INVESTIGATION OF THE EXPLOSIVE ATMOSPHERES EXTENT OF HYDROGEN AND METHANE GAS MIXTURES BY CALCULATION AND FLACS-CFD SIMULATION

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Abstract

Explosive atmosphere is defined as a mixture of dangerous substances with air, under atmospheric conditions, in the form of gases, vapours, mist or dust in which, after ignition has occurred, combustion spreads to the entire unburned mixture. Methane-hydrogen mixtures will become more and more important for energy use in the near future. It has many positive economic and environmental benefits, while the risk of explosion is partly forgotten. It is necessary to identify hazardous areas in the interpretation of technological equipment. The applicable standard, EN IEC 60079-10-1:2020, defines the extent of the explosive atmosphere and zones for a given material, but does not cover mixtures. The objective of the study is to determine the explosive hazard areas of different mixtures of hydrogen and natural gas (methane), by adding additional possible relationships to the initial equations of the standard, and to compare them with the results of the models built in the FLACS-CFD simulation.

Keywords: *hazardous area classification, explosive atmosphere, ATEX, FLACS-CFD, hydrogen-methane mixtures*

1. Introduction and motivation

In the case of a technology e.g. pharmaceutical, oil refinery, chemical industry, explosive mixtures caused by different multi-component gas/vapour mixtures may occur. Explosives manufacturing, as an explosive engineering, also has the role of explosion protection, which needs to be addressed by protective measures (Daruka, 2023), thus the relevance of different explosive gas/vapour mixtures for these manufacturing technologies. It should be noted that the legislative background in these two areas needs to be reviewed (Daruka et al., 2024) as some points are difficult to decide where they belong and so-

called grey zones may develop. Nowadays, the hydrogen-natural gas (methane) mixture is growing importance in the 21st century, particularly in the fields of energy production, environmental protection and industrial applications.

Use as an energy source when hydrogen is burned as a clean energy, only water is produced, so no carbon dioxide is emitted. In the case of fuel cells, hydrogen fuel cells are efficient and clean, and are particularly important for transport and the stability of the electricity grid. Methane is widely available as the main component of natural gas (Tugyi et al., 2023) and is abundant worldwide. In addition, it can be well stored and transported for energy storage, which is beneficial for power grids. The use of a blend allows the combination of good storage of methane and clean combustion of hydrogen, reducing carbon dioxide emissions while maintaining energy supply reliability (Elam et al., 2003).

Environmental benefits include a reduction in carbon dioxide emissions as the addition of hydrogen to methane reduces the amount of carbon dioxide produced by burning fossil fuels (Elam et al., 2003). Furthermore, the use of such blends can provide an incentive to address methane emissions as reducing greenhouse gas emissions is a global priority.

From an economic and infrastructural point of view, the use of existing infrastructure, where the use of a hydrogen-methane mixture allows the use of existing natural gas infrastructure (pipelines, storage), so that it can be integrated cost-effectively and integrated into the energy system cost-effectively and quickly (Nyangon and Darekar, 2024).

In terms of sustainability and vision, the hydrogen-methane gas mix could be an important step in the transition from fossil fuels to renewable energy sources. For a sustainable energy future, the use of gas mixtures offers a transitional solution that can contribute to reduce global warming and pollution while ensuring continuity and stability of energy supply (Nyangon and Darekar, 2024).

For the different technological units, which are not user/residential areas but reservoirs, extraction wells, compressor stations and distribution stations, the extent of explosion hazard areas should be identified in order to determine the potential explosion risk. The standard applicable in the European Union for such technologies is EN IEC 60079-10-1:2020 (International Electrotechnical Commission, 2020), which for mixtures adds a reference in Chapter 6.2 need to take into account the components of flammable materials with different characteristics such as relative density, temperature class and thus whether the ratio of components is sufficient for the relevant parameters (application group, temperature class). However, no guidance is given on the extent of the zones. The EN IEC 60079-10-1:2015 standard also included a so-called safety factor (k), which was intended to provide additional safety in the uncertainties in the determination of the lower explosive limit for flammable substances, in particular for gas mixtures, but this was considered unnecessary and confusing and has therefore been removed from the 2020 version.

