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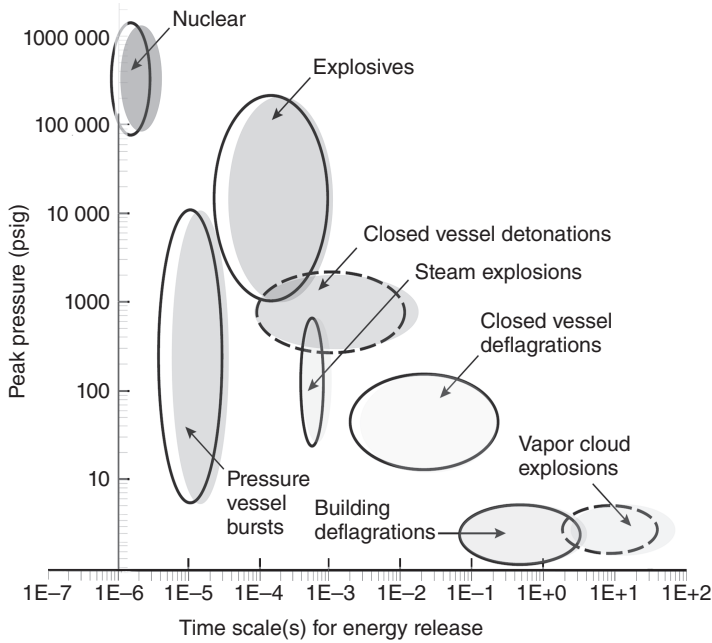
## Introduction

### 1.1 What Is an Explosion? Types of Explosions Covered in this Book

To introduce the concept of explosion protection, one must first understand what is an “explosion?” The dictionary definition of an explosion is “the action of going off with a loud noise or of bursting under the influence of a suddenly developed internal energy.” A more relevant definition related to the scientific study of the problem is the release of energy *to generate a pressure wave of finite amplitude traveling away from the source. This energy may have been stored in various forms such as nuclear, chemical, electrical, or pressure energy* [1]. The release of energy is not considered explosive unless it is rapid and concentrated enough to produce a pressure wave that one can hear. Even though many explosions damage their surroundings, an explosion doesn’t need to create external damage.

Explosions can occur in any media, such as air or condensed phases like liquid or solids. In all cases, the critical aspect is the generation of energy and pressure, which is released in a short time. The magnitude of energy release and its rate of release thus constitute the basis of the classification of different types of explosions. Zalosh [2] describes this using a peak pressure generated vs. a time scale for energy release, as shown in Figure 1.1. The peak pressure is directly related to the total amount of energy<sup>1</sup>, and the time scale is a result of the spatial scale and reaction rate or the speed with which the energy is released during the explosion. For example, when dynamite is ignited, the chemical reaction front proceeds through the solid at a speed of 4900 m/s. Thus, a 50 cm (0.5 m) stick would release all of its energy in  $0.5/4900 = 102 \mu\text{s}$ . For a gas detonation explosion, typical detonation velocities are in the range of 1500–4000 m/s. For example, stoichiometric acetylene ( $\text{C}_2\text{H}_2$ )–air mixture’s detonation velocity can be calculated from a chemical equilibrium code [3] and equal to 1868 m/s. Thus, in this case, the energy release in a 0.5 m radius would occur in  $0.5/1868 = 268 \mu\text{s}$ . The corresponding energy released would be the heat of combustion of acetylene in air (48.22 kJ/g) times its density ( $1.2 \text{ kg/m}^3$ ) times

<sup>1</sup> Pressure can be conceived as the energy released per unit volume. Both quantities have the same units of  $\text{J/m}^3$ .



**Figure 1.1** Classification of different types of explosions based on peak pressure and time to different kinds of energy release. Source: Zalosh [2].

the volume ( $\frac{4}{3}\pi(0.5\text{ m})^3$ ) given by 30.3 MJ! The corresponding pressure is equal to 18.2 atm (267.5 psig).

Explosions can be either deflagrations or detonations, depending on whether the speed of the chemical reaction front propagating through the combustible mixture is less than or greater than sound speed in the unburned fuel–air mixture. (Sound speed is approximately equal to 347 m/s if the fuel concentration is small compared to the air concentration.<sup>2</sup>) As shown in Figure 1.1, the peak pressures generated in detonations are at least twice as large as those in deflagrations, and the time scale is often at least an order of magnitude smaller. To begin, let us briefly describe the different types of explosions shown in Figure 1.1 to understand the significance of peak pressure and time for energy release.

### 1.1.1 Nuclear Explosions

As shown in Figure 1.1, nuclear explosions release the most amount of energy per unit volume. Therefore, they generate the highest pressure on the top right-hand corner of Figure 1.1. Also, the reaction speed is exceptionally high for nuclear explosions, with a tremendous amount of energy released in a microsecond. Both the

<sup>2</sup> For an ideal gas, speed of sound =  $\sqrt{\gamma \bar{R}T}$ , where  $\gamma$  is the ratio of specific heats = 1.4 for air,  $\bar{R}$  is the specific gas constant for air =  $\frac{8.314\text{J/kmol}\cdot\text{K}}{28.7\text{kg/kmol}} = 287\text{J/kg}\cdot\text{K}$ , and  $T$  is the temperature say 300 K.

Thus, speed of sound =  $\sqrt{1.4 \times 287\text{J/kg}\cdot\text{K} \times 300\text{K}} = 347\text{m/s}$ .

exceptionally high magnitude of pressures and the extremely short time scales make nuclear explosions extremely damaging.

### 1.1.2 Pressure Vessel Bursts

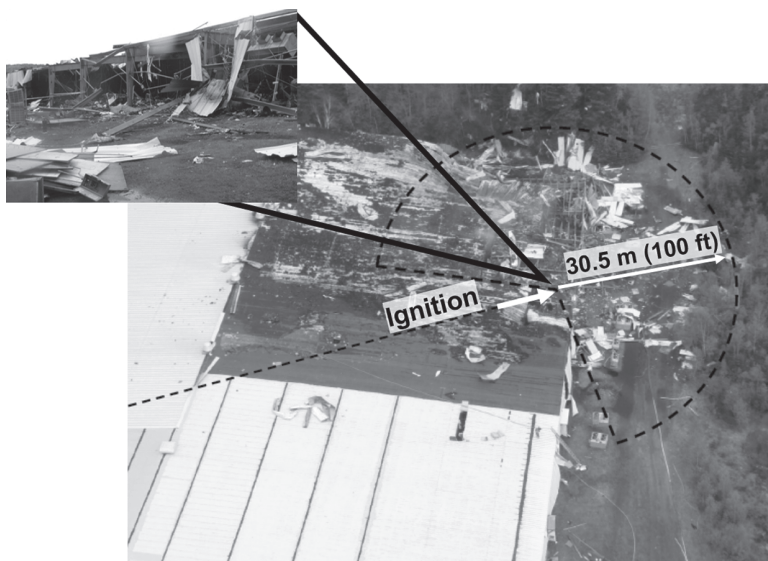
Progressing further in a direction of increasing time scale in Figure 1.1, a pressure vessel burst is the release of energy of compression in high-pressure vessels. The release of pressure takes place in a time for a crack<sup>3</sup> to propagate sufficiently far to allow the vessel shell to split open. This is typically on the order of 10  $\mu$ s. The peak pressure is approximately equal to the vessel pressure at the time of bursting,  $P_b$ . The isentropic expansion energy,  $E_{\text{burst}}$ , for an ideal gas released during the vessel burst is [1]:

$$E_{\text{burst}} = \frac{(P_b - P_a)}{\gamma - 1} V, \quad (1.1)$$

where  $P_b$  = vessel pressure at the time of bursting,  $P_a$  = pressure of ambient air (1 atm = 14.7 psia = 101 kPa at sea level),  $V$  = vessel volume, and  $\gamma$  = ratio of specific heats for the gas in the vessel (equals 1.4 for air).

### 1.1.3 Explosives

Explosions caused by explosives, usually condensed phase have time scales of the order of 100  $\mu$ s. Figure 1.2 shows an aerial view of the aftermath of an explosion



**Figure 1.2** Aerial view of damage and debris caused by a black powder explosion, with arrow indicating origin. Source: U.S. Department of Justice.

<sup>3</sup> If the crack is caused in a vessel containing a high-pressure liquefied gas by a structural loss because of an external fire, the resulting explosion is called a Boiling Liquid Expanding Vapor Explosion (BLEVE).

incident involving a special black powder composed of ascorbic acid (combustible powder), potassium nitrate (strong oxidizer), and potassium perchlorate (highly reactive oxidizer). The latter two ingredients were in the form of granular solids requiring milling prior to being mixed in two combination milling/blending machines located where indicated by the arrow in Figure 1.2. There were about 34 kg (75 lb) of black powder in each machine, and the first explosion triggered a second explosion, with the combined effects causing two fatalities in addition to the destruction shown in the photograph. As shown, the relatively small amount of explosive created significant damage to property in a radius of 30.5 m (100 ft). This radius is also called as a “blast debris radius,” associated with a blast wave, i.e. a pressure disturbance propagating into the atmosphere away from the source of energy release. We will discuss the damage potential of blast waves based on the initial energy release and distance from the release point in Chapter 7. The knowledge is useful for safe citing of industrial facilities.

Energies released by condensed-phase explosives are often quoted in terms of the trinitrotoluene (TNT) equivalent weight. One kilogram of TNT has an explosive energy of  $4.2 \times 10^6$  J. Most condensed-phase high explosives have an explosive energy per unit mass that is similar to that of TNT. For example, the explosive energy of pentolite (50/50) is  $5.1 \times 10^6$  J/kg, and that of royal demolition explosive (RDX) is  $5.4 \times 10^6$  J/kg. The corresponding TNT equivalent of pentolite is  $5.1/4.2 = 1.2$  kg-pentolite/kg-TNT, and that of RDX is  $5.4/4.2 = 1.3$  kg-RDX/kg-TNT.

