

What is an Explosion?

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Abstract

We are going to focus our discussion on “Explosions”, its definitions from a scientific, regulatory, and societal perspective. We will point out that as defined these definitions are not consistent and lead to ambiguity. Of particular interest to this work is how this current ambiguity affects the emerging Regulation Codes and Standards (RCS) as applied to hydrogen technologies. While this manuscript has its roots in combustion science with extension to both the standard development and regulatory communities for hazards at large, the unique behavior of hydrogen in many configurations motivates examining the relevant definitions and language used in these communities.

We will point out the ambiguities, how this leads to confusion in supporting definitions, and how it leads to overly restrictive RCS for hydrogen applications. We will then suggest terminology which is not ambiguous, internally self-consistent, and allows appropriate RCS to be promulgated to ensure the safety of the public and capital, to ensure the correct response of first responders, and allow cost effective development of hydrogen technologies in our infrastructure.

Introduction

In this paper we examine the definitions of explosion and related phenomena as articulated in the Regulations Codes and Standards (RCS), the hazards mitigation literature and in the combustion literature. We demonstrate that taken as a whole and sometimes in part the definitions of these phenomena are ambiguous as presented in the RCS literature. This leads to hazards mitigation that is overly conservative, and leads to less than optimal mitigation strategies.

We contrast the language from the combustion literature with the language from the RCS literature. We then suggest unifying language to provide an unambiguous set of definitions that span the combustion literature and the RCS literature. We also suggest that adopting this language then provides a rigorous structure to identify those regions of combustion

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phenomenon that can grow into a hazardous situation and those regions that cannot grow to hazardous situations. This is particularly important to hydrogen combustion phenomenon, which exhibits unique combustion behavior as compared with hydrocarbon combustion due to hydrogen's very low molecular weight resulting in very high buoyancy. As currently interpreted the RCS language leads to an overly conservative set of constraints which result in overly conservative and hence expensive implementation of the regulations. Adopting our suggestions for explosions and related phenomena allows the RCS community to defensibly differentiate hazardous from non-hazardous conditions and how to set the appropriate limits to prevent a hazardous condition from occurring.

Problem statement

The RCS community needs internally self-consistent language to effectively communicate. Terminology that is not precisely defined and understood by all leads to inappropriate and confusing code development (overly restrictive or worse not restrictive enough). It can lead to confusion over what is the hazard that presents itself and thus the appropriate safety measures need to be executed to ensure the safety of the public and capital investments. Also, this can lead to exaggeration of a hazard by the public causing damage to an emerging technology by creating exaggerated images of danger.

Examples of "Explosion"

Now we focus on the notion of an "explosion" and we will demonstrate that in common usage (society) and in the regulatory and standard development community (RCS) the term "explosion" is ambiguously defined. Indeed, at times it is circularly defined, in that certain phenomenon is categorized as an "explosion" then later in the same document "explosion" is used to define that phenomenon. Which is it?

Consider the images shown in Figures 1-5. Each image in these figures represents an "explosion" from some perspective. The images shown in Figure 1 depict the use of the word in non-technical world. Figure 2 shows images of "explosions" that originated by a large point source of energy release. Figure 3 shows examples of Boiling Liquid Expanding Vapor Explosion, (BLEVE). Neither example shown in Figure 3 involves combustion inside the tank yet it is labeled an explosion. Figure 4 shows examples of non-premixed (or partially premixed) flames. And Figure 5 shows examples of premixed combustion.

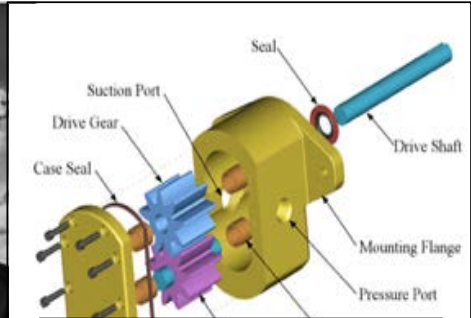
Figure 1. Images depicting every day uses of the word explosion, which have nothing to do with large point sources of chemical or nuclear energy release.



