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Why a Hydrogen Fireball should not be Modelled as a BLEVE Event

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The rapid increasing interest in the usage of Hydrogen has obviously triggered a lot of safety related questions. Apart from non-trivial questions about failure frequencies and ignition probabilities, the consequence modelling of potential events also contains significant uncertainties. Something to be aware of is, that even when assuming the straightforward scenario of direct ignition of the Hydrogen release, the resulting phenomena ”jet fire” (continuous event) or “fireball” (instantaneous event) are still being modelled using traditional and potentially misleading methods. While the Hydrogen jet fire is known to have a very small impact zone around the flame itself, the commonly applied “Chamberlain” approach would result in a flame Surface Emissive Power (SEP) which is highly unrealistic for Hydrogen. Furthermore, for the instantaneous release of compressed Hydrogen, the fireball phenomenon is often modelled using typical BLEVE models. The relations in these BLEVE models correlate a radiative fraction to a vapor pressure, which is irrelevant for situations where non-Pressurized Liquefied Gases (PLG) are being studied. Both approaches result in a very high flame emissive power, while the BLEVE fireball growing and rising behaviour is also based upon experiments with liquefied gas flashing, which is a different phenomenon than the compressed gas expansion situation. Other methods that correlate fireball diameter to the expansion to the Upper Flammability Limit (UFL), are non-conservative for Hydrogen due to its very high UFL.
Because of the big uncertainty and unrealistic approaches in the current modelling, Gexcon started applying a dedicated gas fireball model in its consequence modelling tool EFFECTS. This model differs from the commonly applied BLEVE fireball approaches. While experimental data about compressed Hydrogen fireballs is still scarce, the gas fireball model is based upon relations from available literature, focussing on non PLG fireball data and available experiments providing Hydrogen flame radiation fluxes. The selected relations for fireball diameter and lift-off are similar to those for the BLEVE fireball model, but the rising and growing velocity is different, because it does not include flashing liquid behaviour. During the research of an appropriate model to simulate gas fireballs, it has been encountered that there is very little information in literature that suggests how to correlate the SEP of the fireball to the chemical properties of the substance. This radiative behaviour is highly influenced by the flame’s temperature, gas composition and potential soot formation. Because usage of a “soot fraction” would be unrealistic for substances like Hydrogen, experimentally derived values have been applied for the fireball radiative flux. Apart from the heat radiation effect, the overpressure phenomenon (blast) is also being derived using equations that differ from expanding vapour explosions.

1. Introduction

The ongoing energy transition towards CO_2 neutral energy carriers also raises new safety related questions. Although Hydrogen has been used as an energy carrier for a long time, the type of applications and process conditions tend to change. In this perspective, it is relevant to realize that from the 1940s to the 1970s gas distribution networks were installed, and town gas (also known as coal gas) was the main energy carrier for the industry and households. Town gas consists of up to 50 % of Hydrogen (beside other hydrocarbons and Carbon monoxide). With the discovery and exploitation of natural gas reserves, town gas was replaced by

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natural gas, and now it is being considered to switch to energy carriers without any CO_2 footprint, such as "green" produced Hydrogen. In this "new" situation, however, the use of pure Hydrogen is being evaluated at potentially very high pressures, for instance to apply as a fuel for cars. While pure Hydrogen at elevated pressures may be a standard practice in the carefully controlled chemical industry, now this material is going to be applied in our common environment, consequently turning its use into an external safety issue.
Obviously pure Hydrogen gas has other properties than town gas or natural gas. Common concerns about the use of Hydrogen are usually around its broad flammability region (4 - 75 vol %), the huge pressures applied to make transportation efficient (>700 bar), its large laminar burning velocity (potentially leading to higher blast loads in case of a Vapour Cloud Explosion), or its low ignition energy which has caused a lot of attention towards ignition probabilities to consider in case of a Loss of Containment situation. Those properties justify the attention for its safety aspects. It is important to realize that one accident in a start-up phase of a "new" technology can ruin its reputation and its future. While nobody wants any "Hindenburg" associations, that was a clear lesson to be learned.
When evaluating the safety of compressed Hydrogen gas as an energy carrier, the applicability of predictive models to assess potential consequences of leaks of Hydrogen gas needs to be carefully considered.

2. Current Hydrogen applications in use

First, it is important to realize that in the majority of the foreseen applications, (highly) compressed Hydrogen (or CGH_2 as opposite to LH_2) is used. Although some marine applications are talking about liquefied Hydrogen (LH_2), this is still a rare situation in The Netherlands. LH_2 requires extreme cryogenic and expensive cooling, which makes it economically less attractive. Incentives to use Hydrogen as an automotive fuel are already being rolled out, where a fuelling station either generates its own Hydrogen gas by means of electrolysis or receives Hydrogen from delivery trucks. These trucks were originally tube trailers, carrying 9 to 14 steel cylinders of approximately 3 m^3 at pressures around 200 bar, ending up with a storage capacity of 350 kg of H_2.