#### 1.1.4 Closed Vessel Detonation

As discussed earlier, a detonation propagates at a speed greater than the speed of sound. A closed vessel detonation is usually the detonation of a flammable gas that is enclosed in a vessel, for example, a pipeline. In this case, ignition leads to a deflagration, which starts slowly, but rapidly accelerates to a detonation after propagating through the pipe for a distance called a run-up distance. These distances are usually large (60–100 tube diameters) and the transition occurs in piping but is very improbable in vessels and equipment unless there is a combination of a fast-burning gas mixture and a highly turbulent flame accelerating situation. The transition from deflagration to detonation is also highly complex. A flammable gas can also be made to detonate without a “run up” by providing a sufficiently large ignition energy. For example, Carlson [4] determined the minimum energy for initiation of detonation in stoichiometric gas–oxygen mixtures, using exploding wires to initiate detonation. The ignition energy to cause direct detonation of a stoichiometric propane–oxygen mixture is 2.5 J [4]. On the other hand, the minimum ignition energy (MIE) to ignite (sustain a propagating flame) in the same mixture is four orders of magnitude lower at 0.26 mJ as shown in Table 1.1. Thus, a combustible gas–air mixture likely will form a sustained flame, which may accelerate to a detonation rather than detonate directly since ignition with such a large energy source is usually unlikely.

**Table 1.1** Flammability properties of some common gas air mixtures in air.

Fuel	$T_{ad}$ (K) [3]	$S_L$ (cm/s) [5]	MIE (mJ) [6]	$d_q$ (mm) [6]	AIT (K) [6]	LFL %Fuel [7]	UFL %Fuel [7]	$\phi_{FL}$ [8]	$\phi_{UFL}$ [8]	LOC $N_2$ -air [9]	LOC $CO_2$ -air [9]	$r_{st}$ %Fuel [6]	$\Delta H_c$ (kJ/mol) [6]	$\Delta H_c$ (kJ/g) [6]
H <sub>2</sub>	2400	312	0.018	0.55	673	4	75	0.14	2.54	4.6	4.6	29.5	241.8	119.96
CO	2370	46	—	1.73	882	12.5	74	0.34	6.76	5.1	5.1	29.5	283	10.1
CH <sub>4</sub>	2226	40	0.28	2.5	810	5	15	0.46	1.64	11.1	13.1	9.47	802.3	50.1
C <sub>2</sub> H <sub>2</sub>	2541	166	0.017	0.55	578	2.5	100	0.19	$\infty$	NA	NA	7.74	1255.5	48.22
C <sub>2</sub> H <sub>4</sub>	2370	80	0.09	1.25	763	2.7	36	0.41	6.1	8.5	10.2	6.53	1323.1	47.16
C <sub>2</sub> H <sub>6</sub>	2260	42.5 [10]	0.25	2	745	3	12.4	0.5	2.72	9.5	11.9	5.65	1428.6	47.5
C <sub>3</sub> H <sub>8</sub>	2257	46	0.26	2.10	743	2.1	9.5	0.51	2.83	10.7	12.8	4.02	2043.1	46.3
C <sub>4</sub> H <sub>10</sub>	2260	45	0.26	2.20	638	1.8	8.4	—	—	10.6	13.0	3.12	2656	45.7

$T_{ad}$ : Adiabatic flame temperature;  $d_q$ : Quenching distance; UFL: Upper flammability limit;  $S_L$ : Laminar burning velocity; AIT: Auto-ignition temperature;  $\phi$ : Equivalence ratio; MIE: Minimum ignition energy; LFL: Lower flammability limit; LOC: Limiting oxygen concentration;  $r_{st}$ : Stoichiometric volume concentration of fuel;  $\Delta H_c$ : Heat of combustion.

### 1.1.5 Steam Explosions

A steam explosion produces peak pressures in the range of 2–70 bar (30–1000 psig), within a millisecond. As shown in Figure 1.1, steam explosions have similar time scales as a closed vessel detonation but lower peak pressures. A steam explosion is not caused by combustion. Instead, a steam explosion is a physical explosion caused by the extremely rapid vaporization of water due to heat transfer from a second liquid that is at a temperature far in excess of the water's boiling point and in direct contact with the water. As the second liquid is usually either molten metal or some other melt, a steam explosion is a violent melt–water interaction. If the water is replaced with some other liquid that has a much lower boiling point than the hot liquid, the more general term is *vapor explosion*. Vapor explosion examples include Freon-22 and heated mineral oil, water and liquid nitrogen, and liquid ethane and water [11]. Steam and vapor explosions are a concern in nuclear power plant accidents with water-cooled reactor core temperatures sufficiently high to produce molten nuclear reactor fuel rods or cladding [11].

Vapor explosions occur only if certain thermodynamic and hydrodynamic conditions are satisfied. The thermodynamic condition is that the liquid–liquid contact surface temperature,  $T_{\text{contact}}$ , must be greater than the spontaneous nucleation temperature,  $T_{\text{sn}}$ , for water, that is, the temperature at which vapor bubbles first appear in the absence of any heated surfaces. The equation for  $T_{\text{contact}}$  is:

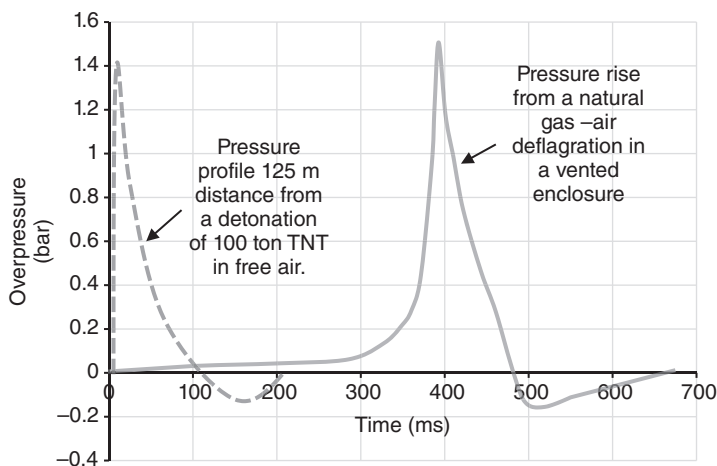
$$T_{\text{contact}} = \frac{T_H + T_C \sqrt{\frac{(k\rho c_p)_C}{(k\rho c_p)_H}}}{1 + \sqrt{\frac{(k\rho c_p)_C}{(k\rho c_p)_H}}}, \quad (1.1)$$

where  $T_H$  is the hot liquid temperature,  $T_C$  is the cold liquid temperature, and  $k\rho c_p$  is the product of thermal conductivity, density, and specific heat for either the cold or hot liquid depending on the subscript.

For example, if molten copper at a temperature of 1400 °C is immersed in 20 °C water, the interfacial contact temperature as per Eq. (1.1) is 1341 °C. If molten cuprous oxide at a temperature of 1330 °C is immersed in 20 °C water, the calculated interfacial contact temperature is 954 °C. In both cases, the contact temperature is substantially higher than the spontaneous nucleation temperature for water, which is very sensitive to surface tension changes due to additives or contaminants but can be as high as 270 °C. Thus, molten copper interactions with water can indeed be explosive. Similar results are observed with many other molten metals and with kraft smelt immersions into water. The latter have been associated with black liquor recovery boiler accidents at paper mills. For the vaporization to occur rapidly enough and in sufficient volume to generate potentially damaging pressures, it is necessary to have ample liquid–liquid interfacial contact area.

### 1.1.6 Closed Vessel Deflagrations

All the explosions discussed earlier, except steam explosions, and pressure vessel bursts were detonations, where the speed of propagation of the reaction front is greater than the speed of the sound. Such explosions are particularly dangerous



**Figure 1.3** Comparison of pressure profiles between a detonation and a confined deflagration. Pressure profile for the 100-ton TNT detonation (dashed curve) at 125 m (410 ft) from the blast center [12]. The natural gas-air deflagration occurs in a large scale  $25.6 \times 8 \times 8$  m test rig [13]. Natural gas concentration equals 9.4% (equivalence ratio = 1.05), and ignition is at the center. Total vent area =  $160 \text{ m}^2$ .

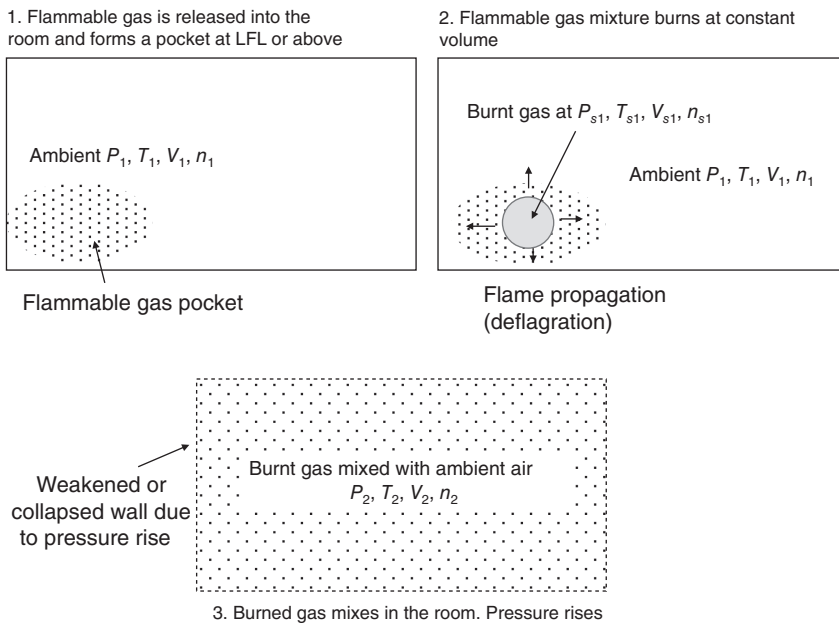
because of the high detonation pressures and the short time scale of energy release. We will now move on to explosions in which the speed of propagation is slower than the speed of the sound. Such explosions are called deflagrations. In small closed vessel deflagrations, peak pressures can reach up to 8–10 bar with time scales in the range of 1–10 ms. Deflagrations in buildings have longer time scales. Such accidental deflagration causes the enclosure to open or burst (because of either deflagration venting or structural failure), and the released blast wave will exert pressure loads on adjacent structures. The pressure vs. time trace because of confined deflagration is much different from pressures discussed earlier from condensed-phase explosives and burst pressure vessels. Figure 1.3 shows the pressure wave generated by a blast wave generated by a condensed-phase explosive (100-ton TNT) at a location 125 m away by a dashed curve. The experiments were performed by Kingery et al. [12] where pressure rise vs. time at different distances from a 100-ton TNT explosion were measured. As shown, a peak pressure of 1.4 bar is attained in a short time scale of  $\sim 1$  ms. The overpressure then decays over a time scale of  $\sim 100$  ms followed by a smaller negative pressure pulse. The solid line in Figure 1.3 is obtained from test data published by the Steel Construction Institute [13]. It shows the pressure felt by the walls of an enclosure ( $25.6 \times 8 \times 8 \text{ m}^3$ ) during the deflagration of a 9.4% natural gas-air mixture ignited in the center. The deflagration pressure cannot reach the peak pressure of  $\sim 8$  bar because of the venting and occurs at 1.5 bar instead because of three openings in the enclosure walls with a total coverage area of  $160 \text{ m}^2$ . The peak pressure of 1.5 bar occurs much slower than the detonation at 400 ms. In addition, it should be noted that the pressure trace by the TNT explosion in Figure 1.3 is 125 m away from the source. At  $\sim 30$  m from the TNT explosion, the peak pressure is 26 bar [12]!