Food Explosion



Blew my Mind

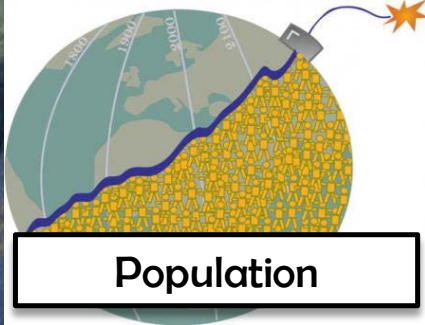


An "exploded" view



Tires

Please hold down the lid of Salad Dressing while **"SHAKING"**..... this prevents messy **"EXPLOSIONS"**



Population



Champagne

Figure 2, Point source of energy release.



Figure 3. Examples of BLEVEs (Boiling Liquid Expanding Vapor Explosion). A) Boiler failure due to overpressure (non-combustible water), B) LPG tank failure due to overpressure (no combustion inside the tank (LPG present in the tank no air).

Boiler Tank catastrophic failure due to over pressure (no combustion)



Tank catastrophic failure due to over pressure (no combustion in side the tank)



Examples of BLEVE – Boiling Liquid Expanding Vapor Explosion. Top steam, bottom LPG

Figure 4. Non-premixed flames (note the stove top burner is an example of combustion process known as a partially premixed flame. The center cone is a rich premixed combustion the outer cone is the non-premixed part of the flame. We show it here as another example of a non-premixed combustion process.)