Figure 1: A tube trailer and composite cylinders battery pack as operated by Linde gas

Most recently, suppliers started using trailers carrying battery packs (racks) of interconnected composite cylinders. Those composite packs are much lighter and might contain more than 100 cylinders of 350 L, operated at 500 bar, already providing a capacity of 1,100 kg of H_2.
At the Hydrogen delivery station, similar composite tanks are being applied. However, pressures here might be as high as 900 bar (buffer storage), while the car fuelling itself can be performed at 750 bar.
While Hydrogen may be the same material, it is those new applications of highly compressed Hydrogen in our surroundings that need to be evaluated in terms of safety. In order to do a safety assessment, potential following events of any leak situation need to be identified.

3. The event tree for potential accidents with gaseous Hydrogen

When dealing with gas releases, an event tree as illustrated in Figure 2 can be sketched, which distinguishes instantaneous from continuous, and direct from delayed ignition events. Even though the toxic event would play a role for town gas due to the presence of Carbon monoxide, toxic consequences can be skipped for pure Hydrogen. Furthermore, some guidelines claim an ignition probability of 1 for Hydrogen (combined direct plus delayed ignition), which implies that the "No ignition" branch of the tree is irrelevant. For the instantaneous event, it is important to be aware of the fact that this not only creates a fireball, but the sudden expansion of the highly pressurized gas will also create an expansion wave.

This phenomenon is being referred as the “gas blast” event. Apart from the damage due to this overpressure wave, fragments of the ruptured pressure vessel may create additional damage resulting from penetration of surrounding equipment. Such cascading or domino events may have to be evaluated separately.
Our previous approach of evaluating the instantaneous direct ignition event was based upon a Purple Book approach (CPR18E, 2005), which assumed a sort of direct ignition flashfire. This was modelled as a hemisphere with dimensions based on the resulting expanded volume at the UFL concentration level. H_2 has an UFL of 75 vol % leading to a non-conservative estimation of the flashfire footprint dimensions. Because it is also known that this event will create a rising and growing fireball (for which radiation might be as important as direct flame contact), this approach was abandoned. Instead, a more suitable fireball model is now being used.