Thus, with a good engineering approach and considering the conservative option, the properties of the more hazardous material that will give the larger zone extent should be considered, but it is necessary to consider what will be the relevant mixture in terms of Ex characteristics (e. g. IIA, T1). The standard also states in Chapter 8.1 that, in the case of potential zone overlap, the more stringent classification criteria for the different zone types, including temperature class and equipment group, should be applied in the area of overlap.

The NFPA 497:2021 (National FireProtection Association Quincy, 2021) also does not include a zone area definition for hydrogen-natural gas (methane) mixtures, but only defines the requirements for single-component materials.

IGEM/SR/25 Edition 2 with amendments 2013 Hydrogen Supplement 1 (Institution of Gas Engineers and Managers, 2022) provides detailed requirements for the classification of hazardous areas for

the handling of hydrogen and hydrogen/natural gas mixtures. The supplement deals with pure hydrogen and 20% hydrogen/natural gas mixtures, including appropriate ventilation systems, modelling of the dispersion of escaping gases and the designation of hazardous areas.

The API RP 505:2018 standard, Chapter D.5.3 (American Petroleum Institute, 2018) mentions the risk of explosion hazards from mixtures, that the radius of the zone extents in such cases is often quite difficult to determine. There are two reasons for this, one is that the extent of dispersion of a hydrocarbon mixture during an emission is sometimes difficult to know. The other reason is that most of the technical data and material properties for the determination of explosive atmospheres deal only with pure components and not with mixtures. It is suggested that the first problem can be addressed to some extent by using commercially available propagation modelling programs because as such programs can be used to estimate both the lower flammability limit (LFL) and upper flammability limit (UFL) – explosive range – of gas mixtures. However, this is not possible with all programs or requires special *programming* skills and knowledge to complement the basic initial equations of the software. The FLACS-CFD software used in this research (Tugyi et al., 2024) software can be used to set this up in a user-friendly manner. The standard recommends that for mixtures, the mass emission rate of the volatile part of the mixture should be determined first. Assuming that all volatile hydrocarbons can escape freely from the mixture during the release, the extent of the explosive region can then be determined, which is described as a method that results in a conservative radius of danger.

The CEI 31-35 (2012), Explosive atmospheres Guide for classification guide for classification of hazardous areas for the presence of gas in application of CEI EN 60079-10-1 (CEI 31-87) (Comitato Elettrotecnico Italiano, 2012) already adds recommendations for calculating the extent of specific mixture of explosive atmospheres. It includes the possibility of calculating the molar mass and the lower flammability/explosive limit for multi-component materials according to Le Chatelier's laws (Bozek & Rowe, 2010), which has been used as a basis for further good approximate models of the lower flammability/explosive limit (Addai et al., 2016). In addition, the EN ISO 10156:2017 standard can be used to determine the lower and upper flammability/explosion limit (International Organization for Standardization, 2017), which has a scientific basis in the studies of Schröder V et al. The calculation method in the standard differs from that of EN IEC 60079-10-1:2020, but in its context, by defining the two parameters mentioned above, it can be applied to mixtures, which was used by Molino et al (Molino et al., 2012) in their research. In CEI 31-35, it is recommended that the presence of a component in the mixture in a total volume of less than 5% should not be taken into account in terms of ignition temperature (temperature class) and gas group.

For the hydrogen methane gas sub-group, the literature indicates that IIC or IIB+H2 is expected for the gas sub-group IIC or IIB+H2 if it exceeds 30% (EN IEC 60079-10-1:2020, NFP 497:2021; CEI 31-35:2012). According to API RP 505:2018 clause 5.5.5, if the hydrogen sulphide content is below 25%, the gas sub-group is IIA, and clause 5.5.6 also mentions IIC for hydrogen contents above 30%. In the case of hydrogen mixtures with a hydrogen content between 25–30%, IIA is not appropriate and IIB or higher is required (Askar et al., 2016).