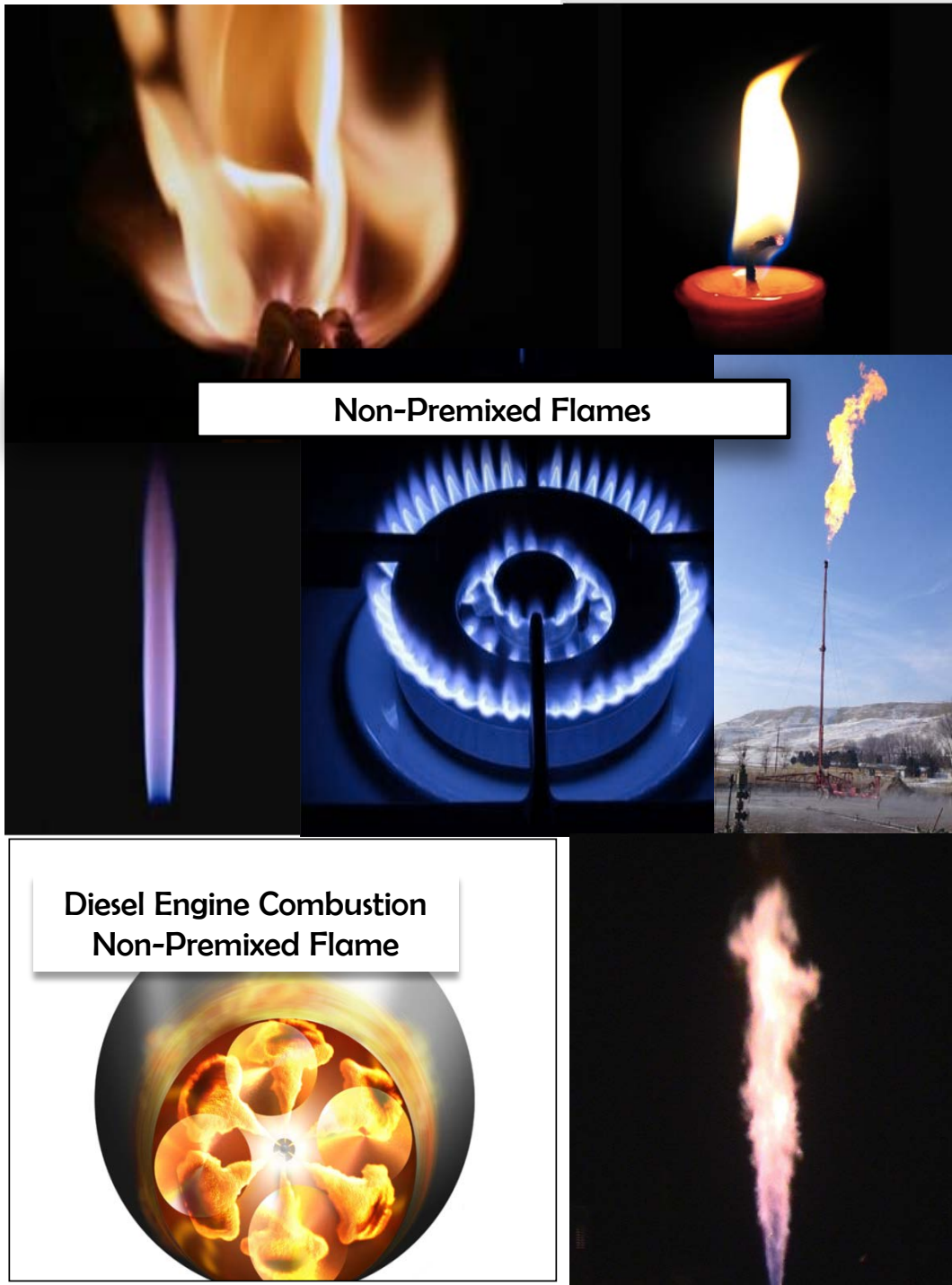
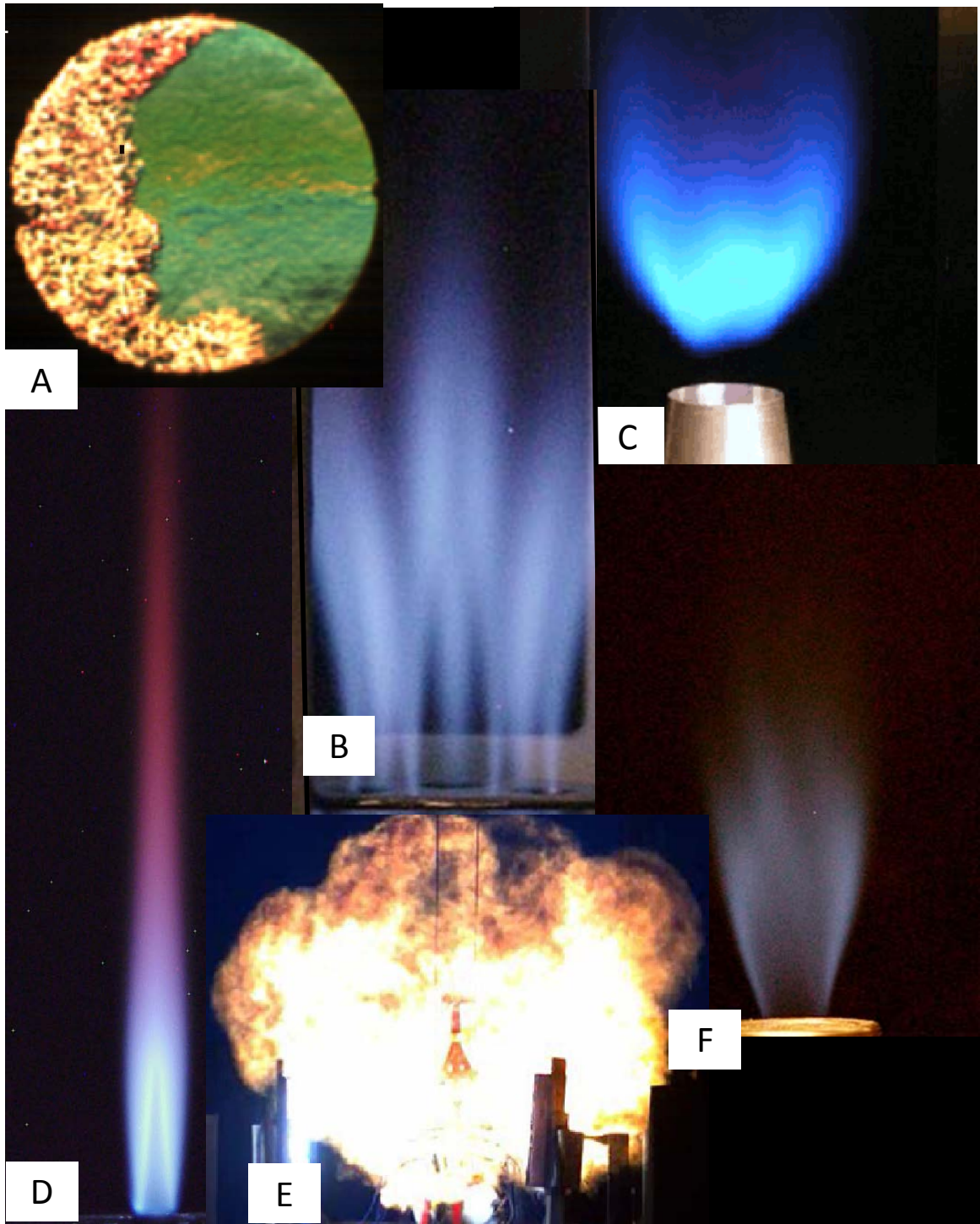


