{LFL}_{\text{mix}} = \frac{1}{\sum_{i=1}^n \frac{y_i}{\text{LFL}_i}} \quad (40.4)$$

$$\text{UFL}_{\text{mix}} = \frac{1}{\sum_{i=1}^n \frac{y_i}{\text{UFL}_i}} \quad (40.5)$$

### Example of lower and upper flammability limits for a mixture

What are the LFL and UFL of a fuel–air mixture when the fuel is composed of 20% hexane, 50% methane, and 30% propane by volume? Take the LFLs as 1.1, 5.0, and 2.2% and the UFLs as 7.5, 15, and 9.6% for hexane, methane, and propane, respectively.

### Solution

Using Le Chatelier's law, the calculations can be made as follows:

$$\begin{aligned} \text{LFL}_{\text{mix}} &= \frac{1}{\sum_{i=1}^n \frac{y_i}{\text{LFL}_i}} \\ &= \frac{1}{\frac{0.2}{1.1} + \frac{0.5}{5.0} + \frac{0.3}{2.2}} \\ &= \frac{1}{0.4182} = 2.39\% \text{ by volume} \end{aligned} \quad (40.6)$$

$$\begin{aligned} \text{UFL}_{\text{mix}} &= \frac{1}{\sum_{i=1}^n \frac{y_i}{\text{UFL}_i}} \\ &= \frac{1}{\frac{0.2}{7.5} + \frac{0.5}{15.0} + \frac{0.3}{9.6}} \\ &= \frac{1}{0.0683} = 14.6\% \text{ by volume} \end{aligned} \quad (40.7)$$

If a competent ignition source is located at a point where the volume concentration of the gas mixture in air is between the two extreme limits of 2.39 and 14.6%, then ignition of the gaseous mixture will take place.

## 40.4.3

**Estimating Flammability Limits**

For some situations, it may be necessary to estimate the flammability limits without experimental data. Then the expressions that the lower limit is 55% and the upper limit is 350% of the stoichiometric value are often used:

$$\text{LFL} = 0.55C_{\text{st}} \quad (40.8)$$

$$\text{UFL} = 3.50C_{\text{st}} \quad (40.9)$$

where  $C_{\text{st}}$  is the stoichiometric volume percentage of fuel in the fuel–air mixture. In general, the flammability range increases with increasing temperature, lowering the LFL and increasing the UFL. Generally, pressure has little effect on the LFL but the UFL increases significantly as the pressure is increased, broadening the flammability range. Further details about temperature and pressure effects on the flammability range may be found in, for example, Crowl and Louvar (1990).

## 40.4.4

**Estimating the Stoichiometric Concentration and LFL and UFL for a Typical C–H–O Fuel**

From standard thermodynamics and combustion principles [see Goodger (1977), Kuo (1986), Turns (2001), and Lilley (2004b)], the concentration by volume is determined using the general stoichiometric combustion reaction:



where  $m$ ,  $x$ , and  $y$  are known for the particular fuel of interest. Note that there is just enough oxygen to oxidize all the carbon to carbon dioxide, but there is not sufficient oxygen to have left-over oxygen on the right-hand side in the products of combustion. There is also nitrogen present, on both sides of the equation, if the oxygen is supplied by way of air, and the molar fraction (or volume fraction) of oxygen in air is 0.21. It follows from the balance equation that the correct amount of the multiplier  $z$  for stoichiometric conditions is

$$z = m + \frac{x}{4} - \frac{y}{2} \quad (40.11)$$

where  $z$  has units of moles of  $O_2$  per mole of fuel. If oxygen is missing from the fuel, then simply put  $y$  equal to zero. Hence additional stoichiometric and unit changes are required to determine the stoichiometric volume percentage of fuel in the fuel–air mixture,  $C_{\text{st}}$ , as a function of  $z$ :

$$\begin{aligned} C_{\text{st}} &= \frac{\text{moles fuel}}{\text{moles fuel} + \text{moles air}} \times 100 \\ &= \frac{100}{1 + \left( \frac{\text{moles air}}{\text{moles fuel}} \right)} \end{aligned}$$

$$\begin{aligned}
 &= \frac{100}{1 + \left(\frac{1}{0.21}\right) \left(\frac{\text{moles O}_2}{\text{moles fuel}}\right)} \\
 &= \frac{100}{1 + \left(\frac{z}{0.21}\right)} \quad (40.12)
 \end{aligned}$$

Hence the LFL and UFL are estimated as

$$\text{LFL} = \frac{0.55 (100)}{4.76m + 1.19x - 2.38y + 1} \quad (40.13)$$

$$\text{UFL} = \frac{3.50 (100)}{4.76m + 1.19x - 2.38y + 1} \quad (40.14)$$

### Example of estimating the LFL and UFL of a hydrocarbon fuel

Estimate the LFL and UFL for propane from the equations and compare the calculated limits with the actual values determined experimentally. The accepted experimental values for propane are 2.2 and 9.6% for the LFL and UFL, respectively.

#### Solution

The stoichiometric balance equation of propane with oxygen is



where  $m = 3$ ,  $x = 8$ ,  $y = 0$ , and  $z = 5$ . With air as the oxidant, there is also nitrogen present with oxygen representing 21% of air by volume. Hence the LFL and UFL are determined using the relevant equations:

$$\begin{aligned}
 \text{LFL} &= \frac{0.55 (100)}{4.76 (3) + 1.19 (8) + 1} \\
 &= 2.218 \text{ vol\% (vs 2.2\% actual)} \quad (40.16)
 \end{aligned}$$

$$\begin{aligned}
 \text{UFL} &= \frac{3.5 (100)}{4.76 (6) + 1.19 (14) + 1} \\
 &= 14.113 \text{ vol\% (vs 9.6\% actual)} \quad (40.17)
 \end{aligned}$$

The agreement for the LFL is very good, but the agreement for the UFL is poor. The methodology is the same with any fuel or mixture of fuels that can always be expressed as  $\text{C}_m\text{H}_x\text{O}_y$ . For example, if the methodology is applied to hexane ( $\text{C}_6\text{H}_{14}$ ), the agreement is excellent for both LFL (1.19 versus 1.1% actual) and the UFL (7.57 versus 7.5% actual).

### Example of calculation of minimum oxygen concentration (MOC) and inerting

Estimate the minimum oxygen concentration (MOC) for the fuel propane ( $\text{C}_3\text{H}_8$ ).

**Solution**

The stoichiometric equation for this reaction with oxygen is



The LFL for propane is 2.2% by volume. From the stoichiometrically balanced equation

$$\begin{aligned} \text{MOC} &= \left( \frac{\text{moles fuel}}{\text{moles fuel} + \text{moles air}} \right) \left( \frac{\text{moles O}_2}{\text{moles fuel}} \right) \\ &= \text{LFL} \left( \frac{\text{moles O}_2}{\text{moles fuel}} \right) \end{aligned} \quad (40.19)$$

By substitution

$$\begin{aligned} \text{MOC} &= (2.2) \left( \frac{5 \text{ mol O}_2}{1 \text{ mol fuel}} \right) \\ &= 11 \text{ vol\% O}_2 \end{aligned} \quad (40.20)$$

The example has illustrated the concept of *inerting*. It shows that the combustion of propane is preventable by adding nitrogen, carbon dioxide, or even water vapor until the oxygen concentration in the entire mixture of fuel, oxygen, nitrogen, and anything else is below 11%. The addition of water, however, is not recommended because any condition which condenses water would make the oxygen concentration in the gaseous mixture higher, and even back into the flammable range.

**40.5****Ignition****40.5.1****Ignition Energy**

The minimum ignition energy (MIE) is the minimum energy input required to initiate combustion, and typically this occurs when the reactants (fuel and oxidizer, usually air) are in the precise proportions not to have any fuel left over and have just enough oxygen to complete the carbon oxidation to carbon dioxide (CO<sub>2</sub>). At fuel-rich or fuel-lean conditions, a greater amount of ignition energy is needed to initiate the chemical reaction. All flammables (including dusts) have an MIE associated with them. The MIE depends on the specific chemical or mixture of fuels, pressure, and temperature. Experimental data indicate that the MIE decreases with increase in pressure. The MIE of dusts are, in general, at levels comparable to those of combustible gases, and an increase in the nitrogen concentration (or decrease in oxygen concentration in the air) increases the required MIE.

A typical MIE for a hydrocarbon fuel is about 0.25 mJ and it must be noted that this is low compared with possible sources of ignition, such as a static discharge of 22 mJ by walking across a rug and 25 mJ from a spark plug in an engine. Note,

therefore, that electrostatic discharges, as a result of fluid flow in some industrial process, typically have energy discharge levels high enough to provide ignition.

#### 40.5.2

##### **Autoignition**

Ignition of a flammable mixture can take place if the temperature is high enough. The concept of the autoignition temperature (AIT) of a vapor, sometimes called the spontaneous ignition temperature (SIT), is the temperature at which the vapor ignites without a specific flame or spark. This temperature is a function of the concentration of vapor, volume of vapor, pressure of the system, presence of catalytic material, and flow conditions. For example, it is known that rich or lean mixtures need a higher temperature to autoignite than stoichiometric mixtures, and an increase in pressure or an increase in oxygen concentration decreases the required temperature for autoignition.

#### 40.5.3

##### **Adiabatic Compression**

Compression without loss of heat is called adiabatic compression. Both pressure and temperature increase when the volume of a gas is decreased. When the compression is sudden, there is little time for the heat generated to escape, and the compression is adiabatic. If the gas being compressed is a gaseous mixture of, for example, gasoline and air in an automobile cylinder, ignition will take place if the compression gives a temperature above the AIT. Preignition knock in gasoline engines that are running too hot and too lean sometimes exhibit this trait. Some overheated engines continue to run on after the spark plug ignition is turned off, for a similar reason. On the other hand, diesel engines use the increase in pressure and temperature to create autoignition deliberately. Note that diesel fuels have a relatively low AIT ( $\sim 250^\circ\text{C}$  or  $\sim 500^\circ\text{F}$ ) compared with gasoline fuels ( $\sim 400^\circ\text{C}$  or  $\sim 750^\circ\text{F}$ ), using values found in tables of data showing AITs at standard pressure; see, for example, Babrauskas (2003). For precise comparisons, data for the actual fuel of interest would need to be used, perhaps utilizing the cetane and octane values, and material data safety sheets (MSDSs).