One example of deflagration in a closed vessel is the Center Wing Tank explosion that occurred during the TWA 800 flight on 17 July 1996. The flammable vapor in the Center Wing Tank of the Boeing 747 on that flight came from a small quantity of Jet A fuel in the tank. As the fuel was heated from air conditioning equipment under the Center Wing Tank, and the partial pressure of tank air was reduced as the Boeing 747 climbed after takeoff, the fuel–air equivalence ratio increased well into the flammable range. Ignition occurred at an altitude of 4300 m (14 000 ft), at which the ambient pressure is 0.585 bar. The closed vessel deflagration pressure  $P_m$  of 6 bar was significantly higher than the strength of the Center Wing Tank structures, leading to a massive breakup of the Boeing 747 [14].

### 1.1.7 Building Deflagrations

Building deflagrations can be because of gas, droplet, or dust (tiny solid particles suspended in air) explosions. Although small in terms of peak pressures generated, compared to the other types of explosions shown in Figure 1.1, it should be noted that it is of sufficient magnitude to cause building collapse. For example, to cause significant damage to a brick wall takes only approximately 2 psig or 0.14 bar (14 kPa)! For typical hydrocarbon fuels, the maximum explosion pressure is roughly 8–10 bars. Since this pressure is enormous when compared to the strength of most industrial structures, small pockets of flammable gasses in a building as shown in Figure 1.4 are sufficient to cause extensive damage.

Figure 1.4 shows a conceptual model for a confined deflagration in a room partially filled with flammable gas. If gas is ignited, a flame will grow spherically



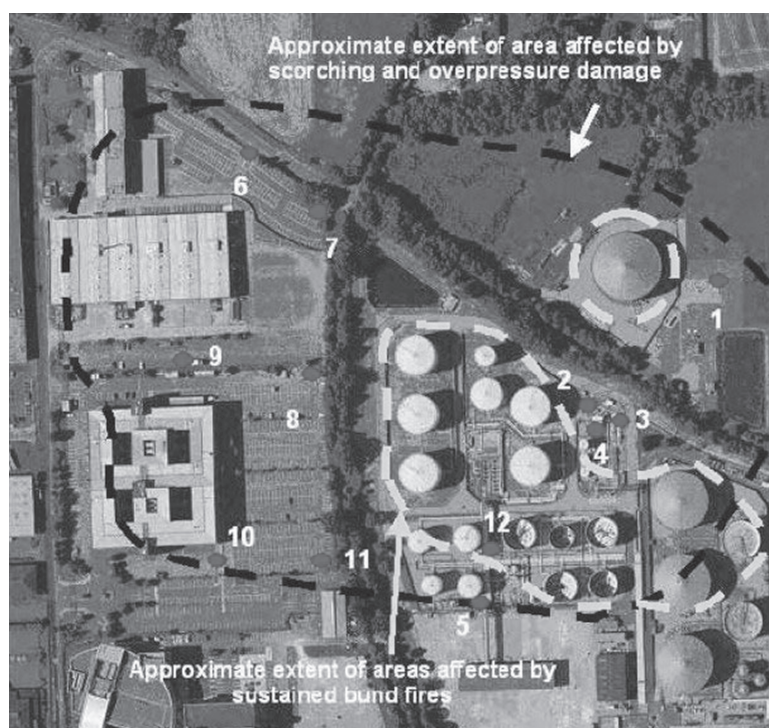
**Figure 1.4** Conceptual flow of events in a building explosion,  $P$ ,  $T$ ,  $V$ , and  $n$  are pressure, temperature, volume, and number of moles. Subscript 1 represents the initial state of the gas pocket and subscript 2 represents the final state after combustion of the small pocket of gas of initial volume  $V_1$ .



outward from the point of ignition. As the flame grows, it consumes fuel and causes a rise in pressure that depends on the volume and concentration of the flammable gas. Building partial volume deflagrations are one of the most common industrial accidents. A case study related to this (Danvers Explosion) is discussed in Chapter 2.

### 1.1.8 Vapor Cloud Explosions

Vapor cloud explosions (VCE) usually occur because of a large vapor cloud release and consequent mixing with ambient air, combined with highly obstructed or partially confined areas. The obstructions and partial confinements create zones, where the deflagration accelerates because of turbulence and in some cases can lead to detonations. Peak pressures in VCEs are of the same order of magnitude as those in building deflagrations, but the energy release times are usually longer because the flammable clouds are usually much larger than those that form inside buildings. One of the most significant industrial accidents recently in Buncefield, UK, was a vapor cloud explosion [15] as shown in Figure 1.5.



**Figure 1.5** Vapor cloud explosion (VCE) at Buncefield, UK, on 11 December 2005. The explosion originated because of a vapor cloud release from a Jet A fuel storage facility. The resulting vapor cloud was estimated to be  $120\,000\text{ m}^2$  with an average height of 3 m. The black dashed line indicates the area affected by scorching and overpressure damage. The white dashed line shows the areas in the tank farm where sustained bund fires occurred after the explosion. The numbers indicate the location of vehicles, drums, and other enclosures, which exhibited damage consistent with overpressures above 200 kPa. Source: Taveau [15]/John Wiley & Sons.

**Example 1.1** Calculate the burst energy for a  $10 \text{ m}^3$  vessel that ruptures when it is filled with air at a pressure of 6890 kPa (1000 psi).

**Solution**

The solution of this problem is based on Eq. (1.1)

$$E_{\text{burst}} = \frac{(P_b - P_a)}{\gamma - 1} V$$

At sea level,  $P_b - P_a = 6890 - 101 = 6789 \text{ kPa}$ ,  $\gamma = 1.4$ .

Thus,

$$E_{\text{burst}} = \frac{6789 \text{ kPa}}{1.4 - 1} 10 \text{ m}^3 = 169 \text{ MJ}$$

The burst energy is  $169 \text{ MJ} = 169/4.2 = 40.2 \text{ kg}$  of TNT.

## 1.2 Controlling Parameters of a Combustible Gas/Vapor Explosion Hazard

Given a combustible gas–air or vapor–air or dust–air mixture, the following parameters must be evaluated by an engineer to analyze the magnitude of the explosion hazard:

1. The laminar burning velocity defined, in a spatial frame fixed to the flame front, as the velocity of the unburned mixture approaching the reaction front in the normal direction. The velocity is a function of the concentration or equivalence ratio of the mixture, ambient pressure, and temperature.
2. Volume of mixture and geometry of the space.
3. The rate of pressure rise denoted by  $\frac{dP}{dt}$ .

A *flame* is a surface in the gas phase where a rapid chemical change occurs in a thin layer accompanied by heat generation. The unburned gas velocity approaching normal to the flame surface in the absence of turbulence is called the *laminar burning velocity*  $S_L$ . The laminar burning velocity is a fundamental thermokinetic property of the mixture composition and concentration, indicating the fuel consumption rate at the reaction zone or flame surface. Hence, it does not change with the increase or decrease of the flow speed. The laminar burning velocity of typical hydrocarbon air flames range from 10 to 80 cm/s with a flame thickness of  $\sim 0.1 \text{ mm}$ . The highest velocity is that of  $\text{H}_2$ –air mixtures, which can be up to 300 cm/s (6.3 mph), or around an average jogging speed. Further details about the laminar burning velocity, its formulation, and its variation with pressure and temperature will be discussed in Chapter 3.

The speed with which the flame travels through the gas–air mixture, measured with respect to some fixed position, is called the *flame speed*. Flame speed is not the same as burning velocity. The flame speed and the burning velocity are related by the expression

$$S_f = S_L \beta E, \tag{1.2}$$

where  $E$  is an expansion ratio caused because of an increase in temperature. Typical flame temperatures of hydrocarbon–air mixtures are around 2500 K, and thus the expansion ratio is  $\sim 2500/300 \text{ K} \sim 8$ .  $\beta$  is a parameter that is related to the fact that the unburned gas may be in motion and the combustion reaction is enhanced because of instabilities and turbulence ( $\beta > 1$ ), as is often manifested in a wrinkled flame surface. The flame speed in gas deflagrations can be very high  $\sim 100 \text{ m/s}$  because of turbulent flame acceleration. An important aspect of both flame speed and pressure development is the degree of confinement or the geometry of the space in which the combustible mixture is contained. Usually, if the combustible vapor–air mixture is not at least partially confined, then pressure effects are not observed. The deflagration is usually in the form of a flash fire and poses a thermal hazard rather than an explosion hazard. For example, unconfined gunpowder (75%  $\text{KNO}_3$ , 15% charcoal, and 10% sulfur) will burn rapidly if ignited. Still, it will not explode if it is not wrapped tightly in a cartridge to make a firework. Increasing the gunpowder volume will result in more energy being produced, thereby creating more power in the explosion [16].