Figure 5. Premixed combustion, Deflagrations, A) Spark ignited internal combustion engine, B) Premixed Turbine Combustor, C) Swirl stabilized combustion, D) Turbulent premixed jet, E) Premixed open deflagration, F) puffy swirl stabilized flame. Flames D,E, and F are Hydrogen air flames.



Explosion and related phenomenon from the RCS literature

Shown in Figures 1-5 depict different events all of which can be considered an explosion. Indeed, in the RCS literature some definitions become circular, in that explosion is used to define a deflagration and then this is used to define an explosion. Consider the following definitions taken from the regulatory community.

Explosion:

1. "a sudden increase of pressure and temperature, due to oxidation or other exothermic reaction."¹
2. "a rapid temperature and pressure rise resulting in an audible spherically propagating pressure wave."²
3. "abrupt oxidation of decomposition reaction producing an increase in temperature, pressure or in both simultaneously"³
4. "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."⁴
5. "In contrast to burning in a fire, an explosion is essentially a self-sustained propagation of the reaction zone (flame) through the explosive atmosphere."⁵
6. "In addition to the familiar fire triangle of oxygen, heat, and fuel (the dust), dispersion of dust particles in sufficient quantity and concentration can cause rapid combustion know as a deflagration. If the event is confined by an enclosure such as a building, room, vessel or process equipment the resulting pressure rise may cause an explosion."⁶
7. "A smoke or fire gas explosion occurs when unburned pyrolysis products accumulate and mix with explosion of the pre-mixed fuel gases and air. This phenomenon generally occurs remote from the fire (as in an attached exposure) or after fire control."⁷
8. "A self-sustained combustion of a gas mixture (flammable plus oxidizing gas) which releases energy as heat and a shock wave."⁸
9. "Deflagration and detonation are the two main subtypes of an explosion as a phenomenon"⁹
10. "The bursting or rupture of an enclosure or a container due to the development of internal pressure from a deflagration."¹⁰

11. "An effect produced by the sudden violent expansion of gases, which may be accompanied by a shock wave or disruption, or both, of enclosing materials or structures. An explosion could result from any of the following:
 1. Chemical changes such as rapid oxidation, *deflagration* or *detonation*, decomposition of molecules and runaway polymerization (usually *detonations*).
 2. Physical changes such as pressure tank ruptures.
 3. Atomic changes (nuclear fission or fusion)."¹¹
12. "Fast Combustion of a gas mixture releasing heat, hot combustion gases, and a shock wave. Explosions can be further subdivided into the two main cases of deflagration and detonation.
Note: This definition excludes pressure sources not related to chemical reactions (like burst of a pressure vessel)"¹²

Explosive atmosphere:

- "a mixture with air, under atmospheric conditions, of flammable substances in the form of gas, vapour, mist or dust in which, after ignition, combustion spreads throughout the unconsumed mixture"¹³

Hazardous explosive atmosphere:

1. "an explosive atmosphere which, if it explodes, causes harm"¹⁴
2. "Flammable and/or combustible substances shall be considered as materials which can form an explosive atmosphere unless an investigation of their properties has shown that in mixtures with air they are incapable of self-sustained propagation of an explosion."¹⁵

Explosion/Flammability limits:

1. "The explosion limits vary with pressure and temperature. As a rule, the concentration range between explosion limits increases with increasing pressure and temperature. ..." ¹⁶
2. "limits of explosion range"¹⁷
3. "In order for ignition of a vaporized fuel to occur, the mixture of oxygen and fuel vapor must fall into a range commonly called the flammable or explosive limits...The flammable or explosive limits have a lower point and upper point that represent the percentage of fuel vapor... When the fuel vapor percentage is between the lower and upper flammable or explosive limits ignition will occur. And if the volume of fuel is significant (as in a house filled with natural gas) the ensuing ignition will have explosive consequences."¹⁸
4. "Essentially no distinction is drawn between the two limits in the basic training packages, not surprising that some portion of the community needs further understanding of the definition, particularly since for transportation hydrogen at retail service stations the industrial mitigations are overly conservative."¹⁹

Authors note: the two limits referred to here are flammability limits and explosion limits.