However, the relationships applicable to EN IEC 60079-10-1:2020 include variables that can be calculated mathematically for mixtures or determined using process simulation software (Unisim Design, ChemCAD).

In this study, the definitions of these variables will be presented, how they can be implemented in the initial equations used to determine the explosive region of a mixture, and then the calculations will be compared with the results of the FLACS-CFD simulation program.

2. Initial equations and dates

For a technology, to determine the extent of the explosive zones, we need to know the state of the medium and its phases. Different equations have to be used for liquid and gas/vapour emissions. This study only considers gaseous/vapour emissions. As input data, it is necessary to know the maximum pressure and temperature of the process equipment under normal operating conditions. It is also necessary to have as an important initial parameter the value of the critical pressure, which gives the information whether the nature of the discharge is subsonic or sonic. This variable depends on the molar fraction, but generally speaking, above 1.89 bar(g) (Tugyi et al., 2023), we are talking about flow above the speed of sound. The two equations from which it is necessary to start are:

Subsonic outflow

$$W_g = C_d \cdot S \cdot p \cdot \sqrt{\frac{M}{Z \cdot R \cdot T} \cdot \frac{2 \cdot \gamma}{\gamma - 1} \cdot \left(1 - \left(\frac{p_a}{p}\right)^{\frac{(\gamma - 1)}{\gamma}}\right) \cdot \left(\frac{p_a}{p}\right)^{\frac{1}{\gamma}}} \tag{1}$$

Sonic outflow

$$W_g = C_d \cdot S \cdot p \cdot \sqrt{\gamma \cdot \frac{M}{Z \cdot R \cdot T} \cdot \left(\frac{2}{\gamma + 1}\right)^{\left(\frac{\gamma + 1}{\gamma - 1}\right)}} \tag{2}$$

where

- W_g is mass release rate of gas or vapour $\left(\frac{\text{kg}}{\text{s}}\right)$,
- C_d is discharge coefficient $(-)$,
- S is cross section of the opening (hole) (m^2),
- p is pressure inside the equipment (Pa),
- M is molar mass $\left(\frac{\text{kg}}{\text{kmol}}\right)$,
- Z is compressibility factor $(-)$, valuse is 1.0 to 50 bar(g)
- R is universal gas constant $\left(8314.5 \frac{\text{J}}{\text{kmol} \cdot \text{K}}\right)$,
- T is temperature of the substance (K),
- γ is polytropic index of adiabatic expansion $(-)$,
- p_a is atmospheric pressure (101 325 Pa).

Subsequently, using the gas/vapour density and the lower flammability/explosive limit (both parameters will be molar fraction dependent in the following), the volumetric release characteristic of the source can be determined, which, using Figure D.1 of IEC 60079-10-1:2020, allows the extent of the explosive zones to be determined:

$$Q_c = \frac{W_g}{\rho_g \cdot LFL} \tag{3}$$

where

- Q_c is volumetric release characteristic of the source $\left(\frac{\text{m}^3}{\text{s}}\right)$,
- ρ_g is gas or vapour density at the ambient conditions $\left(\frac{\text{kg}}{\text{m}^3}\right)$,
- LFL is lower flammability/explosion limit (vol. %).

From the equations described and the molar fraction dependent variables already mentioned in the previous paragraphs, the polytropic index of adiabatic expansion is required, and the specific heat (at constant pressure) is also required:

– molar mass,
– polytropic index of adiabatic expansion,
– specific heat,
– critical pressure,
– gas or vapoure density,
– lower explosion limit.

3. Variables depending on the mole fractions

The following relationships, which relate to the properties of a possible multicomponent mixture, are based on these basic physicochemical laws. They are applied consistently in the design of chemical engineering technologies and in flow equations. Process simulation programs also use these relationships, built on similar principles, to calculate the results of a given simulation model.