Under certain conditions, especially with significant vapor releases, pressure effects can occur if the flame or reaction front accelerates as it propagates through the gas–air mixture. This acceleration and corresponding enhanced reaction rate are usually because of either initial turbulence in the gas cloud, turbulence induced by unburned gas flow around obstacles, or instabilities in the flame front that lead to turbulence. Such explosions, discussed earlier, are called VCEs. VCEs are rare compared to the more common confined gas deflagration explosions. This is because it is unlikely that large quantities of vapor (usually in tens to hundreds of tons) are released in the open.

A more likely scenario is the release of smaller quantities of vapor, dust, and mist within some form of confinement, which is provided by the equipment or the industrial process compartment or section of the industrial plant. If a flammable mixture is formed under such conditions and is ignited, then a confined gas explosion will occur. Such equipment and building explosions usually cause damage to the structure in which they originate. In the case of dust explosions, propagation into adjacent compartments is also possible because the pressure wave from the initial explosion causes built-up dust layers in ceilings and joists in the entire facility to get suspended. The explosion hazard in equipment can be controlled using explosion suppression or deflagration venting systems, and the compartment explosions can be further protected by using deflagration vents, whose design is covered in NFPA 68 [5]. We will also discuss deflagration venting in Chapter 4.

The energy released in explosions can be propagated from the source by three mechanisms:

- i. Shock/blast wave
- ii. Projectiles often in the form of fragments
- iii. Thermal radiation.

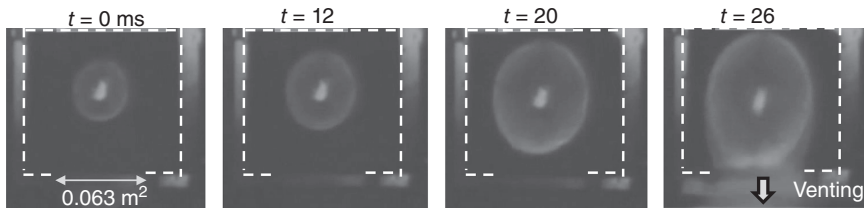
Of these, the blast wave is the common form of far-field damage from explosions where large quantities of explosive mixtures are involved. Damage by flying

fragments is important in building explosions and in pressure vessel bursts. Thermal radiation is an important consideration in dust explosions. In addition, during dust explosions, besides fragments, burning particles can also lead to injury to personnel.

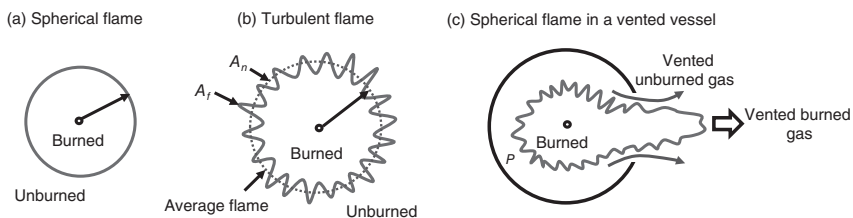
### 1.3 Flame Propagation

In many industrial explosion accidents, the explosion develops because of a chemical combustion reaction. High amounts of energy release occur because of the self-sustained propagation of a localized combustion zone propagating through the given gas–air or combustible dust cloud mixture. Figure 1.6 shows an example of an explosion in a  $0.56\text{ m} \times 0.56\text{ m} \times 0.56\text{ m}$  ( $0.18\text{ m}^3$ ) cubic vessel with a vent of area  $0.063\text{ m}^2$ . The vessel is filled with an 8% ethylene–air mixture and ignited in the center as shown in Figure 1.6 [17]. The flame propagates spherically as shown in Figure 1.7. Initially, at  $t = 12\text{ ms}$  it is laminar but at  $t = 20\text{ ms}$  the flame shows signs of wrinkling, and at  $t = 26\text{ ms}$ , burned gasses are observed escaping from the vent at the bottom. The venting leads to additional turbulence. Higher burning rates and consequently higher pressures are achieved because of the venting.

The speed at which the combustion wave propagates with respect to a fixed position is called the flame speed. The velocity at which the unburned gas enters the flame front in a direction normal to it is called the laminar burning velocity  $S_L$ .



**Figure 1.6** The evolution of an 8% ethylene–air flame in a cubic vessel of volume  $0.18\text{ m}^3$ , with a bottom vent area of  $0.063\text{ m}^2$ . The flame grows spherically till around  $t = 26\text{ ms}$  when venting of the gasses causes the flame shape to become nonspherical. The surface of the flame also becomes wrinkled at around  $t = 20\text{ ms}$ . The maximum pressure in the vented compartment equals  $0.87\text{ atm}$  or  $12.8\text{ psig}$ . Source: Zalosh [17], American Institute of Chemical Engineers.



**Figure 1.7** Flame propagation in: (a) spherical freely propagating flame (laminar), (b) spherical freely propagating flame (turbulent), and (c) spherical flame propagating in a confined vessel with a vent.

The laminar burning velocity,  $S_L$ , is a fundamental thermokinetic property of the gas–air mixture and depends on the composition of the gas–air mixture, gas or dust concentration, temperature, and pressure. The flame speed,  $S_f$ , is a function of  $S_L$ , thermal expansion, change in number of moles, and the initial velocity of the gas. To further demonstrate the differences between  $S_L$  and  $S_f$ , three cases of spherical flame propagation with central ignition are shown in Figure 1.7. All gasses are at rest when ignition takes place. The following questions can now be asked:

1. What is the flame speed or what is the rate at which the flame grows in size?
2. What is the consumption rate of unburned fuel at the flame surface?
3. What happens when the flame becomes stretched or wrinkled because of instabilities and/or turbulence as shown in Figure 1.7b?
4. What happens when the flame is confined in a vessel with an opening, as shown in Figure 1.7c?

The answers to the first two questions should clarify the difference between the flame speed  $S_f$  and the laminar burning velocity  $S_L$ . The third question will clarify the important role of flame wrinkling and turbulence in flame propagation and bridge our understanding of industrial accidents where large-scale turbulent premixed flame spread occurs compared to flames studied in the laboratory that cannot be simulated at such large scales. The fourth question is of importance to explosion safety as when the propagating flame is confined, it will cause an increase in pressure within the confinement. Some of this pressure will be relieved by the flow of gasses leaving the enclosure, which is a process called *venting*. The pressure rise in the enclosure with time and corresponding movement of gasses out of the enclosure through an opening are coupled to the propagating flame’s motion that can be turbulent. This complex problem is one of the critical aspects that we will discuss in detail in Chapters 3 and 4.

Let us consider a combustible gas–air mixture that is ignited at the center causing a spherical flame to propagate freely outward without any confinement as shown in Figure 1.7 radially. The flame divides the burned gasses on the inside denoted with a subscript  $b$  and the unburned gasses outside denoted by a subscript  $u$ . Let us assume the following:

- i. The flame front moves at a velocity that is low relative to the velocity of sound. Typical velocities in HC–air mixtures in case 1 are  $\sim 10$  m/s, an order of magnitude lower than sound speed (330 m/s).
- ii. Ideal gas law applies.
- iii. The flame is perfectly spherical, giving:  $V_b = \frac{4}{3}\pi r_b^3$ .

Since the gas mixture flame is assumed to be spherical (at least until the vent opens),

$$\frac{dV_b}{dr_b} = \frac{d}{dr_b} \left( \frac{4}{3}\pi r_b^3 \right) = 4\pi r_b^2 = A_{f,N}, \quad (1.3)$$

where  $A_{f,N}$  is the area of the flame. The subscript “N” denotes that the flame area evolves in a direction normal to the direction of the flame front. It denotes the

minimum area that the flame can acquire, normal to the direction of propagation. This is an important assumption that is made here. If the flame front area is not spherical, for example, it is wrinkled as shown in Figure 1.7b, the actual area of the flame denoted by  $A_f$  will be much more. However, since  $r_b$  has not increased,  $\frac{dV_b}{dr_b}$ , will equal the minimum area possible for the flame to assume a perfectly spherical shape.

The rate of production of burned gas is given by

$$\frac{dm_b}{dt} = A_f \rho_u S_L. \quad (1.4)$$

The left-hand side denotes the production of burned gasses and the term on the right is the product of the mass flux of unburned gas approaching the flame ( $\rho_u S_L$ ), times its actual surface area,  $A_f$ . The subscript  $N$  is dropped here because the flame surface need not be smooth, as shown in Figure 1.7b. If the flame is wrinkled, there is more surface for the chemical reaction of combustion to take place, causing more production of the burned gas. Writing  $m_b$ , equal to the product of the density of burned gas times its volume gives,

$$\frac{d(\rho_b V_b)}{dt} = A_f \rho_u S_L, \quad (1.5)$$

$$\rho_b \frac{dV_b}{dt} + V_b \frac{d\rho_b}{dt} = A_f \rho_u S_L. \quad (1.6)$$

Note that  $S_L$  is the laminar burning velocity or the velocity of the unburned gas approaching the flame in a direction perpendicular to the surface of the flame. So imagine, you are able to be on the flame front. You will see unburned gasses moving toward you at a velocity equal to  $S_L$ . The unburned gasses will combust and exit the flame at a velocity that you will perceive as leaving behind you at a temperature equal to the flame temperature. Also, in Eq. (1.6),  $\frac{dV_b}{dt} = \frac{dV_b}{dr_b} \cdot \frac{dr_b}{dt} = A_{f,N} S_f$ , where  $S_f$  is the velocity with which the spherical flame grows or the flame speed. Equation (1.6) now becomes,

$$\rho_b A_{f,N} S_f + V_b \frac{d\rho_b}{dt} = A_f \rho_u S_L, \quad (1.7)$$

$$S_f = \frac{A_f}{A_{f,N}} \frac{\rho_u}{\rho_b} S_L - \frac{V_b}{\rho_b A_{f,N}} \frac{d\rho_b}{dt}. \quad (1.8)$$

Equation (1.8) gives the relationship between the laminar flame speed and the laminar burning velocity for a generalized case of the spherical flame propagating outward. The second term on the right-hand side of Eq. (1.8) can be simplified using the ideal gas law  $\rho_b = \frac{P_b(MW_b)}{RT_b}$ , where  $MW_b$  equals the molecular weight of the burned gas,  $P_b$  is the pressure and  $T_b$  is the temperature of the burned gas.  $R$  is the universal gas constant (8.314 J/mol-K).