In many applied cases of interest, simplifications are appropriate to use versus the more cumbersome non-ideal gas with specific heats that vary with temperature. The adiabatic temperature rise for an ideal gas is computed from the constant specific heat version of the thermodynamic adiabatic compression of an ideal gas. The pressure ratio is related to the temperature ratio, and the relevant equation is

$$T_f = T_i \left( \frac{P_f}{P_i} \right)^{(\gamma-1)/\gamma} \quad (40.21)$$

where  $T_f$  is the final absolute temperature,  $T_i$  is the initial absolute temperature,  $P_f$  is the final absolute pressure,  $P_i$  is the initial absolute pressure, and  $\gamma = C_p/C_v$  is the specific heat ratio.



**Example of possible ignition of a fuel with adiabatic compression of air above**

What is the final temperature after compressing air over liquid pentane from 14.7 to 400 psia if the initial temperature is 70 °F? Take the AIT of pentane to be 588 °F and the specific heat ratio  $\gamma$  for air to be 1.4. Assume that air behaves as an ideal gas with constant specific heats and therefore constant specific heat ratio.

**Solution**

From the adiabatic compression equation, using absolute temperatures and absolute pressures:

$$T_f = (460 + 70) \left( \frac{400}{14.7} \right)^{0.4/1.4} \quad (40.22)$$

and so the final after compression temperature is  $T_f = 1362^\circ\text{R} = 902^\circ\text{F}$ . This exceeds the AIT for pentane, and therefore ignition is likely at the surface of the fuel.

**Example of possible ignition of oil after adiabatic compression of air in a cylinder**

In a piston-type compressor, assume that there is a small quantity of some lubricating oil in the cylinder bore. To avoid autoignition of this oil, the compressor operation must ensure that the temperature after the compression stroke is well below the AIT of the oil. Typical lubricating oils have AITs of  $\sim 400^\circ\text{C}$ . For extra safety, compute the compression ratio required to raise the temperature of the air to less than this, say  $350^\circ\text{C}$ . Assume an initial air temperature of  $25^\circ\text{C}$  and 1 atm.

**Solution**

The compression equation applies. Solving for the pressure ratio from the required temperature ratio, we obtain

$$\begin{aligned} \frac{P_f}{P_i} &= \left( \frac{T_f}{T_i} \right)^{\gamma/(\gamma-1)} \\ &= \left( \frac{273 + 350}{273 + 25} \right)^{1.4/0.4} \\ &= 13.2 \end{aligned} \quad (40.23)$$

This represents a final pressure of  $13.2 \times 14.7 \text{ psia} = 194 \text{ psia}$ . The actual compression ratio or pressure should be kept below this value, otherwise the final after-compression temperature would be above  $350^\circ\text{C}$  and ignition of the oil might occur.

## 40.6

**Blast Damage Due to Over-Pressurization**

## 40.6.1

**Basics**

The explosion of a dust or gas (either as a deflagration or detonation) results in a reaction front moving outwards from the ignition source preceded by a shock wave or pressure front. After the combustible material has been consumed, the reaction front terminates, but the pressure wave continues its outward movement. A blast wave is composed of the pressure wave and subsequent wind. It is the blast wave that causes most of the damage.

Peak overpressure resulting from the pressure wave impacting on a structure is a function of the rate of pressure rise. Good estimates of blast damage, however, are obtained using just the peak overpressure, and on the basis of the equivalent mass of TNT; see Tables 40.5 and 40.6 for human injury and property damage criteria versus overpressure. Let the equivalent mass of TNT of the explosion be denoted by  $m_{\text{TNT}}$ , and take  $r$  as the distance away from ground zero of the explosion, then the empirically derived scaling law is

$$z_e = \frac{r}{m_{\text{TNT}}^{1/3}} \quad (40.24)$$

where  $z_e$  is a *scaled distance*, in units of  $\text{ft lb}^{-1/3}$  or  $\text{m kg}^{-1/3}$ . This correlation has been found to be good for determining the overpressure produced by an explosion at a particular distance away from the explosion. The equivalent energy of TNT is  $1120 \text{ cal g}^{-1}$  ( $= 4.69 \text{ MJ kg}^{-1}$ ) and this is used in the conversion into the TNT equivalent energy.

## 40.6.2

**Procedure for Estimating the Overpressure at Any Given Distance**

The procedure for estimating the overpressure  $p$  at any distance,  $r$ , due to the explosion of a mass of material is as follows:

- 1) Compute the energy of the explosion using combustion chemistry heat release principles; see Goodger (1977), Kuo (1986), Turns (2001), and Lilley (2004b).
- 2) Convert this energy to an equivalent amount of TNT.
- 3) Calculate the scaled distance  $z_e$  for the particular distance  $r$  away from the seat of the explosion.
- 4) Use the correlations (Figures 40.1 and 40.2 or fitted equations, see below) to estimate the overpressure.
- 5) Use Tables 40.5 and 40.6 to estimate the human and property damage.

The relationship between overpressure and scaled distance away from the explosion is almost linear when plotted on log–log paper (Figures 40.1 and 40.2). Hence the relationship between the variables can be found by the method of least

**Table 40.5** Human injury criteria (includes injury from flying glass and direct overpressure effects); see NFPA (2011).

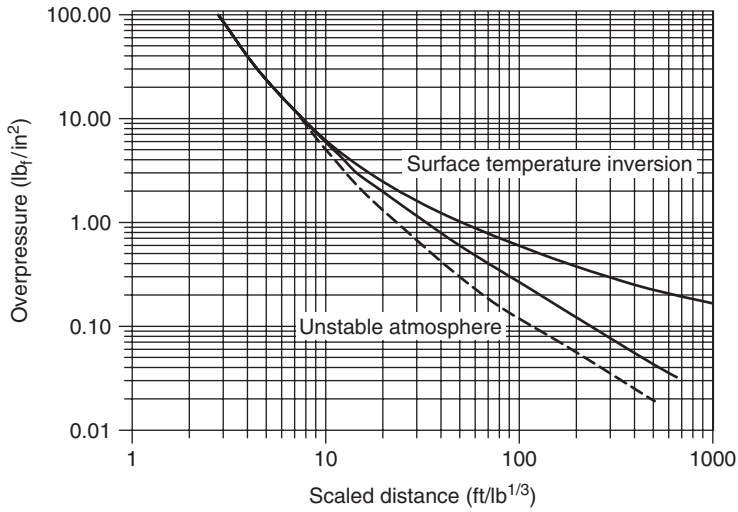
Overpressure (psi) (1 psi = 6.9 kPa)	Injury	Comments	Source
0.6	Threshold for injury from flying glass <sup>a</sup>	Based on studies using sheep and dogs	<sup>b</sup>
1.0–2.0	Threshold for skin laceration from flying glass	Based on US Army data	<sup>c</sup>
1.5	Threshold for multiple skin penetrations from flying glass (bare skin) <sup>a</sup>	Based on studies using sheep and dogs	<sup>b</sup>
2.0–3.0	Threshold for serious wounds from flying glass	Based on US Army data	<sup>c</sup>
2.4	Threshold for eardrum rupture	Conflicting data on eardrum rupture	<sup>c</sup>
2.8	10% probability of eardrum rupture	Conflicting data on eardrum rupture	<sup>c</sup>
3.0	Overpressure will hurl a person to the ground	One source suggested an overpressure of 1.0 psi for this effect	<sup>d</sup>
3.4	1% eardrum rupture	Not a serious lesion	<sup>e</sup>
4.0–5.0	Serious wounds from flying glass near 50% probability	Based on US Army data	<sup>c</sup>
5.8	Threshold for body-wall penetration from flying glass (bare skin) <sup>a</sup>	Based on studies using sheep and dogs	<sup>b</sup>
6.3	50% probability of eardrum rupture	Conflicting data on eardrum rupture	<sup>c</sup>
7.0–8.0	Serious wounds from flying glass near 100% probability	Based on US Army data	<sup>c</sup>
10.0	Threshold lung hemorrhage	Not a serious lesion [applies to a blast of long duration (over 50 m s <sup>-1</sup> ); 20–30 psi required for 3 m s <sup>-1</sup> duration waves]	<sup>e</sup>
14.5	Fatality threshold for direct blast effects	Fatality primarily from lung hemorrhage	<sup>c</sup>
16.0	50% eardrum rupture	Some of the ear injuries would be severe	<sup>e</sup>
17.5	10% probability of fatality from direct blast effects	Conflicting data on mortality	<sup>c</sup>
20.5	50% probability of fatality from direct blast effects	Conflicting data on mortality	<sup>c</sup>
25.5	90% probability of fatality from direct blast effects	Conflicting data on mortality	<sup>c</sup>
27.0	1% mortality	A high incidence of severe lung injuries [applies to a blast of long duration (over 50 m s <sup>-1</sup> ); 60–70 psi required for 3 m s <sup>-1</sup> duration waves]	<sup>e</sup>
29.0	99% probability of fatality from direct blast effects	Conflicting data on mortality	<sup>c</sup>

<sup>a</sup>Interpretation of tables of data presented in reference.<sup>b</sup>Fletcher, Richmond, and Yelverton (1980).<sup>c</sup>Lees (1980).<sup>d</sup>Brasie and Simpson (1968).<sup>e</sup>US Department of Transportation (1988).