3.1. Molar mass of the mixture

To determine the molar mass of a mixture, we need to know the composition of the mixture, i.e. the molar ratio and molar mass of the individual components. The molar mass of a mixture is the weighted average of the molar mass and molar ratio of each component. The general formula for determining the molar mass of a mixture is as follows (Nesbitt, 2007):

$$M_{\text{mix}} = \sum_{i=1}^{n} y_i \cdot M_i \tag{4}$$

where

– M_{mix} is molar mass of the mixture $\left(\frac{\text{kg}}{\text{kmol}}\right)$,
– y_i is molar fraction of each component $(-)$,
– M_i is molar mass of each component $\left(\frac{\text{kg}}{\text{kmol}}\right)$.

3.2. Polytropic index of adiabatic expansion of the mixture

Determining the polytropic index during adiabatic expansion can be a complex process, especially for a mixture. To determine the polytropic index of a gas mixture, the molar ratio of the individual components and their specific heat capacities must be taken into account (Çengel et al., 2024).

$$\gamma_{\text{mix}} = \frac{M_{\text{mix}} \cdot C_{p_{\text{mix}}}}{M_{\text{mix}} \cdot C_{p_{\text{mix}}} - R} \tag{5}$$

where

– γ_{mix} is polytropic index of adiabatic expansion of the mixture $(-)$,
– M_{mix} is molar mass of the mixture $\left(\frac{\text{kg}}{\text{kmol}}\right)$,
– $C_{p_{mix}}$ is specific heat of the mixture $\left(\frac{\text{J}}{\text{kmol} \cdot \text{K}}\right)$,
– R is universal gas constant $\left(8314.5 \frac{\text{J}}{\text{kmol} \cdot \text{K}}\right)$.

A fixed value is one approach, since the exact value depends on the exact thermal properties of each component and also on the temperature conditions of the mixture.

3.3. Specific heat of the mixture

The specific heat of the gas mixture is determined as the weighted average of the molar fraction and specific heat of each component. The specific heat may be constant at pressure (Cp) or constant at volume (Cv). To determine the specific heat of a mixture at constant pressure, the molar fraction of each component and its specific heat must be known (Çengel et al., 2024).

$$C_{p_{\text{mix}}} = \frac{1}{\sum_{i=1}^{n} \frac{y_i}{c_{p_i}}} \tag{6}$$

where
- C_{pmix} is specific heat of the mixture $\left(\frac{\text{J}}{\text{kmol} \cdot \text{K}}\right)$,
- y_i is molar fraction of each component $(-)$,
- C_{pi} is the value of each component $\left(\frac{\text{J}}{\text{kmol} \cdot \text{K}}\right)$.

3.4. Critical pressure of the mixture

To determine the critical pressure of the mixture, it is already necessary to know the polytropic index of adiabatic expansion of the mixture:

$$p_{c_{\text{mix}}} = p_a \cdot \left(\frac{\gamma_{\text{mix}}+1}{2}\right)^{\frac{\gamma_{\text{mix}}}{(\gamma_{\text{mix}}-1)}} \tag{7}$$

where
- $p_{c_{\text{mix}}}$ is critical pressure of the mixture (Pa),
- γ_{mix} is polytropic index of adiabatic expansion of the mixture $(-)$,
- p_a is atmospheric pressure (101,325 Pa).

3.5. Gas or vapour density of the mixture

To determine the gas/vapour density of a mixture, it is already necessary to know the molar mass of the mixture:

$$\rho_{g_{\text{mix}}} = \frac{p_a \cdot M_{\text{mix}}}{R \cdot T_a} \tag{8}$$

where
- $\rho_{g_{\text{mix}}}$ is gas or vapour density of the mixture $\left(\frac{\text{kg}}{\text{m}^3}\right)$,
- p_a is atmospheric pressure (101,325 Pa),
- M_{mix} is molar mass of the mixture $\left(\frac{\text{kg}}{\text{kmol}}\right)$,
- R is universal gas constant $\left(8314.5 \frac{\text{J}}{\text{kmol} \cdot \text{K}}\right)$,
- T_a is ambient temperature (K).