5. “Lower (LFL) and upper (UFL) concentrations of fuel gas in a flammable mixture that will ignite and support a flame.

Note 1: These limits are functions of temperature, pressure, diluents, fluid dynamics, and ignition energy.

Note 2: These limits are usually expressed as percent (volume fraction of fuel gas)”²⁰

Authors note: no definition of explosion limits is provided by this reference.

Explosion Range:

- “range of the concentration of a flammable substance in air, within which an explosion can occur”²¹

Explosive behavior:

- “The behavior of the explosive atmosphere after ignition shall be characterized by data such as:
 - Maximum explosion pressure (P_{\max})
 - Maximum rate of explosion pressure rise $(dP/dt)_{\max}$
 - Maximum experimental safe gap (MESG)”²²

Deflagration:

1. “Explosion propagating at subsonic velocity.”²³
2. “Reaction and flame front velocity is below the velocity of sound
 - a. Slow deflagration: laminar flow, $Ma \ll 1$
 - b. Fast deflagration: turbulent flow, $Ma \sim 1$ (effects rather similar to those of a detonation)”²⁴
3. “Propagation of a combustion zone at a velocity that is less than the speed of sound in the unreacted medium”²⁵
4. “An exothermic reaction, such as the extremely rapid oxidation of a flammable dust or vapor in air, in which the reaction progresses through the unburned material at a rate less than the velocity of sound. A deflagration can have an explosive effect.”²⁶
5. “Explosion process in which a flame or chemical reaction moves through a flammable mixture at a rate less than the speed of sound in the unburned mixture.

Note1: Fast deflagrations are characterized by velocities in the hundreds of metres per second, where confinement causes elevated pressures, and their effects to not differ much from those of a detonation.

Note 2: some deflagrations proceed so slowly that they do not produce any pressure wave: they should not be considered as explosions”²⁷

Detonation:

1. “Explosion propagating at supersonic velocity and characterized by a shock wave”²⁸
2. “Spreads with $Ma \gg 1$; shock wave is much higher and sharper, damage more severe”²⁹
3. “Propagation of a combustion zone at a velocity that is greater than the speed of sound in the unreacted medium.”³⁰
4. “An exothermic reaction characterized by the presence of a shock wave in the material which establishes and maintains the reaction. The reaction zone progresses through the material at a rate greater than the velocity of sound. The principal heating mechanism is one of shock compression. Detonations have an explosive effect.”³¹
5. “Explosion characterized by an exothermic chemical reaction coupled to a shock wave that propagates through a detonable mixture or medium.

Note1: The thermal energy of the reaction sustains the shock wave, and the shock wave compresses unreacted material, producing the high temperatures necessary to drive the reaction.

Note2: The detonation process is characterized by a propagation speed that is greater than the speed of sound in the unburned mixture.”³²

Fire Ball:

- “Unconfined accidental fuel gas releases often result in a fireball once ignited. “However, if the gas mixture is unconfined or if confinement is breached, the burning gas expands as a fireball at normal atmospheric pressure, and the maximum fireball volume is approximately ten times the initial volume of the mixture.”³³

Harm:

- “physical injury or damage to the health of people, or damage to property or the environment”³⁴

Harmful event:

- “occurrence in which a hazardous situation results in harm”³⁵

Hazard:

- “potential source of harm
NOTE: the term hazard can be qualified in order to define its origin or the nature of the expected harm (e.g. electric shock hazard, crushing hazard, cutting hazard, toxic hazard, fire hazard, drowning hazard).”³⁶

Hazardous situation:

- “circumstance in which people, property or the environment are exposed to one or more hazards.”³⁷

From these definitions the reader cannot discern an internally self-consistent definition of “explosion”. Sometimes it is defined to a sudden release of energy requiring a shock, and deflagrations and detonations are subsets of an explosion, however, a deflagration is a subsonic event and hence does not create a shock. Sometimes an explosion is defined to be a large release of energy that does not involve a rupture of a vessel, however, in other definitions an explosion is only associated with the rupture of a vessel. In some instances an explosion requires a flammable gas/oxidant mixture or fine dust.