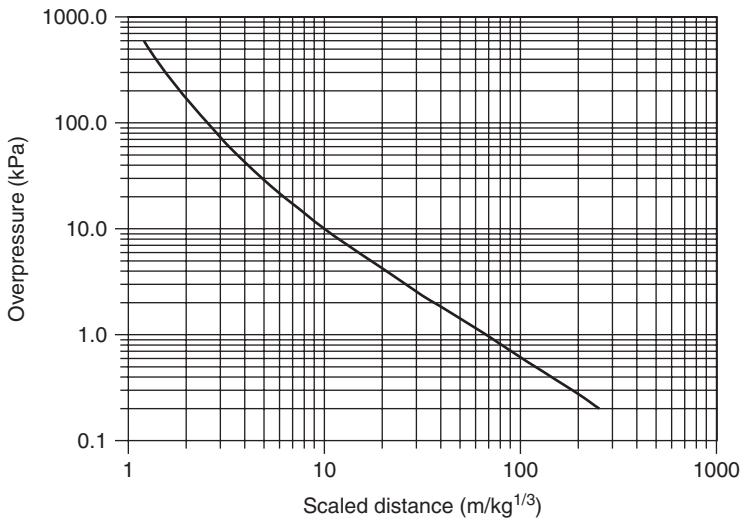
**Table 40.6** Property damage criteria; see NFPA (2011).

Overpressure (psi) (1 psi = 6.9 kPa)	Damage	Source
0.03	Occasional breaking of large glass windows already under strain	<sup>a</sup>
0.04	Loud noise (143 dB). Sonic boom glass failure	<sup>a</sup>
0.10	Breakage of small windows, under strain	<sup>a</sup>
0.15	Typical pressure for glass failure	<sup>a</sup>
0.30	“Safe distance” (probability 0.95 no serious damage beyond this value) missile limit. Some damage to house ceilings, 10% window glass broken	<sup>a</sup>
0.4	Minor structural damage	<sup>a, c</sup>
0.5–1.0	Shattering of glass windows, occasional damage to window frames. One source reported glass failure at 0.147 psi (1 kPa).	<sup>a, c, d, e</sup>
0.7	Minor damage to house structures	<sup>a</sup>
1.0	Partial demolition of houses, made uninhabitable	<sup>a</sup>
1.0–2.0	Shattering of corrugated asbestos siding, failure of corrugated aluminum-steel paneling, failure of wood siding panels (standard housing construction)	<sup>a, b, d, e</sup>
1.3	Steel frame of clad buildings slightly distorted	<sup>a</sup>
2.0	Partial collapse of walls and roofs of houses	<sup>a</sup>
2.0–3.0	Shattering of non-reinforced concrete or cinder block wall panels 1.5 psi (10.3 kPa) according to another source	<sup>a, b, c, d</sup>
2.3	Lower limit of serious structural damage	<sup>a</sup>
2.5	50% destruction of brickwork of house	<sup>a</sup>
3.0	Steel frame building distorted and pulled away from foundations	<sup>a</sup>
3.0–4.10	Collapse of self-framing steel panel buildings, rupture of oil storage tanks, snapping failure – wooden utility tanks	<sup>a, b, c</sup>
4.0	Cladding of light industrial buildings ruptured	<sup>a</sup>
4.8	Failure of reinforced concrete structures	<sup>e</sup>
5.0	Snapping failure – wooden utility poles	<sup>a, b</sup>
5.0–7.0	Nearly complete destruction of houses	<sup>a</sup>
7.0	Loaded train wagons overturned	<sup>a, b, c, d</sup>
7.0–8.0	Shearing/flexure failure of brick wall panels (8–12 in (20.3–30.5 cm) thick, not reinforced), sides of steel frame buildings blown in	<sup>d</sup>

<sup>a</sup>Interpretation of tables of data presented in reference.<sup>b</sup>Fletcher, Richmond, and Yelverton (1980)<sup>c</sup>Lees (1980).<sup>d</sup>Brasie and Simpson (1968)<sup>e</sup>US Department of Transportation (1988).



**Figure 40.1** Correlation between overpressure and scaled distance, English engineering units; see Crowl and Louvar (1990).



**Figure 40.2** Correlation between overpressure and scaled distance, SI units; see Crowl and Louvar (1990).

squares for a straight line of the transformed variables, and in terms of the original variables the relationship is of the form

$$y = \alpha x^\beta \quad (40.25)$$

where  $\alpha$  and  $\beta$  are best-fit constants.

### 40.6.2.1 English Engineering Units

When  $\gamma$  is equal to  $p$  (the overpressure in pounds of force per square inch) and  $z_e$  is the *scaled distance* in units of  $\text{ft lb}^{-1/3}$ , then, using five points for the curve fit,  $\alpha = 29.579$  and  $\beta = -1.054$ . Hence

$$p = 29.6z_e^{-1.054} \quad (40.26)$$

### 40.6.2.2 SI Units

When  $\gamma$  is equal to  $p$  (the overpressure in kilopascals) and  $z_e$  is the *scaled distance* in units of  $\text{m kg}^{-1/3}$ , then, using five points for the curve fit,  $\alpha = 572.678$  and  $\beta = -1.685$ . Hence

$$p = 573z_e^{-1.685} \quad (40.27)$$

### Example of overpressure at a given distance

A mass of 2 kg of TNT is exploded. Compute the overpressure at a distance of 20 m from the explosion.

#### Solution

The value of the scaling parameter is determined as

$$z_e = \frac{r}{m_{\text{TNT}}^{1/3}} \quad (40.28)$$

$$z_e = \frac{20 \text{ m}}{(2 \text{ kg})^{1/3}} = 15.8 \text{ m kg}^{-1/3} \quad (40.29)$$

Hence, from Figure 40.2, the overpressure is estimated to be about 6 kPa = 0.9 psi. According to Table 40.5, this is almost sufficient to cause partial demolition of houses, certainly shattering glass windows.

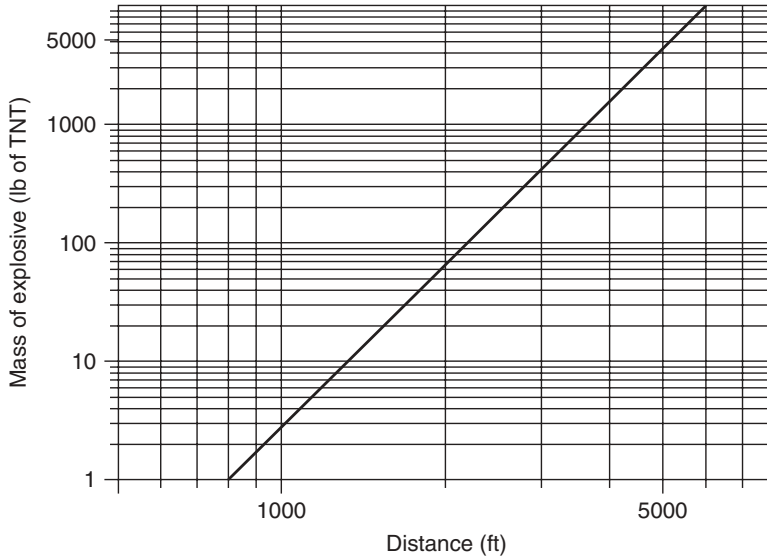
## 40.7

### Blast Fragment Missile Damage

#### 40.7.1

##### Basics

An explosion occurring in a confined structure can rupture the structure, resulting in the projection of debris over a wide area. This debris, or missiles, can cause appreciable injury to people and damage to structures and process equipment. Unconfined explosions also create missiles by blast wave impact and subsequent translation of structures. The mass of explosive and the maximum horizontal range of the fragments can be estimated from first expressing the mass as an equivalent mass of TNT, and then using the figure to estimate the maximum horizontal range



**Figure 40.3** Maximum horizontal range of blast fragments, English engineering units; see Crowl and Louvar (1990) (with data from Clancey (1972).)

of fragments. The relationship between distance  $x$  away from the explosion and the equivalent mass  $m$  of TNT explosive (see Figure 40.3), is almost linear when plotted on log-log paper. Hence the relationship between the variables can be found by the method of least squares for a straight line of the transformed variables, and in terms of the original variables the relationship is of the form

$$y = \alpha x^\beta \quad (40.30)$$

where  $\alpha$  and  $\beta$  are best-fit constants.

#### 40.7.1.1 English Engineering Units

When  $y$  is equal to  $x$  (the maximum distance away in feet that a fragment will go) and  $m$  is the equivalent mass of TNT in pounds of the explosive, then, using five points for the curve fit,  $\alpha = 797.680$  and  $\beta = 0.221$ . Hence

$$x = 798m^{0.221} \quad (40.31)$$

#### 40.7.1.2 SI Units

When  $x$  is the distance in meters and  $m$  is the equivalent mass of TNT in kilograms of the explosive, then the relationship becomes

$$x = 290m^{0.221} \quad (40.32)$$

These relationships are useful during accident investigations for calculating the energy level required to project fragments to an observed distance from the location of the explosion.

**Example of blast damage**

A reactor contains the equivalent of 5000 lb of TNT. If it explodes, estimate the injury to people and the damage to structures 300 ft away.

**Solution**

The scaled distance is:

$$z_e = \frac{r}{m_{\text{TNT}}^{\frac{1}{3}}} = \frac{300 \text{ ft}}{(5000 \text{ lb})^{\frac{1}{3}}} = 17.5 \text{ ft lb}^{-\frac{1}{3}} \quad (40.33)$$

Then the overpressure is about 2 psi using Figure 40.1. This indicates from Table 40.5 that serious wounds could well occur and from Table 40.6 that houses will be severely damaged at this location.

**40.8****Evolution of Flammable Material****40.8.1****Basics**

Explosive breakages in fuel-carrying conduits and tanks will result in the release of flammable material. This topic falls within the science of chemical process safety, health, and loss prevention, which are addressed in Lees (1980), AIChE (1990), Crowl and Louvar (1990), NFPA (2008), and SFPE (2008). These and other publications discuss the many principles, guidelines, and calculations that are necessary for safe design and operation and analysis of failures, including: fires and explosions, vessel overpressure protection, hazards identification and risk assessment, source models, and dispersion modeling. For example, material may be released from holes and cracks in tanks and pipes, from leaks in flanges, pumps, and valves, and a large variety of other sources.