3.6. Lower flammability/explosion limit of the mixture (LFL)

The lower flammability/explosion limit (LEL) of a gas or vapour mixture can be determined by knowing the LEL and molar ratio of each component. A commonly used approximation is the application of Le Chatelier's law (Addai et al., 2016; Bozek & Rowe, 2010; Comitato Elettrotecnico Italiano, 2012; International Organization for Standardization, 2017; Molino et al., 2012) which is used to calculate the explosion limit values of gas mixtures:

$$\text{LEL}_{\text{mix}} = \frac{1}{\Sigma_{i=1}^{n} \frac{y_i}{\text{LEL}_i}} \tag{9}$$

where

- LEL_{mix} is lower explosion limit of the mixture (vol. %),
- y_i is molar fraction of each component ($-$),
- LEL_i is lower explosion limit of each component (vol. %).

It is important to note that this approximation is based on the simple Le Chatelier law. For a more precise definition, experimental data or more advanced model applications may be needed, although this approach can be considered conservative. However, for mixtures where there are significant interactions between individual components, it is important to have experimental data to support this. In addition, simulation programs such as FLACS-CFD, already mentioned and used, and Breeze Incident Analysist (Tauseef et al., 2017) can be used to determine lower and upper flammability/explosion limits for mixtures.

4. New initial equations

By implementing the complementary equations in the initial equations already mentioned, the following relationships for mixtures with several components are obtained:
Subsonic outflow

$$W_{g_{\text{mix}}} = C_d \cdot S \cdot p \cdot \sqrt{\frac{M_{\text{mix}}}{Z \cdot R \cdot T} \cdot \frac{2 \cdot \gamma_{\text{mix}}}{\gamma_{\text{mix}}-1} \cdot \left(1 - \left(\frac{p_a}{p}\right)^{\frac{(\gamma_{\text{mix}}-1)}{\gamma_{\text{mix}}}}\right) \cdot \left(\frac{p_a}{p}\right)^{\frac{1}{\gamma_{\text{mix}}}}} \tag{10}$$

Sonic outflow

$$W_{g_{\text{mix}}} = C_d \cdot S \cdot p \cdot \sqrt{\gamma_{\text{mix}} \cdot \frac{M_{\text{mix}}}{Z \cdot R \cdot T} \cdot \left(\frac{2}{\gamma_{\text{mix}}+1}\right)^{\left(\frac{\gamma_{\text{mix}}+1}{\gamma_{\text{mix}}-1}\right)}} \tag{11}$$

where

- $W_{g_{\text{mix}}}$ is mass release rate of the mixture $\left(\frac{\text{kg}}{\text{s}}\right)$.

By this the volumetric release characteristic of the source can be determined for mixtures:

$$Q_{c_{\text{mix}}} = \frac{W_{g_{\text{mix}}}}{\rho_{g_{\text{mix}}} \cdot \text{LEL}_{\text{mix}}} \tag{12}$$

where

- Q_c is volumetric release characteristic of the source $\left(\frac{\text{m}^3}{\text{s}}\right)$.

Thus, according to EN IEC 60079-10-1:2020, the extent of hazardous areas can be determined.

5. The results of the mathematical calculation for mixtures

The components of the medium under investigation are hydrogen-methane, for this mixture, the values of the molar fraction variables for different concentration distributions are given in *Table 1*.

Table 1

Values of molar fraction variables for hydrogen-methane mixtures of different proportions

Hydrogen [vol.%]	Methane [vol.%]	Critical pressure [Pa]	Polytropic index [-]	Molar mass [kg/kmol]	Gas density [kg/m³]	LFL [vol.%]	Specific heat [J/(kmol·K)]
0	100	185904	1.30	16.04	0.63	4.40	2224.36
10	90	185985	1.31	14.64	0.58	4.36	2429.38
20	80	186083	1.31	13.24	0.52	4.31	2676.01
30	70	186205	1.31	11.83	0.47	4.27	2978.36
40	60	186359	1.31	10.43	0.41	4.23	3357.75
50	50	186563	1.31	9.03	0.36	4.19	3847.90
60	40	186843	1.32	7.63	0.30	4.15	4505.61
70	30	187253	1.33	6.23	0,25	4.11	5434.51
80	20	187909	1.34	4.82	0.19	4.07	6845.91
90	10	189128	1.36	3.42	0.14	4.04	9247.59
100	0	192188	1.41	2.02	0.08	4.00	14245.28