The notion of explosion limits, as given above, gets confusing also. If an explosion is characterized by a shock (see definition 8), and the combustion process creating shocks is a detonation then the explosive limits are the limits of detonation. Deflagration can exist in a very lean mixture (more oxidizer than fuel), indeed for hydrogen and air mixtures as low as 4% of hydrogen by volume. And indeed, for hydrogen air flames mixtures this lean do not propagate throughout the entire flammable mixture and therefore are not explosions by definition number 5.^{38 39 40 41} However, compared to deflagration, the direct initiation of a detonation process requires mixtures closer to the stoichiometric ratio (29.5% by volume) of one and stronger initiation sources. Detonability limits are therefore always within the explosion limits. In addition, the lower limit for detonation is usually noted as 18% by volume for hydrogen air mixtures; however, the literature has values as low as 11%. The limits of detonation are also a strong function of local geometry and the ensuing fluid dynamics, and therefore cannot be rigorously defined, unlike a lower limit on flammability.

As long as flammability and explosion limits are used interchangeably, the community will continue to find itself in this and similar paradoxes. In addition, communication with the non-technical world becomes confusing if the technical (RCS) community cannot unambiguously define precisely the phenomenon of interest.

Explosion and related phenomenon from the combustion literature

The definitions from the RCS literature (see above) are at odds with definitions one finds in the combustion literature. (See discussion in Chapter 3 of reference 42)⁴² Consider the following:

Explosion:

- A runaway chemical reaction, one which the reaction rate increases with time. This can be caused by the chemical kinetic path way creating more radicals (chain branching) than it destroys (chain termination) or by a thermal process, the reaction runs away.

Explosive atmosphere:

- A mixture, temperature and pressure environment that supports a spontaneous explosion as defined here.

Explosion limits:

- Those values of temperature and pressure for a given mixture of reactants that bound the region where a spontaneous explosion can occur. See Figure 6.⁴³

Flammability limits:

- Those mixture limits for a given pressure and temperature which bound the region where a flame (deflagration and/or detonation) can occur.⁴⁴

Note: Given these definitions explosion limits are not flammability limits. Explosion limits are the pressure-temperature boundaries for a specific fuel-oxidizer mixture ratio that separate the regions of slow and fast reaction. For a given temperature and pressure, flammability limits specify the lean and rich fuel oxidizer mixture ratio beyond which no flame will propagate.

Figure 6 depicts the regions of pressure and temperature for a given mixture that divides fast reactions from slow reactions for a stoichiometric mixture of hydrogen and oxygen. In the “explosive” regions the chemical kinetic rates increase unbounded. This can be caused by thermal effects or the chemical reaction pathways produce more radicals than it consumes (chain branching out paces chain termination), the reaction runs away – it explodes; these are noted as “fast reactions”. Outside that region, the reaction is self-limiting creating “slow reactions”. Reading from figure 6 shows that for stoichiometric Hydrogen / Oxygen mixtures at 760 mm Hg the explosion limit is about 580 °C. (Note that under atmospheric pressure (760 mm Hg), a stoichiometric mixture of hydrogen and air has an autoignition temperature of about 585 °C above which the mixture is “explosive” below which it is not “explosive”). This explains why a stoichiometric mixture of hydrogen and oxygen (and air for that matter) will not “explode” under atmospheric conditions as defined here. If, however, one supplies an ignition source to locally raise the temperature to move the mixture beyond the third limit (raise the local temperature above 585° C) as shown in the figure then the reaction becomes explosive. Since it is exothermic it heats the local environment above the explosion limit and it propagates, producing a thin reaction zone (a flame).