$$\frac{V_b}{\rho_b A_{f,N}} \frac{d\rho_b}{dt} = \frac{V_b}{\rho_b A_{f,N}} \frac{d}{dt} \frac{P_b(MW_b)}{RT_b}. \quad (1.9)$$

With an assumption that  $T_b$  and  $MW_b$  will not change with time,<sup>4</sup> the differential term in Eq. (1.9) is equal to  $\frac{dP_b}{dt}$  denoting the rate of pressure rise in the burned gas. For a freely expanding flame Figure 1.7a or b, this quantity is small and can be neglected, causing the second term on the right-hand side of Eq. (1.8) to be equal to zero. Thus the flame speed is given by

$$S_f = \frac{A_f}{A_{f,N}} \frac{\rho_u}{\rho_b} S_L, \quad (1.10)$$

And for a case where the flame is smooth (Figure 1.7a), can be further simplified as  $A_f = A_{f,N}$ ,

$$S_f = \frac{\rho_u}{\rho_b} S_L = \frac{T_b(MW_u)}{T_u(MW_b)} \frac{P_u}{P_b} S_L. \quad (1.11)$$

For freely propagating premixed hydrocarbon gas flames,  $\frac{P_u}{P_b} \sim 1.01$  and  $\frac{(MW_u)}{(MW_b)} \sim 1$ , thus making  $S_f$  related to  $S_L$  in the simplest case as

$$S_f = \frac{T_b}{T_u} S_L = E S_L, \quad (1.12)$$

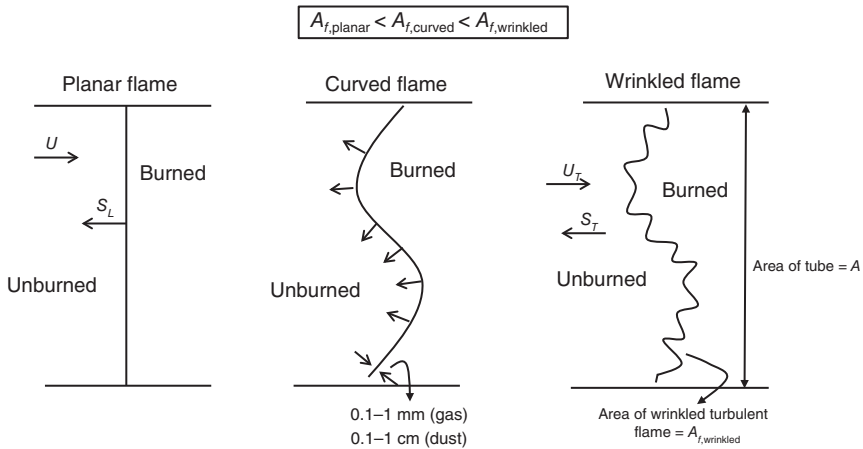
where  $E$  is called an expansion factor and is a measure of the increase in volume created by combustion

$$E = \frac{T_b}{T_u}. \quad (1.13)$$

Assuming no losses, the burned gas temperature is equal to the flame temperature and  $E \sim \frac{T_f}{T_u} \sim 8$  for most hydrocarbon–air flames. Equation (1.13) shows that, in a simplified case with similar molecular weights of unburned reactants and products, flame speed is equal to the burning velocity multiplied by an expansion ratio that is equal to the flame temperature divided by the unburned gas temperature. However, in practice, as the flame grows its surface can no longer be considered planar and the assumption of  $A_f = A_{f,N}$  no longer applies. Figure 1.8 shows a sketch of a flame propagating in a tube. Instabilities and turbulence create flame distortions causing the smooth planar flame to transition to a wrinkled flame front, which is usually the shape of the flame in industrial deflagrations. The first sketch shown in Figure 1.8 shows a planar flame. However, such a flame occurs only during the initial stages of the flame propagation when the flow is laminar. Very soon the flame becomes wrinkled as shown in the middle sketch of Figure 1.8. The wrinkling increases with increased turbulence as shown by the last sketch. Importantly, the capability of the curved flame and then the wrinkled flame to consume fresh unburned fuel increases dramatically. As the flame gets more and more wrinkled, its flame speed will increase because the area of turbulent wrinkled flame is significantly greater than the planar flame ( $A_{f,\text{laminar}} < A_{f,\text{curved}} < A_{f,\text{wrinkled}}$ ). In the case of combustible dust flame propagation discussed in Chapter 8, there is inherently turbulence

<sup>4</sup>  $T_b$  can change due to adiabatic compression for confined deflagrations. In this case,  $T_b$  will be a function of  $dP_b/dt$ . However, for now, we will assume this is negligible and discuss the details further in Chapter 3.

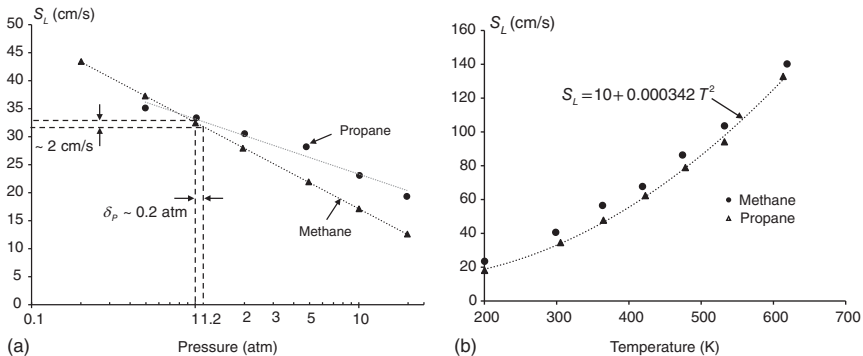




**Figure 1.8** Planar, curved, and wrinkled flame. The area of the flame increases as the flame becomes wrinkled because of instabilities and turbulence effects. The laminar burning velocity and turbulent burning velocity are related as  $S_L A_{f,wrinkled} = S_T A$ , where  $S_L$  = laminar burning velocity,  $S_T$  = turbulent burning velocity,  $A$  is the area of the planar flame, and  $A_{f,wrinkled}$  = surface area of the turbulent flame.

present and the flame is always distorted and may not even be one contiguous surface.

Finally, a note on the case with a propagating flame in a confined enclosure (either completely confined or with a vent as shown in Figure 1.7c) is warranted. In this case, the laminar burning velocity  $S_L$  will increase as the temperature of the unburned gas increases with compression and decreases with an increase in pressure as shown in Figure 1.9a,b. However, the influence of pressure is not significant given the range of pressure increase observed in building explosion accidents because the buildings cannot withstand high pressures. For example, as discussed



**Figure 1.9** (a) Laminar burning velocity (cm/s) vs. pressure (atm) and (b) Laminar burning velocity (cm/s) as a function of unburned gas temperature  $T_u$  (K). Source: Adapted from Zabetakis [7].



earlier, a brick wall fails at an overpressure of 0.14 atm. The consequent reduction in burning velocity is only 5–10% and can be ignored (Figure 1.9a). However, unburned gas temperature,  $T_u$ , can easily increase to 700 K, thereby causing an increase in the burning velocity by nearly three to four times (Figure 1.9b).

**Example 1.2** A stoichiometric mixture of methane–air at 298 K and 1 atm initially is ignited in a closed spherical vessel. Evaluate the adiabatic flame temperature. Also, evaluate the final pressure inside the vessel. Compare the result with adiabatic flame temperature for methane–air flame propagation in a tube that is open at both ends.

### Solution

The solution to this problem requires the student to go through Appendix A covering basic chemistry and thermodynamics necessary to solve many problems discussed in this book. For methane–air mixture in a closed vessel, the adiabatic flame temperature is evaluated using the first law of thermodynamics (see Appendix A), which can be simplified to state that there is no change in internal energy between reactants and products, as there is no heat loss (adiabatic). Thus,

$$U_u = U_b$$

where  $U$  is internal energy, and subscripts  $u$  and  $b$  represent unburned reactants and burned product gasses, respectively. The stoichiometric reaction for methane is shown below:



Internal energy of unburned gas can be written in terms of enthalpies as:

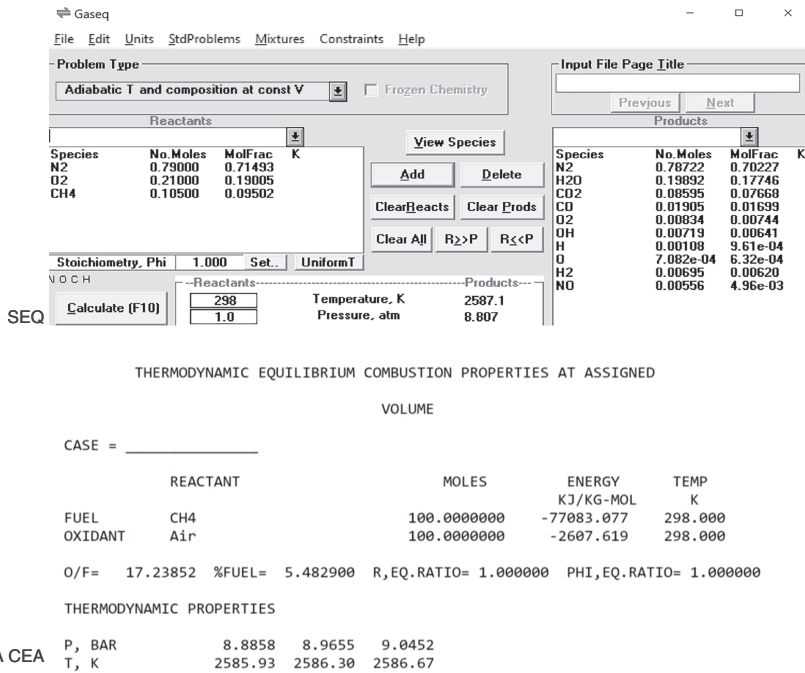
$$\begin{aligned} U_u &= H_u - p_u V = H_u - n_u RT_u \\ &= \sum n_i h_i - RT \sum n_i = [1(-74831) + 0 + 0] - 8.314 \\ &\quad \times 298 \times (1 + 2 + 2 \times 3.76) \\ &= -100\,895 \text{ kJ} \end{aligned}$$

where  $H$  is the enthalpy,  $n$  is the number of moles,  $R$  is the universal gas constant, and  $T$  is the temperature.