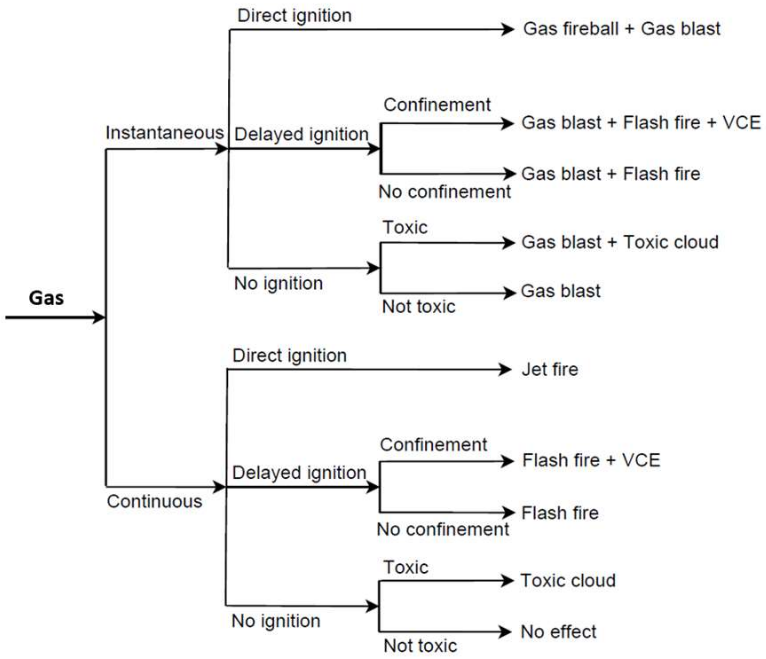

Figure 2: Event tree of a gas Loss of Containment event

4. A gas fireball is not a BLEVE phenomenon

The direct ignition of an instantaneous release of compressed flammable gas will lead to a fireball. A standard empirical model to describe this scenario is the method provided in (CCPS,1994), which can be traced back to (Roberts, 1982). The equations in (Roberts, 1982) method describe the fireball as a growing and rising radiating sphere. This approach describes equations for the assessment of the maximum diameter and maximum duration of the fireball and describe its diameter and height as a function of time. The resulting heat radiation is calculated using a solid flame approach, where the SEP (radiation flux emitted by the fireball) is a function of the available heat of combustion, duration, and radiative fraction.
However, when digging into the original literature, it became clear that most of the experimental data used to derive the empirical formulas was coming from Propane and Butane experiments and was referring to a BLEVE fireball event. However, when dealing with a release of compressed Hydrogen gas (CGH_2), there is no flashing liquid. This implies that the growing and rising behavior of the fireball is not affected by evaporating liquid and might be different as obtained from pressurized liquefied fireball situations. During the evaluation of the relevant literature, experiments conducted by (Lihou and Maund, 1982) were selected, who also used Methane experiments to derive fireball characteristics. Different from typical flashing liquid fireball behavior they obtained a constant growing and rising velocity, independent of the fuel type. Based on the available gas fireball literature the following equations can be applied:

<u>Maximum diameter of the fireball</u>:

$$D_{max} = 5.8 \cdot m_f^{\frac{1}{3}} \quad (1)$$

If vapor is treated as an ideal gas, the initial diameter of the expanded sphere (D_0) can be calculated from the released mass of gas fuel (m_f) and the density of the released gas (ρ_g) by:

$$D_0 = \left[\frac{6}{\pi} \cdot \frac{m_f}{\rho_g}\right]^{\frac{1}{3}} \quad (2)$$

Duration of the fireball:
While the maximum size of the fireball is independent of the release pressure, the dynamics of the fireball are dependent upon the momentum of the release. For momentum-dominated fireballs, the burning duration (t_d) is given by the equation below (CCPS, 1994).

$$t_d = 0.45 \cdot m_f^{\frac{1}{3}} \quad (3)$$

For buoyancy-dominated fireballs, such as would be expected for atmospheric pressure releases, the burning duration is given by the expression below (CCPS, 1994).

$$t_d = 2.6 \cdot m_f^{\frac{1}{6}} \quad (4)$$

Growing and rising behavior
From measurements of rising fireballs, (Lihou and Maund, 1982) found that the velocity of rise (expressed as "v" in the equation below) equals the rate of increase of the diameter, and that, for methane and butane, dD/dt is close to 10 m/s. Therefore, they suggested a simple relationship to calculate the fireball's lift-off duration (t_e):

$$t_e = \frac{D_{max} - D_0}{2 \cdot v} \quad (5)$$

Combining the relations into explicit relations for diameter:

$$D(t) = min\ (D_0 + 2 \cdot v \cdot t, D_{max}) \quad (6)$$

After the time of lift-off (which is the time that it takes the fireball to reach its maximum height), the fireball may continue to rise at a constant velocity. The height of the fireball($h_{fireball}$) also adjusted for the initial elevation of the vessel (H_{vessel})

$$h_{fireball} = \left(H_{vessel} + \frac{D_{max}}{2}\right) + v \cdot \Delta t \quad (7)$$

This leads to an important difference with the BLEVE fireball model: during the lift-off time (or growing period) the gas fireball will grow and rise with a constant rate, and not a third order rate (which relates to the evaporating / flashing behavior of the BLEVE).
For the associated overpressure (and fragmentation) effects of the "gas blast" phenomenon, the "BLEVE" overpressure calculation would be inappropriate. Thus, a "gas expansion" vessel rupture prediction model must be applied. The coexistence of both phenomena in the same event is also highly relevant because the blast wave may already destroy windows which would have a protective function for non-destructive but injuring heat radiation.

5. Surface emissive power uncertainty

The fireball predictive model uses a solid-flame approach to calculate the heat radiation. The model addresses the fireball's dimensions, its surface emissive power (SEP), atmospheric transmissivity (τ_a), and view factor (F_{view}). The heat flux (q") at a certain distance from the fire, which is experienced by the receiver per unit area, can be calculated by:

$$q" = F_{view} \cdot \tau_a \cdot SEP \quad (8)$$

While the view factor and transmissivity can be calculated using standard relations identical to those used for a BLEVE fireball, the SEP itself should be based on fuel substance characteristics. View factor, transmissivity and SEP are time dependent parameters, because the fireball itself grows, burns and rises as a function of time.
In standard fireball models, the SEP is calculated based upon an energy balance relation which uses on the fraction of the heat radiated (F_s), the heat of combustion (h_c) the burning rate (q_s) and the surface of the fireball ($A_{fireball}$).

$$SEP_{max} = \frac{F_s \cdot h_c \cdot q_s}{A_{fireball}} \quad (9)$$

The surface of the fireball ($A_{fireball}$) corresponds to the surface of a sphere, where D_{max} is the maximum diameter of the fireball:

$$A_{fireball} = \pi \cdot D_{max}^2 \quad (10)$$

The burning rate (q_s) depends on the total mass of fuel involved in the fireball (m_f) and its duration (t_d).