It can be seen that for the values of pure hydrogen and methane, and for the different concentration distributions, the calculated values show a quasi-steady decreasing or increasing trend with respect to the two extremes. The specific heat values were determined using the Hyperbolic Functions (Green and Southard, 2019) approximation in Chapter 2 of Perry's Handbook at 25 °C, which is temperature dependent, not pressure dependent. In three cases, I also checked the specific heat values using UniSim Design software, which already takes pressure into account. The results are shown in *Table 2*.

Table 2

Perry's Handbook and UniSim Design comparison of specific heat results

Hydrogen [vol.%]	Methane [vol.%]	Perry's Handbook [J/(kmol·K)]	5 bar(g) [J/(kmol·K)]	160 bar(g) [J/(kmol·K)]
10	90	2429.38	2422.54	3400.79
50	50	3847.90	3600.98	4118.79
90	10	9247.59	8560.06	8910.03

Using the software, the specific heat of the mixture was lower for all concentration distributions tested at 5 bar(g) pressure and at 160 bar(g) for 90–10% hydrogen methane concentration. The specific heat value is important in determining the extent of the zones, but for two extreme values, 2429.38 J/kmol·K and 9247.59 J/kmol·K, the difference in the extent of a possible zone was 0.12 m for the same conditions, in favour of the lower specific heat. This is not a significant difference compared to a difference of more than three times between the two values, but it may be worthwhile to deviate in the direction of safety and increase the calculated zone extent by 0.1 m or more.

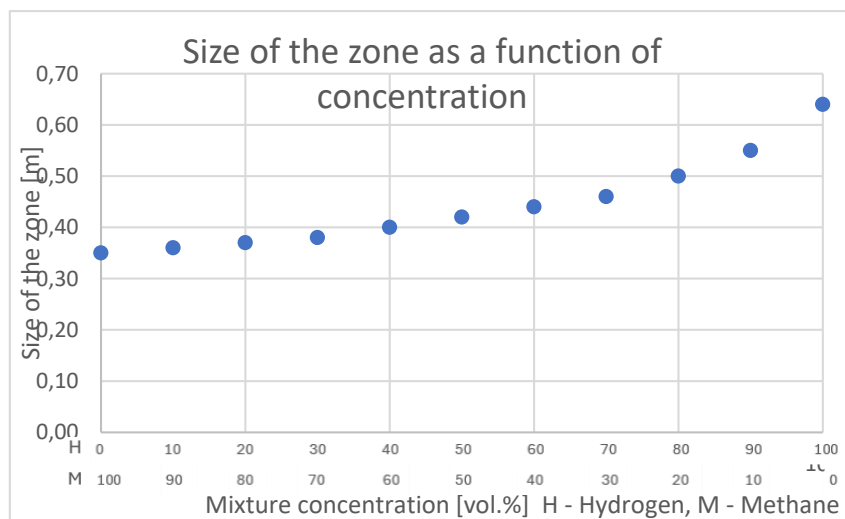### 5.1. Size of the explosive zones - Small hole, low pressure

In the case where the process equipment has a pressure of 5 bar(g), a temperature of 25 °C and an assumed hole size (e. g. for a flange connection) of $1.375 \cdot 10^{-6}$ m². This means a diameter of $6.615 \cdot 10^{-4}$ m.

Holes can be caused by corrosion, material changes due to vibration, expansion due to pressure and temperature, exposure to chemicals or improper installation due to human error, poorly selected gaskets, weak welds, loosely tightened bolts and joints.

Table 3 shows the mass release rate, volumetric release characteristic and zone extents for different distributions. *Figure 1* shows concentration and zone extent as a function of results.