Internal energy of burned gas:

$$\begin{aligned} U_b &= H_b - p_b V = H_b - n_b RT_b \\ &= \sum n_i h_i - RT \sum n_i = \sum n_i (h_o + C_p(\Delta T)) - RT \sum n_i \\ &= [1(-393\,546 + 56.21(T_b - 298)) + 2(-241\,845 + 43.87(T_b - 298)) \\ &\quad + 7.52 \times (0 + 33.71(T_b - 298))] - 8.314 \times T_b \times (1 + 2 + 2 \times 3.76) \\ &= -877\,236 - 118\,440 + 309.9 \times T_b \end{aligned}$$

Equating the internal energy, we get  $T_b = 2887$  K. It should be noted that the values obtained using GASEQ [3] and NASA CEA are 2587 and 2586 K, respectively. Figure 1.10 shows snapshots from GASEQ and NASA CEA. The calculated value of



**Figure 1.10** Snapshots of GASEQ, Source: Morley [3], Gaseq and NASA CEA code by NASA [18] for calculating constant volume flame temperature and composition for a methane–air reaction at stoichiometric conditions.

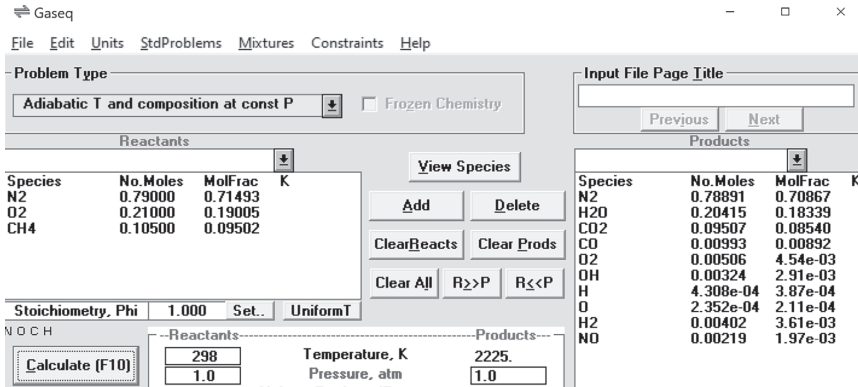
2887 K is higher than the numerical solvers because of the assumptions involved in the calculation: (i). Constant specific heat for species, and (ii) complete combustion of fuel to form  $\text{CO}_2$  and  $\text{H}_2\text{O}$  as products.

The final pressure is evaluated as  $P_b = P_u \times \frac{T_b}{T_u} = 1 \times \frac{2887}{298} = 9.7$  atm. This value as obtained from GASEQ and NASA CEA is about 8.9 atm.

For flame propagation in a tube open at both ends, the adiabatic flame temperature is evaluated at constant pressure. By using first law of thermodynamics, enthalpy of the reactants and products remains the same. Hence,

$$H_u = H_b \Rightarrow [1(-74831) + 0 + 0] = [1(-393546 + 56.21(T_b - 298)) + 2(-241845 + 43.87(T_b - 298)) + 7.52 \times (0 + 33.71(T_b - 298))]$$

Hence,  $T_b = 2317$  K. The value obtained from GASEQ is 2225 K. Again, this value is lower because we did not account for the variation of specific heat with temperature and dissociation of product species (mostly conversion of  $\text{CO}_2$  to  $\text{CO}$ ). Figure 1.11 shows a snapshot of the GASEQ code using adiabatic temperature and composition at constant pressure this time.



**Figure 1.11** Snapshot of GASEQ, Source: Morley [3], Gaseq, adiabatic temperature, and composition at constant pressure for a methane–air reaction at stoichiometric conditions.

**Example 1.3** A stoichiometric propane–air mixture is contained in a spherical cloud initially at 300 K. Evaluate the flame speed considering a spherical flame front as shown in Figure 1.7a.

### Solution

Flame speed ( $S_f$ ) is given by Eq. (1.10) as

$$S_f = \frac{A_f}{A_{f,N}} \frac{T_b}{T_u} S_L,$$

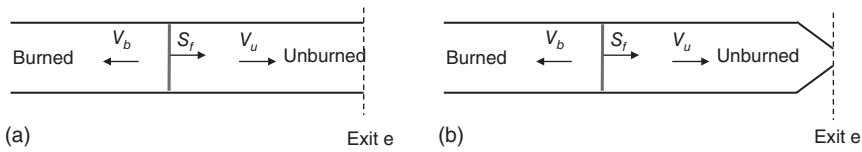
Here, the unburned gas temperature is  $T_u = 300$  K. Using Table 1.1, the laminar burning velocity of propane–air at stoichiometric ( $S_L$ ) = 46 cm/s, and the temperature of burned gas is assumed to be the adiabatic flame temperature given as,  $T_b = T_{ad} = 2257$  K for propane–air mixture. The adiabatic flame temperature can also be calculated using GASEQ [3] or NASA CEA [18] at constant pressure for a propane–air cloud at stoichiometric conditions.

For a planar flame front,

$$A_f = A_{f,N} \Rightarrow \frac{A_f}{A_{f,N}} = 1.$$

Thus, flame speed  $S_f = \frac{2257}{300} \times 46 = 346.07$  cm/s  $\sim 3.5$  m/s.

Note that it is assumed that there is no pressure build up. If the propane–air mixture were confined, then pressure would increase and unburned gas temperature would increase because of compression. The influence of decrease in laminar burning velocity with pressure (Figure 1.10a) and the increase in laminar burning velocity with temperature (Figure 1.10b) will need to be included to obtain an accurate solution. These influences are further explored in Chapter 3.



**Figure 1.12** Flame propagation in a tube with (a) open ends, and (b) nozzle exit.

**Example 1.4** Consider propagation of flame in a 2 cm horizontal tube open at both ends with a stoichiometric mixture of propane and air at 1 atm and 300 K initially. The planar flame propagates from left to right as shown in Figure 1.12a. Evaluate the velocity of burned gas and velocity of the flame with respect to the tube for the following exit conditions:

- (i) Exit “e” shown in Figure 1.12a is open to the atmosphere at 1 atm, and  $V_u = 0$
- (ii) Exit “e” is a convergent nozzle of 0.2 cm diameter opening as shown in Figure 1.12b and  $V_u \neq 0$ .

Assume that pressure of the burned gasses is at atmospheric = 101 325 Pa for both exit conditions.

### Solution

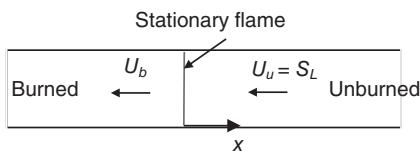
- i. Figure 1.12a shows the velocities with respect to the tube, namely, the burned gas velocity ( $V_b$ ), the unburned gas velocity ( $V_u$ ), and the flame velocity ( $S_f$ ). The subscripts  $u$  and  $b$  represent unburned and burned gas, respectively. For solving the problem, we will convert to a flame-fixed coordinate system as shown in Figure 1.13. We do this because we can easily write down the conservation equations of mass, momentum, and energy. Thus, if the coordinate system is on the flame (Figure 1.13), the unburned gasses approach the flame at the laminar burning velocity  $S_L$ , and burned gasses have a velocity of  $U_b$ . Further, for propane–air mixture at stoichiometric proportion,  $S_L = 46$  cm/s (Refer Table 1.1). From Figure 1.13, we can write:

$$U_b = S_f + V_b,$$

$$S_L = S_f - V_u.$$

Assuming 1D flame propagation, the equation for conservation of mass (continuity equation) can be written as:

$$\frac{d(\rho u)}{dx} = 0 \Rightarrow \rho u = \text{constant}$$



**Figure 1.13** Burned and unburned gas velocities with the coordinate system on the flame.

Momentum conservation can be written as:

$$\frac{dP}{dx} + \rho u \frac{du}{dx} = 0$$

since  $\frac{d(\rho u)}{dx} = 0$ ,  $\rho u = \text{constant}$ , and the momentum conservation equation can be rewritten as:

$$\frac{d(P + \rho u^2)}{dx} = 0 \Rightarrow P + \rho u^2 = \text{constant}$$

Thus, the equations that have to be solved simultaneously are:

$$\rho_u U_u = \rho_b U_b \text{ (Continuity)}$$

$$P_u + \rho_u U_u^2 = P_b + \rho_b U_b^2 \text{ (Momentum conservation)}$$

$$P_u = \rho_u \bar{R} T_u, P_b = \rho_b \bar{R} T_b \text{ (Equation of state)}$$

In these equations,  $U_u = S_L = 46 \text{ cm/s}$ , or the velocity of the unburned gases approaching normal to the flame. The unburned gas temperature is  $T_u = 300 \text{ K}$  and the temperature of burned gas is the adiabatic flame temperature,  $T_b = T_{\text{ad}} = 2257 \text{ K}$  for propane–air stoichiometric mixture.  $\bar{R}$  is the gas-specific constant that can be evaluated approximately using molecular weight of nitrogen as it is the abundant species on both reactant and product side.

$$\bar{R} = \frac{8.314 \text{ J/mol-K}}{28 \text{ kg/kmol}} = 297 \text{ J/kg-K}$$

Since there is no pressure build up, the pressure of the burned gas can be assumed to be  $P_b = 1 \text{ atm}$ . Hence, burned gas density,  $\rho_b$ , can be evaluated as:

$$\rho_b = \frac{P_b}{\bar{R} T_b} = \frac{101325}{297 \times 2257} = 0.151 \text{ kg/m}^3$$

As a result, the unknowns are  $\rho_u$ ,  $U_b$ , and  $P_u$ . Using continuity equation and the momentum equation:

$$P_u + \left( \frac{P_u}{RT_u} \right) U_u^2 = P_b + \frac{(\rho_u U_u)^2}{\rho_b} \Rightarrow P_u + \frac{P_u}{RT_u} U_u^2 = P_b + \frac{1}{\rho_b} \left( \frac{P_u}{RT_u} U_u \right)^2,$$

$$P_b + \frac{P_u^2}{\rho_b} \left( \frac{S_L}{RT_u} \right)^2 - P_u \left( 1 + \frac{S_L^2}{RT_u} \right) = 0,$$

$$101325 + P_u^2 \frac{1}{(0.151)} \left( \frac{0.46}{297 \times 300} \right)^2 - P_u \left( 1 + \frac{0.46^2}{297 \times 300} \right) = 0.$$

The quadratic equation can be solved for  $P_u$  giving,

$$P_u = 101326.6 \text{ Pa.}$$

Observe that the unburned gas pressure,  $P_u$  equals 101326.6 Pa, which is slightly more than the burned gas pressure, which is at atmospheric (101325 Pa). However, the pressure difference is very small and  $\frac{P_b}{P_u} = \frac{101325 \text{ Pa}}{101326.6 \text{ Pa}} = 0.99$ . In general,  $\frac{P_b}{P_u} < 1$  is the case for all deflagrations. This can be proved using the Hugoniot curve explained in combustion textbooks [19], and hence

deflagrations are sometimes called as expansion waves. Note that this is opposite to detonations, which are compression waves where  $\frac{P_b}{P_u} \gg 1$ .