Figure 6. Explosion limits for stoichiometric mixture of Hydrogen and Oxygen

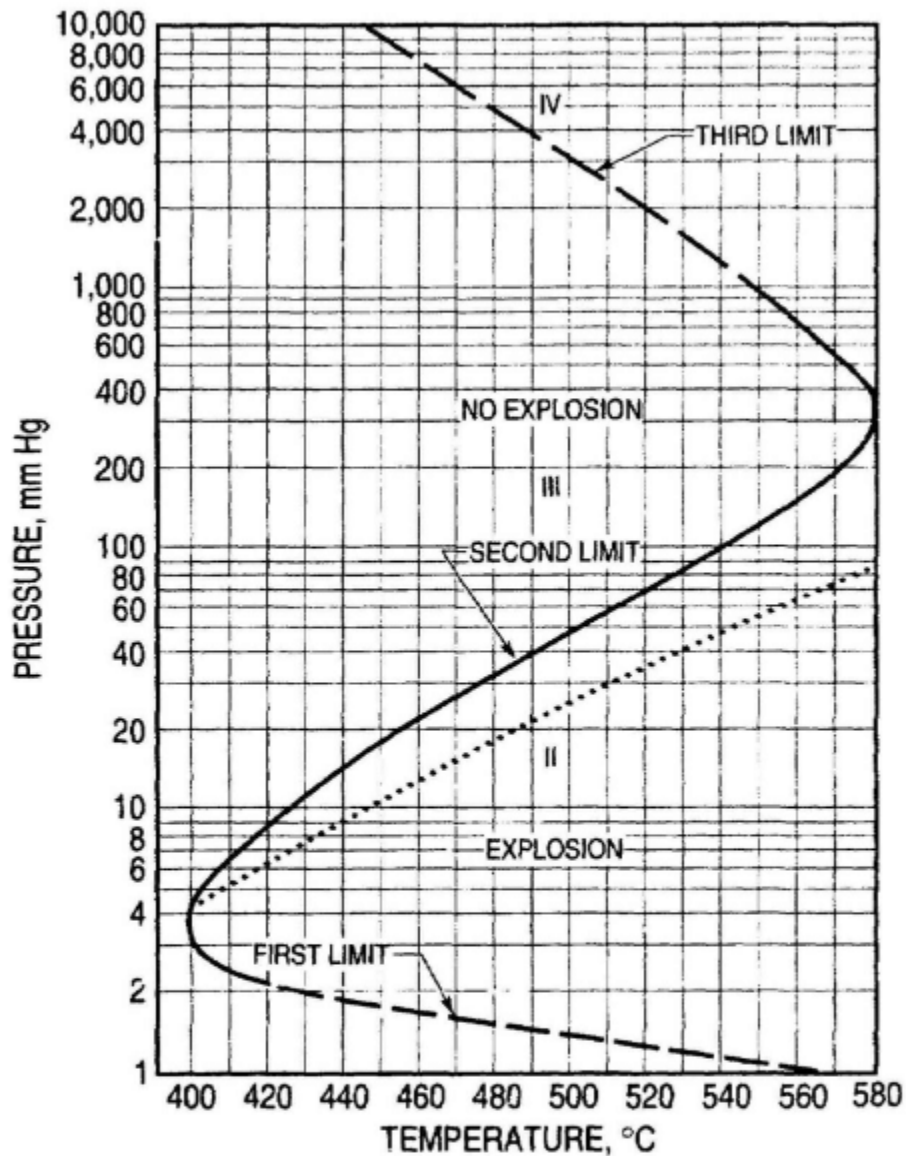


Figure 1. Explosion limits of stoichiometric H_2-O_2 mixture in a spherical KCl-coated vessel of 7.4 cm diameter. First and third limits are partly extrapolated. Dotted line defines condition where $2k_2 = k_{10}[M]$ in stoichiometric H_2-O_2 . (From Ref. 3.)

Deflagration:

- A subsonic propagating flame (thin reaction zone)
 - Negligible pressure difference across the reaction zone
 - Speed of propagation limited to the speed of sound in the unburnt reactants

Detonation:

- A supersonic propagating flame (thin reaction zone)
 - Large pressure difference across the shock (10 to 20 times)

It is instructive to note that under the right conditions a deflagration can accelerate to a detonation. This is referred to as a deflagration to detonation transition (DDT).

What are we interested in?

We need consistent terminology. The best approach for all interested communities places explosion in the context of hazards mitigation. That way, explosion, when used, everyone will understand what we are talking about. Fundamentally the notion is that an “explosion” is an event that once initiated grows rapidly and initially unbounded. Such an event lacks the mechanisms to control its rate of growth and will grow unbounded until some external influence is applied (such as consuming all the fuel). This presents a hazard as it can result in thermal (burns), shrapnel (flying fragments) and/or mechanical (overpressure) exposure to people and structures. By using a consistent definition we may appropriately address conditions which will not, under any circumstances result in an explosion, as we have defined it here, and those conditions which will. Therefore we may most appropriately apply hazard mitigation as needed rather than in response to a supposed, lesser understood or “boogeyman” phenomena.