Table 3

Small hole, low pressure, zone extents for different concentrations

Hydrogen [vol.%]	Methane [vol.%]	W_g [kg/s]	Q_c [m³/s]	Size of zone [m]
0	100	8.62E-04	3.09E-02	0.35
10	90	8.24E-04	3.27E-02	0.36
20	80	7.83E-04	3.47E-02	0.37
30	70	7.41E-04	3.71E-02	0.38
40	60	6.96E-04	3.99E-02	0.40
50	50	6.48E-04	4.33E-02	0.42
60	40	5.97E-04	4,77E-02	0.44
70	30	5.40E-04	5.33E-02	0.46
80	20	4.77E-04	6.13E-02	0.50
90	10	4.04E-04	7.39E-02	0.55
100	0	3.14E-04	9.83E-02	0.64

Figure 1. *Concentration and zone extents as a function of the results (small hole, low pressure)*

It can be observed that as the mixing fraction of hydrogen increases, the zone extents tend to change exponentially from a concentration of 60%.

5.2. Size of the explosive zones – Small hole, high pressure

In the case where the process equipment has a pressure of 160 bar(g), a temperature of 25 °C and an assumed hole size of $1.375 \cdot 10^{-6}$ m^2. This means a diameter of $8.899 \cdot 10^{-2}$ m. *Table 4* shows the mass release rate, volumetric release characteristic and the zone extents for different distributions. *Figure 2* shows the results as a function of concentration and zone extent.

Table 4

Small hole, high pressure, zone extents for different concentrations

Hydrogen [vol.%]	Methane [vol.%]	W_g [kg/s]	Q_c [m^3/s]	Size of zone [m]
0	100	2.56E-02	9.17E-01	2.06
10	90	2.45E-02	9.70E-01	2.12
20	80	2.33E-02	1.03E+00	2.19
30	70	2.20E-02	1.10E+00	2.27
40	60	2.07E-02	1.19E+00	2.36
50	50	1.93E-02	1.29E+00	2.46
60	40	1.77E-02	1.42E+00	2.59
70	30	1.60E-02	1.58E+00	2.74
80	20	1.42E-02	1.82E+00	2.95
90	10	1.20E-02	2.19E+00	3.26
100	0	9.33E-03	2.92E+00	3.78
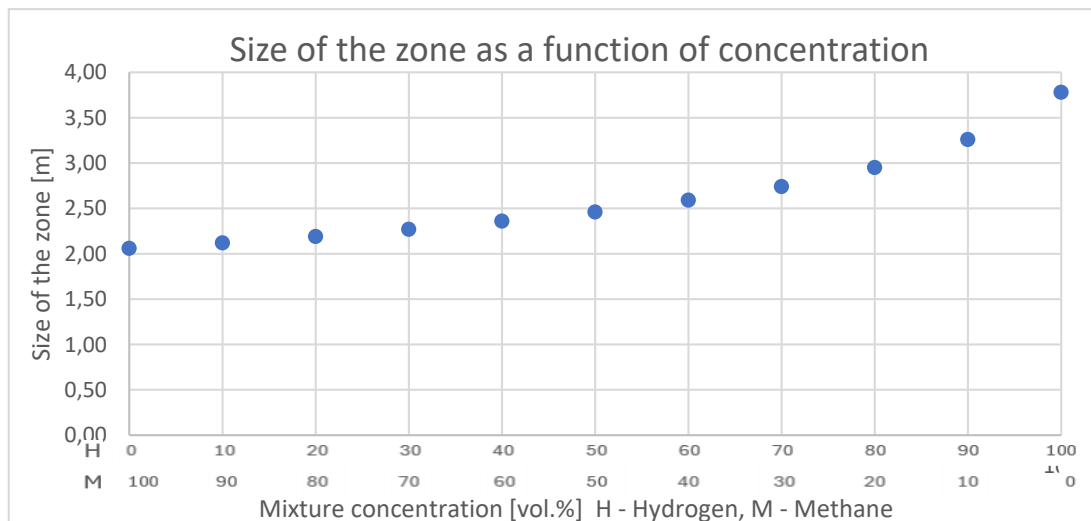
Figure 2. *Concentration and zone extents as a function of the results (small hole, high pressure)*

The same can be observed as for lower pressures, that the zone increases exponentially after the 60% hydrogen concentration mentioned above.