Coming back to the problem, since  $P_u$  is almost equal to atmospheric pressure at the Exit “e,” and the exit is not confined by a nozzle, the velocity at the exit  $V_e = 0$  cm/s, pertaining to quiescent unburned reactants. As a result,  $S_f \simeq S_L = 46$  cm/s. The laminar burning velocity is thus equal to the flame speed in this case.

The unburned gas density can be evaluated as:

$$\rho_u = \frac{P_u}{RT_u} = \frac{101326.6}{297 \times 300} = 1.14 \text{ kg/m}^3.$$

Observe that  $\rho_u$  is much more than the burned gas density. The burned gas velocity is

$$U_b = \frac{\rho_u U_u}{\rho_b} = \frac{1.14 \times 0.46}{0.151} = 3.47 \text{ m/s}.$$

The velocity of burned gas with respect to tube can now be calculated as:

$$V_b = U_b - S_f = 3.47 - 0.46 = 3.01 \text{ m/s},$$

Similarly, the velocity of the unburned gasses with respect to the tube is equal to:

$$V_u = S_f - S_L = 0.46 - 0.46 = 0 \text{ m/s}.$$

The solution shows that with both sides of the tube open, the flame speed is the same as the burning velocity and equals 46 cm/s. Further, the expansion of the burned gas because of combustion causes the burned gas to leave the tube at a velocity that is an order of magnitude higher and equal to 3.01 m/s. We will now examine what happens with the restriction on the unburned side with a nozzle in part (ii).

- ii. When the unburned gasses vent through a convergent nozzle, they are restricted. In this case, the unburned gas velocity in lab coordinate system ( $V_u$ ) can be evaluated using continuity and momentum conservation between unburned gas and Exit “e” (at 1 atm).

$$\rho_u A_t V_u = \rho_e A_e V_e \text{ (Continuity)}$$

$$P_u + \frac{\rho_u V_u^2}{2} = P_e + \frac{\rho_e V_e^2}{2} \text{ (Momentum conservation)}$$

Here,  $A_t$  is the cross-sectional area of the tube and  $A_e$  is the cross-sectional area of the Exit “e” as shown in Figure 1.12b. The ratio of the two areas equals:

$$A^* = \frac{A_t}{A_e} = \frac{2 \times 2}{0.2 \times 0.2} = 100.$$

Assuming that the passage of the unburned gas through the nozzle causes no density changes,  $\rho_u \simeq \rho_e$ . Thus,

$$A_t V_u = A_e V_e,$$

$$V_e = \frac{A_t V_u}{A_e} = A^* V_u.$$

Substituting for  $V_e$  in the conservation of momentum,

$$P_u + \frac{\rho_u V_u^2}{2} = P_e + \frac{\rho_u}{2} [A^* V_u]^2$$

$$\rho_u V_u^2 [(A^*)^2 - 1] = 2[P_u - P_e]$$

$$V_u = \sqrt{\frac{2(P_u - P_e)}{\rho_u [(A^*)^2 - 1]}} = \sqrt{\frac{2(101327 \text{ Pa} - 101325 \text{ Pa})}{1.4 \frac{\text{kg}}{\text{m}^3} (100^2 - 1)}} = 1.7 \text{ cm/s}$$

Hence, the unburned gas velocity in the tube is  $V_u = 1.7 \text{ cm/s}$ .

In this case, velocity of flame =  $S_f = S_L + V_u = 46 + 1.7 = 47.7 \text{ cm/s}$  with respect to the tube. Moreover, the velocity at nozzle exit =  $A^* V_u = 170 \text{ cm/s}$ .

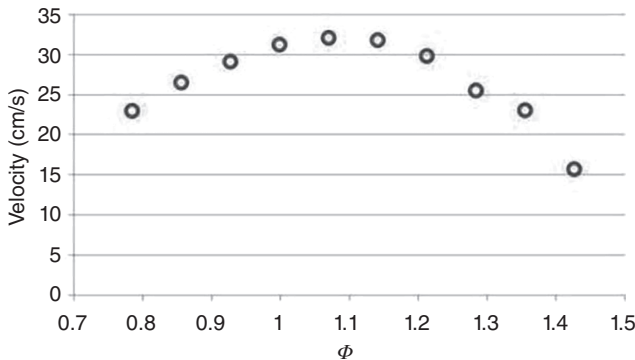
Velocity of burned gas with respect to the tube =  $V_b = U_b - S_f = 3.47 - 0.477 = 3 \text{ m/s}$ .

The pressure difference created because of the slightly higher pressure on the unburned side drives the flow out of the nozzle. In the tube, the flame speed,  $S_f$ , increases by 1.7 cm/s to compensate for this flow out of the nozzle. The most important aspect is the fact that the pressure on either side of a flame in a deflagration is such that the pressure on the unburned side is higher. This difference is necessary to cause the flow of unburned fresh fuel toward the flame.

## 1.4 Mixture Concentration – Definition of Flammability Limits

Figure 1.14 shows that the laminar burning velocity of methane–air flame varies with equivalence ratio, whereby it is maximum for an equivalence ratio slightly greater than 1, but for lean and rich mixtures its value drops.

In fact, at less than  $\sim 1/2$  stoichiometric, or more than  $\sim 3$  times stoichiometric, it is not possible to sustain a self-propagating flame. Such values of  $\Phi_{\min}$  or  $\Phi_{\max}$  establish

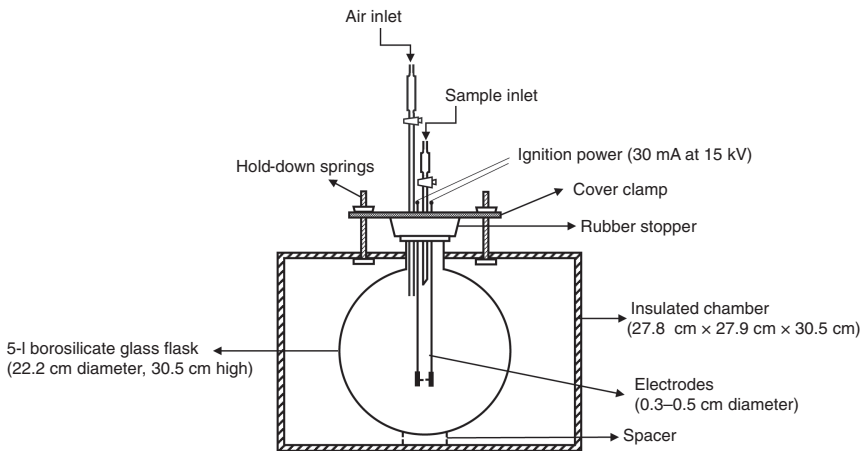


**Figure 1.14** Laminar burning velocity of methane–air premixed flame at different equivalence ratios. Measurements were performed at the Worcester Polytechnic Institute (WPI) combustion laboratory using the cone angle method.

the flammability limits of a fuel–air mixture. Since  $S_L$  is a function of composition, initial temperature, and pressure, a flammability limit can be defined as the limit of one of these quantities beyond which a fuel–oxidizer mixture cannot be made to burn. The flammability limits are usually tabulated in codes and standards [9] and standard textbooks [20] and are shown in Table 1.1 for some practical fuels of interest. Extensive tabulation can be found in Coward and Jones [21] and Zabetakis [7] based on experiments performed by the Bureau of Mines in 1950–1965. An interesting point to note is that lower flammability limit (LFL) is independent of  $O_2/N_2$  ratio in air. For example, if all the  $N_2$  is replaced by  $O_2$ , the LFL will not change. This is because both  $O_2$  and  $N_2$  have the same specific heat, and thus the heat of combustion transferred to either gas will lead to the same reaction temperature. The upper flammability limit (UFL), on the other hand, depends strongly on the concentration of  $O_2$  in air, since this limit is caused by an excess of fuel, i.e. by a deficiency of oxygen. Bartknecht [22] has also shown that the relative humidity has a perceptible influence on the width of the flammability range, with the widest range observed in extremely dry mixtures.

Figure 1.15 shows a spherical vessel [ASTM E681-09] for measuring the UFL and LFL of vapors and gasses. The gas mixture is contained in a 5-l borosilicate spherical glass vessel with a cover clamp, which is held down by light springs. There is provision for gas inlet and air inlets in the cover clamp. The uniform mixture of gas or vapor is ignited by an electric spark from the stainless steel electrodes, and the upward and outward propagation of the flame away from the ignition source is noted by visual observation. The concentration of the flammable component is varied between trials until the composition that will just sustain propagation of the flame is determined.