The definition, “an event that once initiated grows rapidly and unbounded” now works for all those examples in the societal sense of an explosion: population explosion, explosion of emotion, explosion of data, explosion of color ... This notion also embraces those examples of large energy release: cosmic stars, nuclear bombs, point source of stored chemical energy release ... It also embraces combustion phenomenon (run away chemical kinetics), manifesting itself in terms of deflagrations and detonations.

We propose the following internally self-consistent definitions.

Explosion:

- an event that once initiated grows rapidly and initially unbounded

Explosive limits:

- those temperatures and pressures for a given mixture that separate regions of slow and fast reactions. They bound the conditions where chemical kinetics are self-regulated from the conditions where kinetics accelerates unbounded, an explosion which is “an event that once initiated grows rapidly and initially unbounded” as defined above.

Flammability limits:

- the values of the concentration of a fuel and oxidizer for a given pressure and temperature that bound conditions for a flame to exist (both deflagrations and detonations).

Simply identifying and defining the phenomena doesn't mitigate it. Therefore we propose a definition of a term which enables discussion with regard to hazard mitigation:

Hazardous condition:

- a set of circumstances which may result in harm to people or damage to structures.

Hazardous flammability limits:

- the value of the mean concentration for a given pressure and temperature that bound conditions which may grow into a hazardous condition, for example: a deflagration can transition to a detonation or the over pressurization a vessel, or a deflagration becomes rapid enough that will result in a significant overpressure, ...

This definition, when considered with regard to “hazards mitigation” has already been embraced by some code language (see definitions for Hazardous Explosive Atmosphere, Harm, Harmful event, Hazard, and Hazardous situation provided above). Embracing the notion that we want to avoid a hazardous situation, allows us to define the conditions leading to a hazardous condition and to define the limits in concentration for a given pressure and temperature, where outside of which a hazardous condition cannot occur. This is not to dismiss the other boundaries such as limits of flammability that bound the mixture space for a given pressure and temperature where flames can exist, and hazards limits bound the limits where a flame can grow into a hazardous condition. But through use of this simple definition we can embrace the macroscopic notion that a hazardous condition could result from a point source release of energy (chemical, mechanical, nuclear or ...) which would fall under our notion of an explosion as an event that once initiated grows unbounded and can cause harm.

The notion of hazards mitigation is particularly important for hydrogen and air combustion processes. For very lean mixtures of hydrogen and air ($4\% \leq \text{mixture fraction} \leq 8\%$) a deflagration (subsonic propagating thin reaction zone) can exist. The lean flammability limit for hydrogen and air flames is 4% but only for a vertically propagating flame. Mixture fractions below 8% cannot propagate downward, horizontally, spherically, or against a jet, these flames cannot grow into a hazardous situation. This unique property of hydrogen is due to the very low molecular weight resulting in high buoyancy. Note: for hydrocarbon flames the “hazardous flammability limit” and the “flammability limit” will be essentially the same – not true for hydrogen.

The use of hazardous flammability limits, flammability limits and consistent use of the proposed definition of explosion (particularly within regulations, codes and standards) will enable clear a discussion regarding what is “safe,” meaning outside of the hazardous flammability limits, what is “flammable,” meaning where a flame may occur including local overpressure as a result of fast deflagrations or detonations and what is “explosive” meaning where, or when under the wrong conditions an explosion might develop. Using these criteria we can more appropriately apply mitigation strategies guided by the risk of such events occurring.

Summary

In this manuscript we presented examples of “explosion” as viewed from the non-technical societal and from the regulatory and combustion professional perspective. We pointed out that the language taken from the RCS community is frequently ambiguous which leads to confusion and often less than optimal and overly constrictive hazard control. We suggest a definition of the notion of explosion be an event that upon initiation grows, rapidly and unbounded. This can now be applied to all events that we intuitively understand to be an “explosion” within the societal and the professional spheres. We also embrace the notion that we are interested in preventing a hazardous condition, which may or may not involve an overpressure event or a point source of energy release. We conclude that adopting this as a philosophy provides a rigorous framework to differentiate non-hazardous combustion events from those that can grow into hazardous ones. This is particularly important for hydrogen air flames which due to the very low molecular weight exhibit behavior different from hydrocarbon flames. We point out that while the lower flammability limit for hydrogen air flames is recognized to be ~4% this is not the lower limit of a hazardous condition which can be defensibly defined to be 8%.

Acknowledgement

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