When an accidental or deliberate fracture occurs in a fuel line or storage tank, the source models represent the material release process. The relevant model will provide useful information for determining the consequences of the pressurized release, including the rate of material release, the total quantity released, and the physical state of the material. Source models are constructed from fundamental or empirical equations representing the physico-chemical processes that occur during the release of materials. Several basic source models are available, each applicable to the particular release scenario:

- flow of liquids through a hole
- flow of liquids through a hole in a tank
- flow of liquids through pipes
- flow of vapor through holes
- flow of vapor through pipes
- flashing liquids
- liquid pool evaporation or boiling.



and problem parameters come into play in determining the amount of release or rate of release. The purpose of the source model is to determine: the form of material released (solid, liquid, or vapor), the total quantity of material released, and the rate at which it is released. Extensive further information is available in Lilley (2012).

Source releases are driven by pressure differences, and the resulting velocities depend on the density of the fluid (liquid or gas), whether or not the fluid is compressible, and whether or not choking (maximum flow) conditions occur. The volume flow rate ( $\text{m}^3 \text{s}^{-1}$  or  $\text{ft}^3 \text{s}^{-1}$ ) and mass flow rate ( $\text{kg s}^{-1}$  or  $\text{lbm s}^{-1}$ ) may be determined via introduction of the flow passage cross-sectional area and density of the flowing material. A correction factor is introduced to cater for the flow being less than ideal, via multiplication by  $C_0$  (called the discharge coefficient, a number less than 1). Other standard notation includes the following:

- $P$  = absolute pressure ( $\text{N m}^{-2} = \text{Pa}$  or  $\text{lbf ft}^{-2}$ )
- $P_g$  = gauge pressure ( $\text{N m}^{-2} = \text{Pa}$  or  $\text{lbf ft}^{-2}$ )
- $\rho$  = fluid density ( $\text{kg m}^{-3}$  or  $\text{lbm ft}^{-3}$ )
- $V$  = average instantaneous velocity of the fluid ( $\text{m s}^{-1}$  or  $\text{ft s}^{-1}$ )
- $g_c$  = conversion factor constant ( $= 1 \text{ kg m N}^{-1} \text{ s}^{-2}$  or  $32.2 \text{ lbm ft lbf}^{-1} \text{ s}^{-2}$ )
- $g$  = acceleration due to gravity ( $= 9.81 \text{ m s}^{-2}$  or  $32.2 \text{ ft s}^{-2}$ )
- $\bar{R}$  = universal gas constant ( $= 8314 \text{ J kg}^{-1} \text{ mol}^{-1} \text{ K}^{-1}$  or  $1545 \text{ ft} \cdot \text{lbf} \cdot \text{lbm}^{-1} \text{ mol}^{-1} \text{ }^\circ \text{R}^{-1}$ )
- $T$  = absolute temperature ( $\text{K}$  or  $^\circ \text{R}$ )
- $M$  = molecular weight of the gas ( $\text{kg kg}^{-1} \text{ mol}^{-1}$  or  $\text{lbm lbm}^{-1} \text{ mol}^{-1}$ ).

#### 40.8.2

##### Flow of Liquid Through a Hole

There is a trade-off between pressure energy and velocity produced, that is, high pressure and zero velocity inside the container, with the resulting liquid escaping into zero gauge pressure at a high velocity. In practice, the driving pressure gives a lower exit velocity than the idealized equation gives, because of losses associated with the flow going through the area reduction. This is taken into account by multiplying the ideal answer by a number less than unity, this number being called the discharge coefficient,  $C_0$ . The resulting equation for the velocity ( $\text{m s}^{-1}$  or  $\text{ft s}^{-1}$ ) of fluid exiting the leak is

$$V = C_0 \sqrt{\frac{2g_c P_g}{\rho}} \quad (40.34)$$

and the mass flow rate  $Q_m$  (in  $\text{kg s}^{-1}$  or  $\text{lbm s}^{-1}$ ) due to a hole of area  $A$  ( $\text{m}^2$  or  $\text{ft}^2$ ) is given by

$$Q_m = \rho VA = AC_0 \sqrt{2\rho g_c P_g} \quad (40.35)$$

The total mass of liquid spilled is dependent on the total time the leak is active. In these equations,  $P_g$  is the gauge pressure pushing the fluid through the hole to an ambient zero gauge pressure.

The discharge coefficient  $C_0$  is a complicated function of the Reynolds number of the fluid escaping through the leak, the contour of approach to the exit, and the diameter of the hole; see standard texts on fluid mechanics and Lees (1980). Some general guidelines areas follows: for sharp-edged orifices and for Reynolds numbers  $> 30\,000$ ,  $C_0$  approaches the value 0.61; for a well-rounded nozzle, it approaches unity; and for short sections of pipe attached to a vessel (with a length:diameter ratio not less than 3), it is  $\sim 0.81$ . For cases where the discharge coefficient is unknown or uncertain, use a value of 1.0 to maximize the computed flow and thereby overestimate the release rate.

### 40.8.3

#### Flow of Vapor Through a Hole

Free expansion leaks for gas (vapor) through holes differ from those of liquid flow because of the very much lower density of the vapor or gas and the fact that it is compressible and pressure, temperature, and density all change as the gas escapes and its velocity increases as it goes through the exit. Often we can approximate and use the ideal gas law and constant specific heat ratio  $\gamma = C_p/C_v$ . In general,  $\gamma$  is the specific heat ratio of the gas emerging, which is equal to 1.67, 1.40, and 1.32 according to whether the gas is monoatomic, diatomic (or air), and triatomic, respectively. Introducing the discharge coefficient and keeping absolute pressures yields the equation for mass flow rate (in  $\text{kg s}^{-1}$  or  $\text{lbm s}^{-1}$ ) as

$$Q_m = C_0 A P_0 \sqrt{\frac{2g_c M}{\bar{R} T_0} \frac{\gamma}{\gamma - 1} \left[ \left( \frac{P}{P_0} \right)^{2/\gamma} - \left( \frac{P}{P_0} \right)^{(\gamma+1)/\gamma} \right]} \quad (40.36)$$

where  $P$  is the absolute pressure of the external surroundings,  $P_0$  is the absolute pressure of the source (both in  $\text{N m}^{-2}$  or  $\text{lbf ft}^{-2}$ ), and  $\bar{R}$  is the universal gas constant.

The above equation holds only for flows which are not choked, that is, flows with an upstream absolute pressure less than about twice the downstream absolute pressure (which is usually the atmosphere). For high pressure ratios (with the upstream absolute pressure greater than about twice the downstream absolute pressure), the flow becomes sonic at the hole. Then the flow rate depends only on the upstream driving absolute pressure  $P_0$  and the mass flow rate (in  $\text{kg s}^{-1}$  or  $\text{lbm s}^{-1}$ ) is given by

$$(Q_m)_{\text{choked}} = C_0 A P_0 \sqrt{\frac{\gamma g_c M}{\bar{R} T_0} \left( \frac{2}{\gamma + 1} \right)^{(\gamma+1)/(\gamma-1)}} \quad (40.37)$$

where  $M$  is the molecular weight of the escaping vapor or gas and  $T_0$  is the absolute temperature of the source.

For gaseous flows through sharp-edged orifices with Reynolds numbers  $>30\,000$  (and not choked), a constant discharge coefficient  $C_0$  of 0.61 is indicated. However, for choked flows, the discharge coefficient increases as the downstream pressure decreases. For these flows and for situations where  $C_0$  is uncertain, a conservative value of 1.0 is recommended when the maximum (worst) possible scenario is being estimated.

## 40.9

### Dispersion and Possible Ignition of Released Material

Dispersion models describe the airborne transport of materials away from the accident site. After a release, the airborne material (small solid particles, small liquid droplets, and/or vapor) is carried away by the wind in a characteristic plume or a puff. Larger particles and larger drops of liquid fuel form trajectories with air resistance and the flight paths are affected by local wind conditions. The 3D trajectories may be calculated by solving the governing ordinary differential equations for position and speed in all three directions as time progresses; see Lilley (2010). In plume and puff releases, the maximum concentration occurs at the release point (which may or may not be a ground level). Concentrations as the cloud goes downstream are less, because of dispersion, turbulent mixing, and entrainment of surrounding air. Many parameters affect the concentration of released material at a particular downstream  $(x, y, z)$  location and at a particular time after the release, notably wind speed, atmospheric stability, ground conditions, buildings, water, trees, height of the release above ground level, and momentum and buoyancy of the initial material released. For simplicity, in the discussion here, only ground level releases are considered.

Two types of vapor cloud dispersion models are commonly used: the plume and puff models, collectively known as the Pasquill–Gifford model, using dispersion coefficients that empirically specify the rates of spread of the dispersing material. The plume model describes the steady-state concentration of material released from a continuous source. The puff model describes the temporal concentration of material from a single release of a fixed amount of material. Models are available that permit concentration ( $\text{kg m}^{-3}$ ) and volumetric concentration percentage (%) to be calculated at a location  $(x, y, z)$  as a function of time  $(t)$  after initial release. It is important to determine if the mixture is within the flammability limits at a nearby ignition source, in the case of fuel release. Details and sample calculations are given in Lilley (2008) for both plume and puff vapor cloud dispersion, where a simple VBA code behind the Excel spreadsheet is used for making calculations, which are then immediately portrayed in tabular and graphic form on the Excel spreadsheet. Useful references include ASME (1973), Hanna and Drivas (1987), AIChE (1990), Crowl and Louvar (1990), and EPA, NOAA and NSC (1992). Further recommendations for possible modifications of the basic diffusion equation results are given in LaGrega, Buckingham, and Evans (1994) and DeNevers (1995). Sprays of liquid droplets

**Table 40.7** Atmospheric stability classes<sup>a</sup> for use with the Pasquill–Gifford dispersion model; see Crowl and Louvar (1990).