Flammability limits are of practical interest in safety considerations because mixtures outside of these limits can be handled without concern for ignition. For most practical applications, the flammability limits can be correlated using the heat of



**Figure 1.15** ASTM standard test method for measuring upper and lower flammability limits of gasses and vapors. Source: Adapted from Zabetakis [7].



combustion as shown by Suzuki and Koide [23, 24]

$$\begin{aligned} LFL &= \frac{-3.42}{\Delta H_c} + 0.569\Delta H_c + 0.0538\Delta H_c^2 + 1.80 \\ UFL &= 6.30\Delta H_c + 0.567\Delta H_c^2 + 23.5 \end{aligned} \quad (1.13)$$

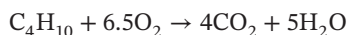
Equation (1.13) is an empirical relationship considering 123 organic materials containing carbon, hydrogen, oxygen, nitrogen, and sulfur. The heat of combustion  $\Delta H_c$  is in kJ/mol and the LFL and UFL are in vol% of fuel in air.

Adding an increasing quantity of inert gas or a noncombustible mixture can also lead to a critical concentration causing a no-flame propagation. This is usually expressed in terms of a limiting oxygen concentration (LOC) and is based on the concentration of inert that needs to be added to prevent ignition of a combustible gas-air mixture. The efficiency of the inert gas is based on the quantity of heat transferred during the flame propagation and ensuring that this heat is absorbed without causing further reaction to sustain flame propagation.

**Example 1.5** Estimate the LOC for butane ( $C_4H_{10}$ ).

**Solution**

The LFL for butane is = 1.9% by volume. The overall chemical reaction of butane at stoichiometric condition is



The LOC can be estimated as:

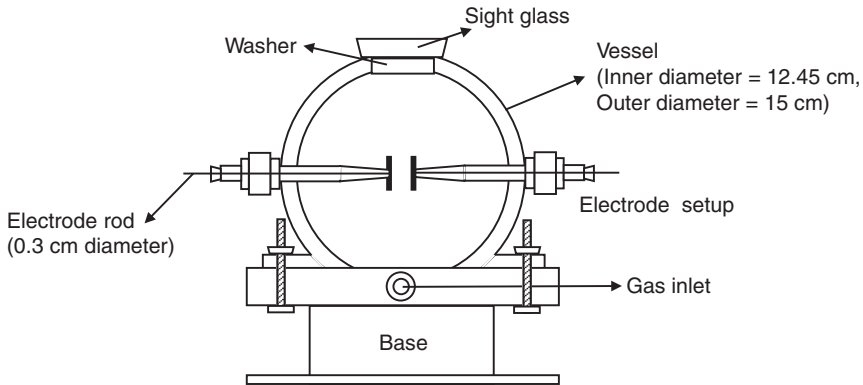
$$LOC = \left[ \frac{\text{moles fuel}}{\text{total moles}} \right]_{LFL} \left[ \frac{\text{moles } O_2}{\text{moles fuel}} \right]_{\text{stoichiometric}} = 1.9 \frac{6.5}{1} = 12.4 \text{ vol\% } O_2$$

Thus the combustion of butane can be prevented by adding an inert until the oxygen concentration is below 12.4%.

## 1.5 Minimum Ignition Energy (MIE) and Auto Ignition Temperature (AIT)

Some energy has to be input initially to initiate a chemical reaction. The MIE is the minimum *energy* input required to initiate combustion. Many hydrocarbons have an MIE of 0.25 mJ. This is low enough to cause ignition by electrostatic discharges due to fluid flow and static electricity. Walking across a rug on a cold winter day initiates a static discharge of around 22 mJ. An ordinary spark plug has a discharge of 25 mJ. Thus, given a flammable gas mixture, ignition is relatively easy. For a dust-air mixture, the MIE is significantly higher and can exceed 1000 mJ in some cases making ignition of dust clouds more energy intensive compared to gas clouds. We will discuss this further in Chapter 8.

MIE decreases with an increase in pressure. The pressure is the net force that gas molecules are exerting when they collide with a container's walls. High pressure means more collisions per second of gas molecules on the container and/or each



**Figure 1.16** ASTM standard test method for measuring minimum ignition energy. Source: Adapted from Mitu et al. [10]/American Chemical Society.

collision is occurring with a greater force. Thus, gas molecules in a high-pressure condition are moving about very fast and therefore have higher energy. This means they will need lesser energy from an ignition source to react. The MIE is related to the burning velocity by  $MIE \equiv \frac{k_u}{S_u}[T_f - T_o]$ , where  $k_u$  is the thermal conductivity of the unburned gas,  $T_f$  is the flame temperature, and  $T_o$  is the ambient temperature.

The standard test method for MIE is shown in Figure 1.16 [ASTM E582-07]. A stainless steel spherical vessel with inner diameter of 12.45 cm (4.9") is used. The gasses enter the vessel through tangential ports to enhance mixing through the induced swirl. Thin 3.175 mm (1/8") stainless steel rods are used as electrodes and the applied voltage is increased such that a spark occurs. The flame initiation and propagation can be observed through a sight glass that is provided to ensure visual access.

The autoignition temperature is different from the MIE and denotes the minimum temperature at which a gas mixture will react spontaneously without the presence of a spark. It depends on the concentration or equivalence ratio of the gas mixture, pressure, flow condition, initial temperature, and the presence/absence of a catalyst. The ignition of vapor is also possible by adiabatic compression. For example, vapors in a gasoline engine ignite when compressed to a temperature that exceeds AIT creating engine knock. Several large accidents have been caused due to flammable vapors sucked into the intake of air compressors. Example 1.6 adapted from Crowl and Louvar [25] illustrates this mode of ignition.

**Example 1.6** A lubricating oil has an AIT of 400 °C. Compute the compression ratio required to raise the temperature of air to the AIT of this oil. Assume an initial air temperature of 25 °C.

### Solution

$$T = P^{(\gamma-1)/\gamma}$$

$$\Rightarrow P = T^{\gamma/(\gamma-1)}$$

$$\Rightarrow \frac{P_f}{P_i} = \left( \frac{T_f}{T_i} \right)^{\gamma/(\gamma-1)} = \left( \frac{400 + 273}{25 + 273} \right)^{1.4/0.4} = 17.3$$

Therefore, compression ratio should be kept below  $17.3 \times 14.7 \text{ psia} = 254 \text{ psia}$ .

Lubricating oil in piston-type compressors is always found in minute amounts in the cylinder bore. Compressor operations must always be kept below the AIT of the oil to prevent explosion.

## Exercise Problems

- 1 Due to a high-pressure steam hose breakage, air above a hexane fuel layer is compressed by 12 times ambient pressure of 1 atm. If the autoignition temperature of hexane is  $487^\circ\text{C}$  (760 K) what should be the temperature of the ambient to ensure no autoignition.
- 2 A full propane cylinder from a camp stove leaks its contents of 1.02 lb (0.464 kg) into a  $12' \times 14' \times 8'$  ( $3.66 \text{ m} \times 4.27 \text{ m} \times 2.44 \text{ m}$ ) room at  $20^\circ\text{C}$  and 1 atm. After a long time, the fuel gas and room air are well mixed. Is the mixture in the room flammable?
- 3 What volume of air is required to burn stoichiometrically 1 mole of propane gas, with the initial air at 25 C and with a pressure of 0.98 bar. If the pressure equals 2.2 bar, what is the volume?
- 4 What will be the most effective diluent to an explosive mixture of H<sub>2</sub> to lower or prevent explosion possibility: Carbon Dioxide, Helium, Nitrogen, or Argon? Arrange in order of effectiveness.
- 5 Consider propagation of flame in a 2 cm diameter horizontal tube open at both ends with a stoichiometric mixture of propane and air at 1 atm and 300 K initially. The planar flame propagates from left to right as shown in Fig. 1.12a. Evaluate the velocity of burned gas, and velocity of the flame with respect to the tube for a convergent section of 0.2 cm diameter opening at the burned side of the tube. Assume that pressure of the unburned gases is at pressure of 101327 Pa.

## Nomenclature

$A$	Area ( $\text{m}^2$ )
$C_d$	Orifice discharge coefficient (—)
$C_p$	Specific heat at constant pressure ( $\text{J}/\text{kg K}$ )
$C_v$	Specific heat at constant volume ( $\text{J}/\text{kg K}$ )
$E$	Expansion ratio $\frac{T_b}{T_u} \sim \frac{T_f}{T_u} \sim 8$ (—)
$h$	Enthalpy per unit mass ( $\text{J}/\text{g}$ )

$k$	Thermal conductivity (W/m K)
$m$	Mass (kg)
$n$	Number of moles (–)
$P$	Pressure (N/m <sup>2</sup> or Pa)
$r$	Radius of spherical enclosure (m)
$R$	Universal gas constant (8.314 J/mol K)
$\bar{R}$	Gas constant for a specific gas $\frac{R}{MW}$ (J/kg K)
$Re$	Reynolds number (–)
$S_L$	Laminar burning velocity (m/s)
$S_T$	Turbulent burning velocity (m/s)
$S_U$	Unburned gas burning velocity (m/s)
$S_f$	Flame speed (m/s)
$T$	Temperature (K)
$u$	Velocity (m/s)
$u'$	Turbulent intensity (m/s)
$U$	Internal energy (J)
$V$	Volume (m <sup>3</sup> )
$W$	Width (m)
$X$	Mole fraction (–)
$Y$	Mass fraction (–)

## Greek Symbols

$\rho$	Density (kg/m <sup>3</sup> )
$\beta$	Multiplication factor in Eq. 1.2 to account for flame acceleration because of turbulence and instabilities (–)
$\phi$	Equivalence ratio (–)
$\gamma$	Ratio of specific heats ( $C_p/C_v$ )

## Subscripts

$a$ or $o$	Ambient
$ad$	Adiabatic
$b$	Burned
$e$	Exit
$f$	Flame
$i$	Initial condition
$min$	Minimum
$max$	Maximum
$N$	Normal
$t$	Total
$u$	Unburned

## Other Notations

<i>AIT</i>	Auto Ignition Temperature (K)
<i>LFL</i>	Lower Flammability Limit (vol %)
<i>LOC</i>	Limiting Oxygen Concentration (vol %)
<i>MIE</i>	Minimum Ignition Energy (mJ)
<i>MW</i>	Molecular Weight (g/mol)
<i>UFL</i>	Upper Flammability Limit (vol%)
$\Delta H_c$	Heat of combustion (J/kg)

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