$$q_s = \frac{m_f}{t_d} \quad (11)$$

In conventional BLEVE fireball models, the fraction of heat radiated F_s is based upon a relation that associates this radiative fraction to the vapour pressure of the expanding vapour cloud. Obviously, for a (CGH_2) Hydrogen fireball, this vapour pressure is totally irrelevant, and experiments have revealed that a Hydrogen flame has a very low radiative flux. This flame radiative flux is highly dependent on the substance: it will be totally different for a Methane fireball compared to a Hydrogen fireball. Because no other sources of trustworthy SEP values were discovered, the experimentally derived "clear flame" data as presented in (Rew and Hulbert, 1996) has been selected. This publication associates a Hydrogen flame with a SEP of 70 kW/m^2, while a clear Methane flame emits heat radiation with a SEP of 265 kW/m^2. This matches very well with observed Methane fireball values mentioned in (CCPS, 1994).
The resulting fireball model has been implemented in Gexcon's consequence modelling software EFFECTS and appears to give larges consequences distances compared to the previous "UFL flashfire" model, but shows smaller distances than a BLEVE fireball model. This is mainly due to the shorter duration of the fireball and smaller SEP values applied.

6. Other potential uncertainties in event modelling

In order to assess the consequences of any Loss of Containment scenario, the first step would be to obtain a leak mass flow rate and (decompressed) release conditions. Although gas release models have been used for ages, a potential "Negative Joule Thompson" effect needs to be considered. This influences the end temperature, and the supercritical pressures applied may lead to a significant inaccuracy in density estimations. Apart from the release rate itself, the high velocity (supersonic) turbulent mixing with air requires special attention if the formation of a flammable cloud has to be evaluated.
Of course, the dispersion of a flammable cloud of Hydrogen requires a predictive model that is validated for rising plume behaviour, and fortunately there is already high awareness of this rising cloud aspect. The modelling of a Vapour Cloud Explosion (VCE) needs paying special attention to the presence of roofs and ceilings. This would require a 3D modelling tool such as Gexcon's CFD software FLACS to account for the surrounding 3D geometries.
However, for the direct ignition event leading to a jet fire (continuous event) or fireball (instantaneous event) these events used to be predicted with the same kind of models applied for Methane or Propane situations. As stated earlier in this paper, this approach can lead to misleading conclusions for a fireball. However, similar doubts about SEP also apply to conventional jet fire modelling. Often applied jet flame models like (Chamberlain, 1987) or (Cook et al, 1990) require a "soot fraction" to correct for radiant fluxes. Obviously, soot should be zero for a Hydrogen jet fire, but this would lead to unrealistic high radiation fluxes. Therefore, based on experimental results it has been decided to limit the SEP of a pure Hydrogen jet fire to 70 kW/m^2, leading to less conservative results for a Hydrogen jet fire. Unfortunately, it is already known that "foreign materials" in a H_2 jet can completely change its radiative behaviour. Even the collision of the jet flame against a wall or neighbouring pipes will change the flame's radiative behaviour, making the flame visible after interaction with an engulfed object. Furthermore, these low SEP values will not apply for jet flames of Methane/Hydrogen mixtures, which are expected to get transported through our natural gas network.

7. Conclusions

Although Hydrogen is not a new gas, its expected application resulting from an ongoing energy transition requires careful consideration of applicability of conventional empirical models. To avoid misuse of BLEVE fireball models, a solution has been proposed to apply a dedicated gas fireball approach, using experimentally derived values for SEP. To be able to assess CGH2 scenarios, this fireball model has been implemented in

Gexcon's consequence modelling tool EFFECTS. Its empirical jet fire models have also been adapted for SEP expected for pure Hydrogen flames. A dedicated technical note (Gexcon, 2020) addresses points of attention when modelling Hydrogen scenarios with the software tool EFFECTS. Unfortunately, several uncertainties will remain, and further improvement of consequence modelling requires new experimental campaigns. At the moment of writing, we are anxiously awaiting results from more recent test campaigns, such as the SH2IFT program, which hopefully also reveals if a BLEVE fireball (Pressurised Liquefied H_2 situation) can occur, and what surface emissive power should be expected for Hydrogen fireballs.

Nomenclature

BLEVE – Boiling Liquid Expanding Vapour Explosion
CGH_2 – Compressed Gas Hydrogen
SEP – Surface Emissive Power
PLG – Pressurised Liquefied Gas
LH_2 – Liquefied Hydrogen (a Cryogenic PLG)
UFL – Upper Flammability Limit
VCE – Vapour Cloud Explosion

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