Wind speed (m s <sup>-1</sup> )	Day radiation intensity			Night cloud cover	
	Strong	Medium	Slight	Cloudy	Calm and clear
<2	A	A–B	B	—	—
2–3	A–B	B	C	E	F
3–5	B	B–C	C	D	E
5–6	C	C–D	D	D	D
>6	C	D	D	D	D

<sup>a</sup>Stability classes for plume model: A, B, unstable; C, D, neutral; E, F, stable. Stability classes for puff model: A, unstable; B, neutral; C, stable.

and particles may be handled via computation of particle trajectories, including air resistance and wind effects, as outlined by Chow (1979) and Lilley (1992, 2010).

#### 40.9.1

##### Plume Model

It is common to utilize the dispersion coefficients,  $\sigma_x$ ,  $\sigma_y$ , and  $\sigma_z$ . These represent the standard deviations of the concentration in the downwind, crosswind, and vertical ( $x$ ,  $y$ ,  $z$ ) directions, respectively. The dispersion coefficients are a function of atmospheric conditions and the distance downwind from the release. The atmospheric conditions are classified according to six different stability classes. The stability classes depend on wind speed and quantity of sunlight. During the day, increased wind speed results in greater atmospheric stability, whereas at night the reverse is true. This is due to a change in vertical temperature profiles from day to night. Stability classes are given in Table 40.7.

The dispersion coefficients,  $\sigma_y$  and  $\sigma_z$ , for a continuous source were developed and are given in figures and tables. Values for  $\sigma_y$  are not provided since it is reasonable to assume that  $\sigma_x = \sigma_y$ . Table 40.8 gives equations for these “plume” release coefficients as functions of downstream distance  $x$ . For a plume with a continuous steady-state source of constant mass release rate  $Q_m$  (kg s<sup>-1</sup>) and a wind velocity  $u$  (m s<sup>-1</sup>) in the  $x$ -direction, the ground concentration is given at  $z = 0$  by [see Wark, Warner, and Davis (1998)]

$$C(x, y, 0) = \frac{Q_m}{\pi \sigma_y \sigma_z u} \exp \left[ -\frac{1}{2} \left( \frac{y}{\sigma_y} \right)^2 \right] \quad (40.38)$$

where  $C$  represents concentration (kg m<sup>-3</sup>). This can also be transferred to volumetric concentration and to parts per million (ppm). The concentration along the centerline of the plume directly downwind is given at  $y = z = 0$  by

**Table 40.8** Equations and data for plume releases; see Crowl and Louvar (1990).

Equation for continuous plumes		
Stability class <sup>a</sup>	Horizontal $\sigma_y = \sigma_x$ (m)	
A	$\sigma_y = 0.493 \times 0.88$	
B	$\sigma_y = 0.337 \times 0.88$	
C	$\sigma_y = 0.195 \times 0.90$	
D	$\sigma_y = 0.128 \times 0.90$	
E	$\sigma_y = 0.091 \times 0.91$	
F	$\sigma_y = 0.067 \times 0.90$	
Stability class <sup>a</sup>	x (m)	Vertical $\sigma_z$ (m)
A	100–300	$\sigma_z = 0.087 \times 1.10$
	300–3000	$\text{Log}\sigma_z = 1.67 + 0.902\text{log}x + 0.181(\text{log}x)^2$
B	100–500	$\sigma_z = 0.135 \times 0.95$
	$500-2 \times 10^4$	$\text{log}\sigma_z = -1.25 + 1.09\text{log}x + 0.0018(\text{log}x)^2$
C	$100-10^5$	$\sigma_z = 0.112 \times 0.91$
D	100–500	$\sigma_z = 0.093 \times 0.85$
	$500-10^5$	$\text{log}\sigma_z = -1.22 + 1.08\text{log}x - 0.06(\text{log}x)^2$
E	100–500	$\sigma_z = 0.082 \times 0.82$
	$500-10^5$	$\text{log}\sigma_z = -1.19 + 1.04\text{log}x - 0.070(\text{log}x)^2$
F	100–500	$\sigma_z = 0.057 \times 0.80$
	$500-10^4$	$\text{log}\sigma_z = -1.91 + 1.37\text{log}x - 0.119(\text{log}x)^2$

<sup>a</sup>Stability classes for plume model: A, B, unstable; C, D, neutral; E, F, stable.

$$C(x, 0, 0) = \frac{Q_m}{\pi \sigma_y \sigma_z u} \quad (40.39)$$

For continuous ground level release, the maximum concentration occurs at the release point. For a plume with a continuous steady-state source of constant mass release rate and wind velocity in the  $x$ -direction, the concentrated equation for elevated source (smoke releases) with reflection can be found in Wark, Warner, and Davis (1998).

#### 40.9.2

##### Puff Model

As with the plume model, dispersion coefficients  $\sigma_x$ ,  $\sigma_y$ , and  $\sigma_z$  are utilized as identified for puff releases in figures and tables. Table 40.9 gives equations for these “puff” release coefficients as functions of downstream distance  $x$ . The downstream concentrations on the ground ( $z = 0$ ) for a puff of mass release  $Q_m^*$  (kg) with a wind velocity  $u$  ( $\text{m s}^{-1}$ ) in the  $x$ -direction as shown in Wark, Warner, and Davis (1998) is given by

**Table 40.9** Equations and data for puff releases; see Crowl and Louvar (1990).

Stability condition <sup>a</sup>	Horizontal $\sigma_y = \sigma_x$ (m)		Vertical $\sigma_z$ (m)	
Unstable	$\sigma_y = 0.14 \times 0.92$		$\sigma_z = 0.53 \times 0.73$	
Neutral	$\sigma_y = 0.06 \times 0.92$		$\sigma_z = 0.15 \times 0.70$	
Very stable	$\sigma_y = 0.02 \times 0.89$		$\sigma_z = 0.05 \times 0.61$	

Stability condition <sup>a</sup>	$x = 100$ m		$x = 4000$ m	
	$\sigma_y$ (m)	$\sigma_z$ (m)	$\sigma_y$ (m)	$\sigma_z$ (m)
Unstable	10	15	300	220
Neutral	4	3.8	120	50
Very stable	1.3	0.75	35	7

<sup>a</sup>Stability classes for puff model: A, unstable; B, neutral; C, stable.

$$C(x, y, 0, t) = \frac{Q_m^*}{\sqrt{2\pi}^{\frac{3}{2}} \sigma_x \sigma_y \sigma_z} \exp \left[ -\frac{1}{2} \left( \frac{x - ut}{\sigma_x} \right)^2 + \frac{y^2}{\sigma_y^2} \right] \quad (40.40)$$

The ground level concentration along the  $x$ -axis is given at  $y = z = 0$  via

$$C(x, 0, 0, t) = \frac{Q_m^*}{\sqrt{2\pi}^{\frac{3}{2}} \sigma_x \sigma_y \sigma_z} \exp \left[ -\frac{1}{2} \left( \frac{x - ut}{\sigma_x} \right)^2 \right] \quad (40.41)$$

The center of the cloud is found at coordinates  $(ut, 0, 0)$ . The concentration at the center of this moving cloud is given by

$$C(ut, 0, 0, t) = \frac{Q_m^*}{\sqrt{2\pi}^{3/2} \sigma_x \sigma_y \sigma_z} \quad (40.42)$$

### 40.9.3

#### Possible Ignition of Released Material

Ignition of the released material occurs if the volume concentration of the leaked substance falls between the flammable limits and a suitable ignition source is present. Flammable limits apply generally to vapors and are defined as the volume concentration range in which a flammable substance can produce a fire or explosion when an ignition source such as a spark or open flame is present. The concentration is generally expressed as percentage fuel by volume in air. Information regarding the combustion properties of common flammable gases can be obtained from Lilley (2004a, 2012).

Above the UFL, the mixture of substance and air is too rich in fuel (deficient in oxygen) to burn. This is sometimes called the upper explosive limit. Below the LFL, the mixture of substance and air lacks sufficient fuel (substance) to burn. This is

sometimes called the lower explosive limit. Any concentration between these limits can cause ignition or explosion. Flammability ranges of specific materials can be obtained from Lilley (2004a, 2012). Being above the upper limit is not particularly safe, either. If a confined space is above the UFL and is then ventilated or opened to an air source, the vapor will be diluted and the concentration will fall into the flammable limit range in many locations.

## 40.10

### Plume Distribution Calculations

#### Example of plume distribution code validation

On an overcast day, an emission of  $10 \text{ kg s}^{-1}$  ( $22 \text{ lbm s}^{-1}$ ) of butane occurs continuously from a ground level release point. The wind speed is  $3 \text{ m s}^{-1}$  ( $10 \text{ ft s}^{-1}$ ). Calculate the mean concentration (in volume percentage) of butane at 20 m (66 ft) downwind and 4 m (13 ft) to the side.

Assume that the gas is neutrally buoyant and omit consideration of the dense gas situation. If a small pilot flame is located at that point, is ignition likely to occur or not?

This problem is taken from Lilley (1997c) and it is solved for the purpose of verification of the code being developed and used to illustrate parameter effects. The agreement is precise.

#### Solution

Let us take stability class C, using Table 40.7. The plume equations give

$$\sigma_x = \sigma_y = 0.195x^{0.90} = 2.89 \text{ m}$$

$$\sigma_z = 0.112x^{0.91} = 1.71 \text{ m}$$

$$C(x, y, z) = \frac{Q_m}{\pi \sigma_y \sigma_z u} \exp \left[ -\frac{1}{2} \left( \frac{y}{\sigma_y} \right)^2 \right] \quad (40.43)$$

- a) First, the centerline concentration is calculated. At  $x = 20 \text{ m}$ ,  $y = 0 \text{ m}$ ,  $u = 3 \text{ m s}^{-1}$ ,  $\exp[\dots] = 1$ :

$$C(20, 0, 0) = \frac{10}{\pi (2.89) (1.71) (3)} = 0.215 \text{ kg m}^{-3} \quad (40.44)$$

Air has  $1.2 \text{ kg m}^{-3}$ , so the volume concentration percentage is

$$= \frac{0.215/58}{12/29} \times 100 = 9.0\% \quad (40.45)$$

The LFL and UFL for butane from Table 40.4 are approximately 1.9 and 8.5%, respectively, so once the continuous plume cloud is established, it is technically just slightly too rich to ignite from an ignition source at this location. However,

this is too close to call, with meandering because of wind variations and the range of fuel:air ratios that will be passing this location as the plume starts from the initial leakage, so ignition is certainly possible.

- b) Second, the concentration at a distance to the side is deduced. At  $x = 20$  m,  $y = 4$  m,  $u = 3$  m s<sup>-1</sup>:

$$\begin{aligned} C(20, 4, 0) &= C(20, 0, 0) \exp \left[ -\frac{1}{2} \left( \frac{4}{2.89} \right)^2 \right]^3 \\ &= (0.215) (0.384) = 0.0825 \text{ kg m}^{-3} \end{aligned} \quad (40.46)$$

The volume concentration percentage is

$$= \frac{0.0825/58}{12/29} = 3.4\% \quad (40.47)$$

This lies well within the flammability range for butane so ignition is very likely.

#### 40.10.1

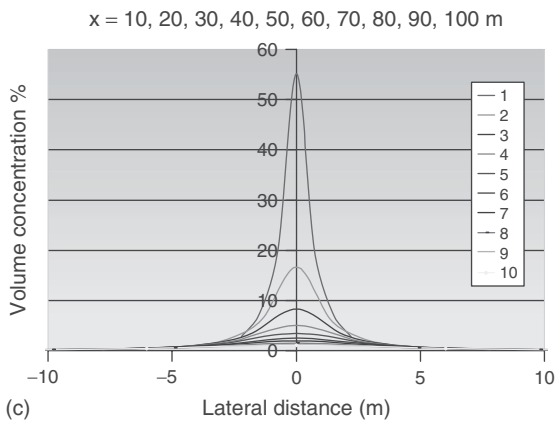
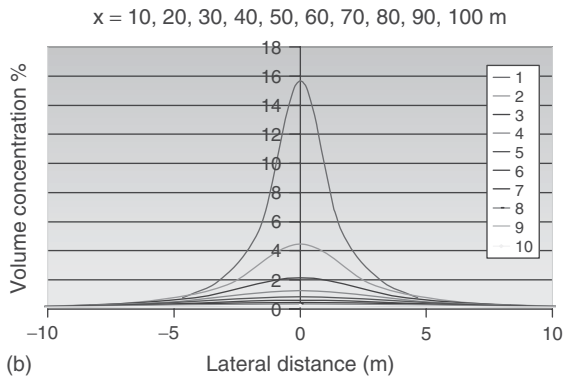
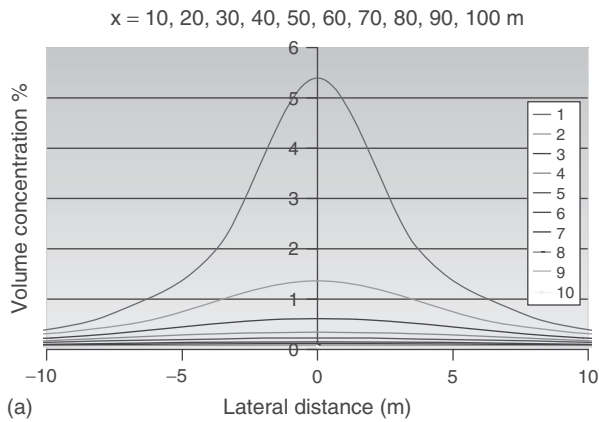
##### Parameter Effects

Calculations are now exemplified from work by Lilley (2008). Figure 40.4a–c show how the volume concentrations vary with lateral distance. Volume concentrations are expressed in percentages on the y-axis and lateral distance is measured in meters on the x-axis. In Figure 40.4, stability classes are varied by keeping the mass flow rate  $Q$  (10 kg s<sup>-1</sup>) of gas released and velocity of wind (6 m s<sup>-1</sup>) constant. Stability classes considered are A, C, and E, representing unstable, neutrally stable, and stable atmospheric conditions, respectively. As can be seen, volume concentrations are higher for the more stable stability classes. Here, volume concentrations for stability class E are higher than those for stability class C, and the latter are higher than those of stability class A. These results are consistent with the plume model equations. For a constant wind speed, the dispersion will be less for a higher than for a lower stability class. Hence one sees that the volume concentrations are higher for the more stable stability classes, and lower for the less stable stability classes. Recall that the stability classes A–F in Tables 40.7 and 40.8 represent the range from unstable through stable classes, respectively.

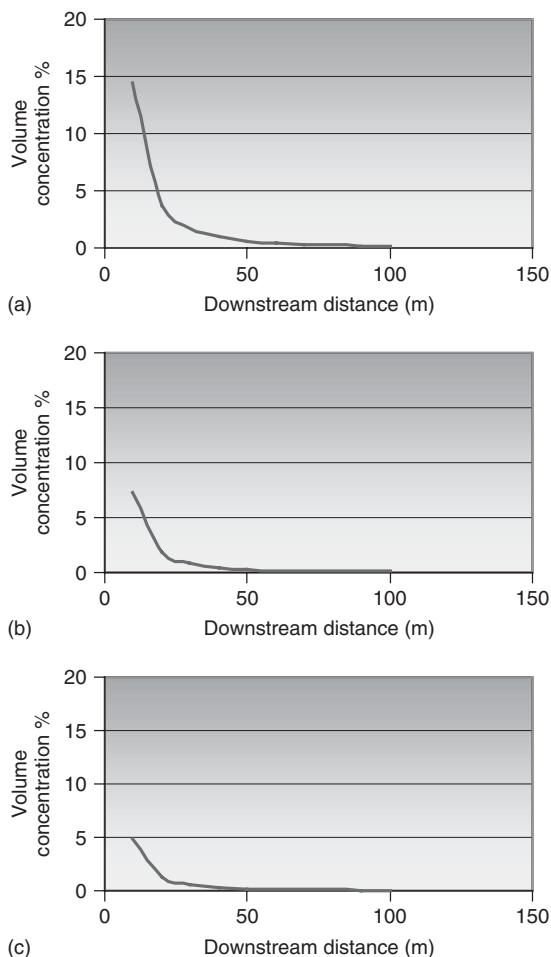
Similar figures may also be generated for wind speeds other than 6 m s<sup>-1</sup> as in Figure 40.4. For example, a summary of the centerline concentration with the unstable atmospheric conditions of stability class A is given in Figure 40.5, with parts (a), (b), and (c) showing how volume concentration changes with lateral distance, with a wind velocity of 3, 6, and 9 m s<sup>-1</sup> respectively. It is observed that the corresponding volume concentrations for which the wind velocity is 3 m s<sup>-1</sup> are higher than those at higher wind speeds. Hence the higher the velocity of the wind, the lower is the volume concentration at a specified downstream location.

Perspective views with dynamic graphics are also generated automatically with the Excel/VBA codes. For example, Figure 40.6a and b present the plan and perspective views, respectively, of volumetric concentration, with the continuous





**Figure 40.4** Volume concentration versus lateral distance at various downstream distances  $x$  in meters, for a  $10 \text{ kg s}^{-1}$  continuous plume release into a  $6 \text{ m s}^{-1}$  wind; see Lilley (2008). (a) Atmosphere unstable, stability class A; (b) atmosphere neutral, stability class C; (c) atmosphere stable, stability class E.



**Figure 40.5** Volume concentration versus downstream distance, for a  $10 \text{ kg s}^{-1}$  continuous plume release in to an unstable atmosphere with stability class A; see Lilley (2008). Wind speed: (a) 3, (b) 6, and (c)  $9 \text{ m s}^{-1}$ .

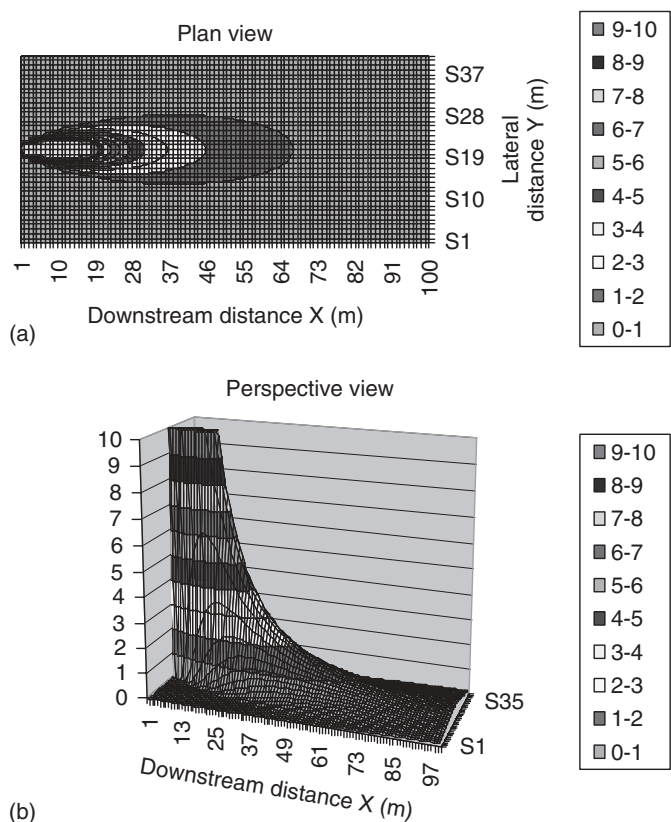
plume model with  $10 \text{ kg s}^{-1}$  release into a  $3 \text{ m s}^{-1}$  wind of a neutrally stable atmosphere of stability class C.

#### 40.11

##### Puff Distribution Calculations

##### Example re puff distribution code validation

A bottle of liquid  $\text{SO}_2$  bursts at ground level and instantaneously releases 80 lb (36.24 kg) of  $\text{SO}_2$ . What is the approximate maximum concentration that will be



**Figure 40.6** (a) Plan view and (b) perspective view for a  $10 \text{ kg s}^{-1}$  continuous plume model with wind velocity  $3 \text{ m s}^{-1}$  in a neutral atmosphere with a stability class C; see Lilley (2008). Both parts of the figure illustrate downstream distance and lateral distance versus volume concentration.

observed by a person who is 1000 m directly downwind under the worst-case meteorological conditions?

This problem is taken from Wark, Warner, and Davis (1998) and it is solved for the purpose of verification of the code being developed and used to illustrate parameter effects. The agreement is precise.

### Solution

For ground level sources, the worst-case meteorological conditions occur with the most stable situation with low wind velocity, so take stability class C at a wind speed of  $1 \text{ m s}^{-1}$ . Based on the equations in Table 40.9, and using a stability condition of very stable, the  $\sigma_y$  and  $\sigma_z$  values at 1000 m downwind are calculated to be 9.4 and 3.4 m, respectively. The value of  $\sigma_x$  is assumed to be equal to  $\sigma_y$ . Substituting the

values into the equation for puff release and setting the exponential term equal to unity, the centerline mass concentration at  $x = 1000$  m becomes

$$C = C(1000, 0, 0) = \frac{(2)(36.24)}{(2\pi)^{3/2}(9.4)(9.4)(3.4)}(1.0) = 0.0153 \text{ kg m}^{-3} \quad (40.48)$$

This agrees precisely with Wark, Warner, and Davis (1998) when the dispersion coefficients are equal to 9.4 m with stable meteorological conditions. In the general computer program, the equations (for dispersion coefficients from fitted curves through limited data) would actually give  $\sigma_x = \sigma_y = 9.35$  and  $\sigma_z = 3.38$ , thereby giving a slight discrepancy versus the other calculations.

Results from the sample validation can be verified for lateral distributions also at 1000 m downstream, and other downstream locations. At this distance, the concentration is about  $0.015 \text{ kg m}^{-3}$  on the centerline. At  $x = 500$  m it is  $0.0815 \text{ kg m}^{-3}$ .

#### 40.11.1

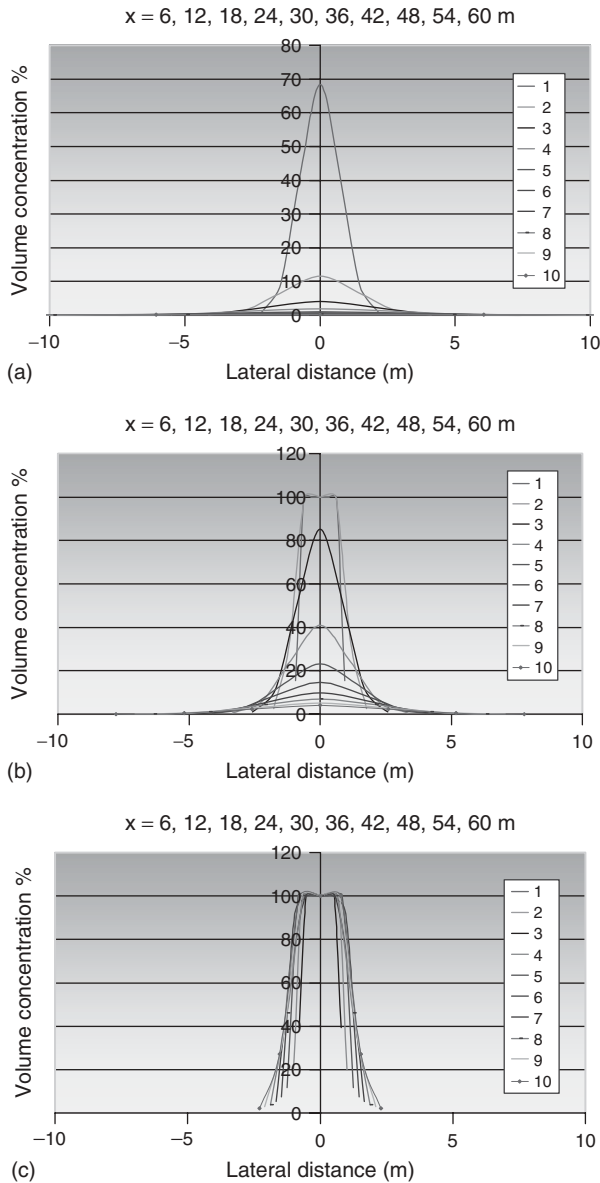
##### Parameter Effects

Calculations are now exemplified from work by Lilley (2008). Figure 40.7a–c show how the volume concentrations vary with lateral distance. Volume concentrations are expressed in percentages on the y-axis versus the lateral distance in meters at several downstream  $x$  locations. The stability classes are unstable, neutrally stable, and stable, called *stability class A, B, and C*, respectively, in the three parts of Figure 40.7. In all cases the mass released  $[Q]^*$  is 10 kg into a wind of speed  $3 \text{ m s}^{-1}$ . As can be seen, volume concentrations are higher for more stable atmospheric conditions. Hence the volume concentrations are higher for the most stable class considered, stability class E. Similar graphs can be developed for other wind speed conditions. Figures 40.8 and 40.9 represent plan and perspective views, respectively, for a 10 kg sudden puff release with a wind velocity of  $4 \text{ m s}^{-1}$  in an unstable atmosphere with stability class A. In each figure, parts (a), (b), and (c) represent views at time 5, 10, and 15 s, respectively. These graphics are generated automatically with the Excel/VBA code as calculations are accomplished for a specific case. For further details, see Lilley (2008).

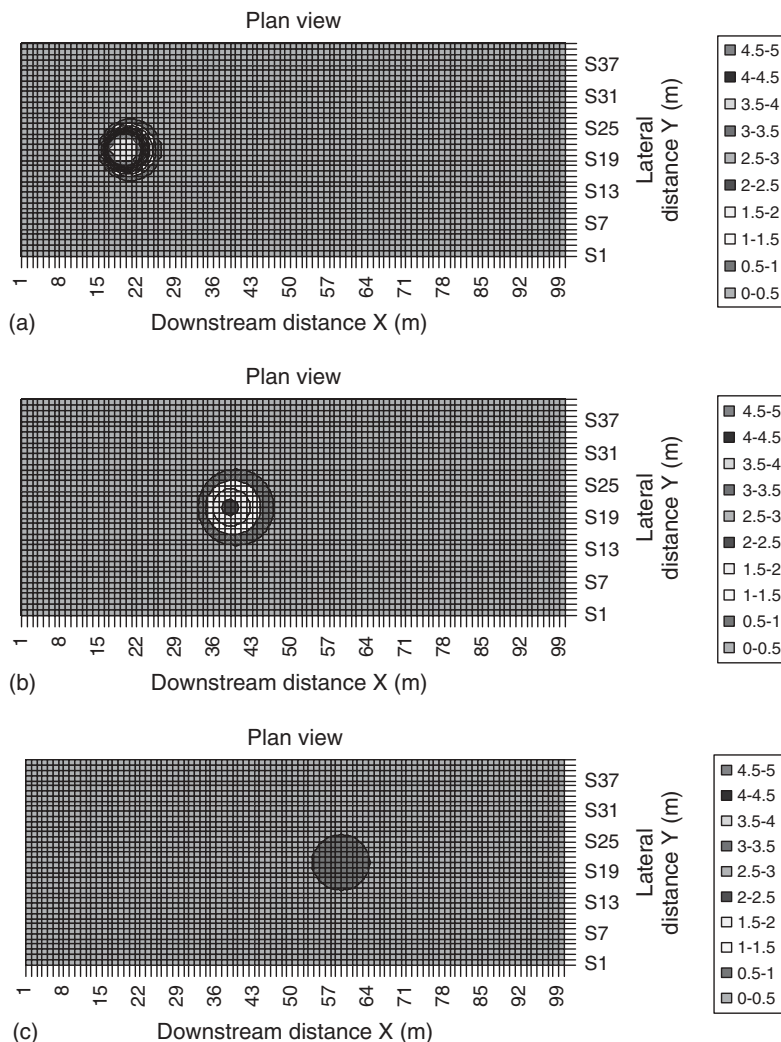
#### 40.12

##### Conclusion

The possibility of internal explosions and/or structural failure in a supply line or tank carrying a combustible material has been considered. The high internal pressure generates the release of toxic, flammable, and explosive materials which may subsequently ignite and explode. The resulting explosion and fire can often be devastating. A review was undertaken of pertinent information related to these

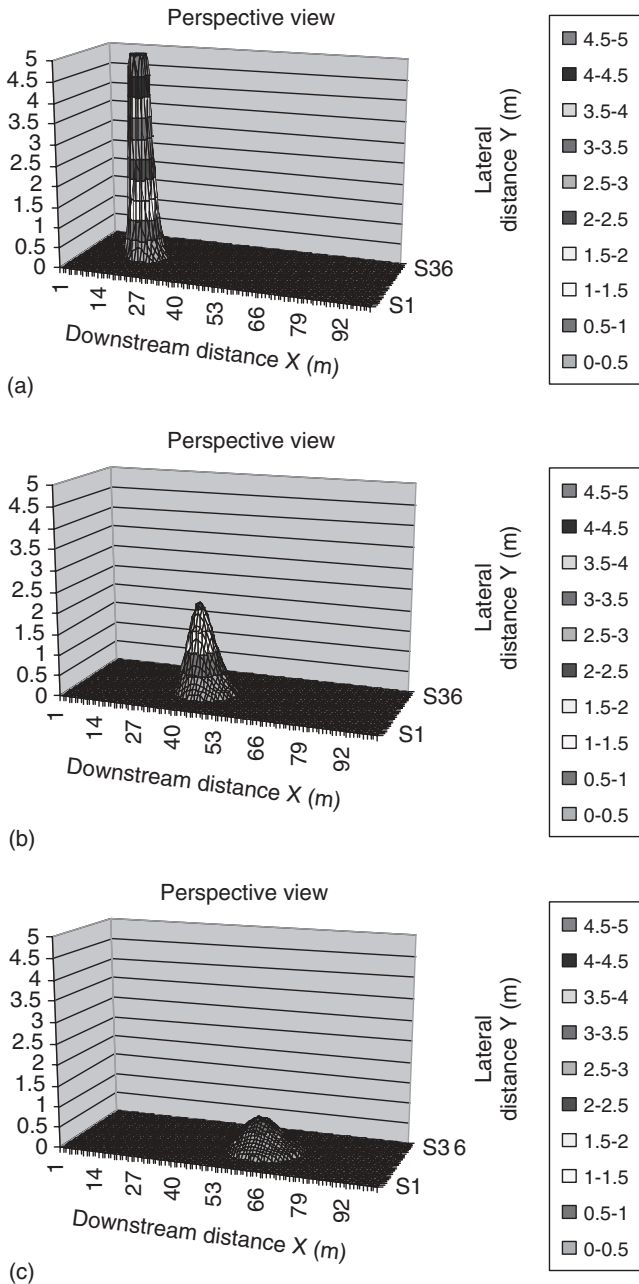


**Figure 40.7** Volume concentration versus lateral distance at various downstream distances  $x$  in meters for a  $10\text{ kg}$  puff release into a  $3\text{ m s}^{-1}$  wind; see Lilley (2008). (a) Atmosphere unstable, stability class A; (b) atmosphere neutral, stability class B; (c) atmosphere stable, stability class C.



**Figure 40.8** Plan view of a 10 kg puff release with a wind velocity of  $4 \text{ m s}^{-1}$  in an unstable atmosphere with stability class A; see Lilley (2008). Downstream distance and lateral distance versus volume concentration at times (a) 5, (b) 10, and (c) 15 s.

industrial problems, with release rates, and vapor clouds with plume and puff release of material, and its potential ignition. Any concentration of fuel between the LFL and UFL can ignite or explode. Being above the upper limit is not safe, since as the released material approaches a potential ignition source, a range of fuel:air ratios pass the location. Information related to explosions and/or the possible ignition of released materials has been given, and several calculations were given to illustrate the phenomena.



**Figure 40.9** Perspective view of a 10 kg puff release with a wind velocity of  $4 \text{ m s}^{-1}$  in an unstable atmosphere with stability class A; see Lilley (2008). Downstream distance and lateral distance versus volume concentration at times (a) 5, (b) 10, and (c) 15 s.

## References

- AGA (American Gas Association) (1988) *Fundamentals of Gas Appliances*, American Gas Association, Arlington, VA.
- AIChE (American Institute of Chemical Engineers) (1990) *Safety, Health and Loss Prevention in Chemical Processes*, AIChE, New York.
- ASME (American Society of Mechanical Engineers) (1973) *Prediction of the Dispersion of Airborne Effluents*, ASME, New York.
- Babrauskas, V. (2003) *Ignition Handbook*, Fire Science Publishers and Society of Fire Protection Engineers, Issaquah, WA.
- Bartnecht, W. (1981) *Explosions*, Springer, New York.
- Berry, D.J. (1989) *Fire Litigation Handbook*, 2nd Printing, National Fire Protection Association, Quincy, MA.
- Chow, C.Y. (1979) *Computational Fluid Mechanics*, John Wiley & Sons, Inc., New York.
- Clancey, V. (1972) Diagnostic features of explosive damage. Presented at the 6th International Meeting of Forensic Science, Edinburgh.
- Combustion Institute (1979) *Colloquium on Fire and Explosion. Proceedings of the 17th Symposium on Combustion*, Combustion Institute, Pittsburgh, PA.
- Cote, A.E. and Linville, J.L. (eds) (1990) *Industrial Fire Hazards Handbook*, National Fire Protection Association, Quincy, MA.
- Crowl, D.A. and Louvar, J.F. (1990) *Chemical Process Safety: Fundamentals with Applications*, Prentice Hall, Englewood Cliffs, NJ.
- DeNevers, N. (1995) *Air Pollution Control Engineering*, McGraw-Hill, New York.
- EPA, NOAA, and NSC (1992) CAMEO, ALOHA and MARPLOT, EPA, NOAA and NSC.
- Goodger, E.M. (1977) *Combustion Calculations*, Macmillan, London.
- Hanna, S.R. and Drivas, P.J. (1987) *Vapor Cloud Dispersion Models*, AIChE, New York.
- Kennedy, J. and Kennedy, P.M. (1985) *Fires and Explosions: Determining Cause and Origin*, Investigations Institute, Chicago, IL.
- Kennedy, J. and Kennedy, P.M. (1990) *Explosion Investigation and Analysis – Kennedy on Explosions*, Investigations Institute, Chicago, IL.
- Kletz, T. (1994) *What Went Wrong? Case Histories of Process Plant Disasters*, 3rd edn, Gulf Publishing, Houston, TX.
- Kuo, K.K. (1986) *Principles of Combustion*, John Wiley & Sons, Inc., New York.
- LaGrega, M.D., Buckingham, P.L., and Evans, J.C. (1994) *Hazardous Waste Management*, McGraw-Hill, New York.
- Lees, F.P. (1980) *Loss Prevention in the Process Industries*, Butterworths, London.
- Lilley, D.G. (1990a) *Fuels, Flammability, Fires and Flames*, Applied Engineering, Stillwater, OK.
- Lilley, D.G. (1990b) *Fire Investigation Technical Information*, Applied Engineering, Stillwater, OK.
- Lilley, D.G. (1992) *Computational Fluid Dynamics: Course Notes*, Applied Engineering, Stillwater, OK.
- Lilley, D.G. (1995a) *Fire Dynamics*. Short Course.
- Lilley, D.G. (1995b) *Fire dynamics*. Presented at the 33rd Aerospace Sciences Meeting, Reno, NV, January 9–12, 1995, Paper AIAA-95-0894.
- Lilley, D.G. (1996a) *Fire hazards of flammable fuel release*. Presented at the 34th Aerospace Sciences Meeting, Reno, NV, January 15–18, 1996, Paper AIAA 96-0405.
- Lilley, D.G. (1996b) *Flammable fuel release*. Presented at the Forum on Industrial and Environment Applications of Fluid Dynamics, ASME Fluids Engineering Conference, San Diego, CA, July 7–11, 1996.
- Lilley, D.G. (1997a) *Structural fire development*. Presented at the 35th Aerospace Sciences Meeting, Reno, NV, January 6–10, 1997, Paper AIAA-97-0265.
- Lilley, D.G. (1997b) *Estimating fire growth and temperatures in structural fires*. Presented at the 35th Aerospace Sciences Meeting, Reno, NV, January 6–10, 1997, Paper AIAA-97-0266.
- Lilley, D.G. (1997c) *Evolution, dispersion and ignition of flammable fuel release*. Presented at the ASME 17th International Computers in Engineering Conference, Sacramento, CA, September 14–17, 1997.



- Lilley, D.G. (1998a) Fuel release and ignition calculations. Presented at the 36th Aerospace Sciences Meeting, Reno, NV, January 12–15, 1998, Paper AIAA-98-0262.
- Lilley, D.G. (1998b) Fire development calculations. Presented at the 36th Aerospace Sciences Meeting, Reno, NV, January 12–15, 1998, Paper AIAA-98-0267.
- Lilley, D.G. (1999) Release and ignition of flammable material. Presented at the International Joint Power Generation Conference, San Francisco, CA, July 25–28, 1999.
- Lilley, D.G. (2003) Explosions: Technical Aspects of Fuel Gas Explosions. Short Course, repeated and updated annually, Lilley & Associates, Stillwater, OK.
- Lilley, D.G. (2004a) Fire Dynamics, Short Course, 2nd edn, repeated and updated annually, Technical Manual, Calculation Manual, Case Studies, and Review Problems, Lilley & Associates Course, Stillwater, OK.
- Lilley, D.G., (2004b) Adiabatic flame temperature calculation: a simple approach for general CHONS fuels. Presented at Aerospace Sciences Meeting, Reno, , NV, January 5–8, 2004, Paper AIAA-2004-0817.
- Lilley, D.G. (2005) Explosions: some fundamentals for investigators. Presented at the 43rd Aerospace Sciences Meeting, Reno, NV, January 10–13, 2005, Paper AIAA-2005-0379.
- Lilley, D.G. (2008) Parameter effects on plume and puff dispersion of released material. Presented at the 46th Aerospace Sciences Meeting, Reno, NV, January 6–10, 2008, Paper AIAA-2008-1141.
- Lilley, D.G. (2010) Trajectories of projectiles in 3-D space with an Excel/VBA code. Presented at the 48th Aerospace Sciences Meeting, Orlando, FL, January 4–7, 2010, Paper AIAA-2010-1359.
- Lilley, D.G. (2012) Fire dynamics, in *Safety Professionals Handbook*, 2nd edn (ed. J.M. Haight), American Society of Safety Engineers, pp. 467–514.
- NFPA (National Fire Protection Association) (2008) *Fire Protection Handbook*, 20th edn (ed. A.E. Cote), National Fire Protection Association, Quincy, MA.
- NFPA (National Fire Protection Association) (2011) *Guide to Fire and Explosion Investigations*, NFPA 921, National Fire Protection Association, Quincy, MA.
- Patton, A.J. (1994) *Fire Litigation Sourcebook*, 2nd edn, John Wiley & Sons, Inc., New York.
- SFPE (Society of Fire Protection Engineers) (2008) *Handbook of Fire Protection Engineering*, 4th edn, National Fire Protection Association and Society of Fire Protection Engineers, Boston, MA.
- Turns, S.R. (2001) *An Introduction to Combustion*, 2nd edn, McGraw-Hill, New York.
- Wark, K., Warner, C.F., and Davis, W.T. (1998) *Air Pollution: Its Origin and Control*, 3rd edn, Addison Wesley Longman, Menlo Park, CA.