5.3. *Size of the explosive zones - Large hole, small pressure*

In the case where the process equipment is repeatedly at a pressure of 5.0 bar(g), a temperature of 25 °C and an assumed hole size of $6.221 \cdot 10^{-3}$ m^2 larger than for a hypothetical skimming, *Table 5* shows the mass release rate, volumetric release characteristic and zone extent for different distributions. *Figure 3* shows concentration and zone extent as a function of results.

Table 5

Large hole, small pressure, zone extents for different concentrations

| Hydrogen [vol.%]	Methane [vol.%]	W_g [kg/s]	Q_c [m^3/s]	Size of zone [m]
0	100	5.15	184.39	33.25
10	90	4.92	195.02	34.32
20	80	4.68	207.20	35.35
30	70	4.43	221.40	36.59
40	60	4.16	238.26	38.03
50	50	3.87	258.78	39.71
60	40	3.56	284.59	41.74
70	30	3.23	318.54	44.29
80	20	2.85	366.29	47.65
90	10	2.41	441.19	52.54
100	0	1.88	586.82	61.01
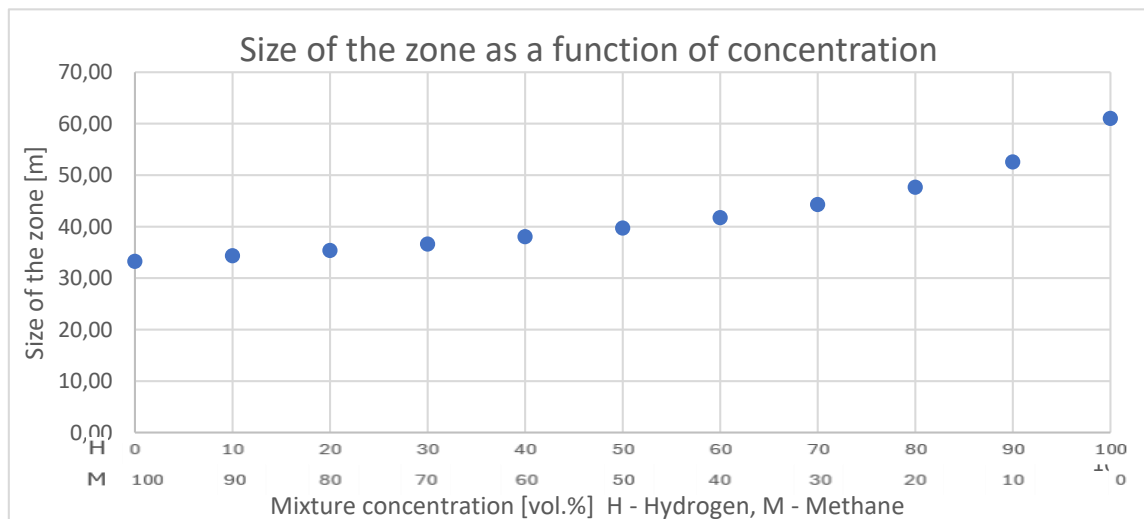
Figure 3. *Concentration and zone extents as a function of the results (large hole, low pressure)*

Similar to the previous two cases, the zones increase exponentially from a hydrogen concentration of 60%.

6. The results of simulation for mixtures

With the FLACS-CFD simulation, the simulations were carried out for the assumed largest release in the three possible releases, since in the other cases, where the release was much smaller in magnitude, it was not possible to investigate the propagation locally. The mathematically calculated results were modelled and compared for three different mixing ratios. If the hydrogen-methane ratio is 50-50%, the simulation gives an explosive region of approximately 15 m, which is illustrated in *Figure 4*. Each simulation was run for 10 seconds and 4.5 seconds from the time point was observed with maximum zone extent (airflow was not included in the models as a boundary condition).
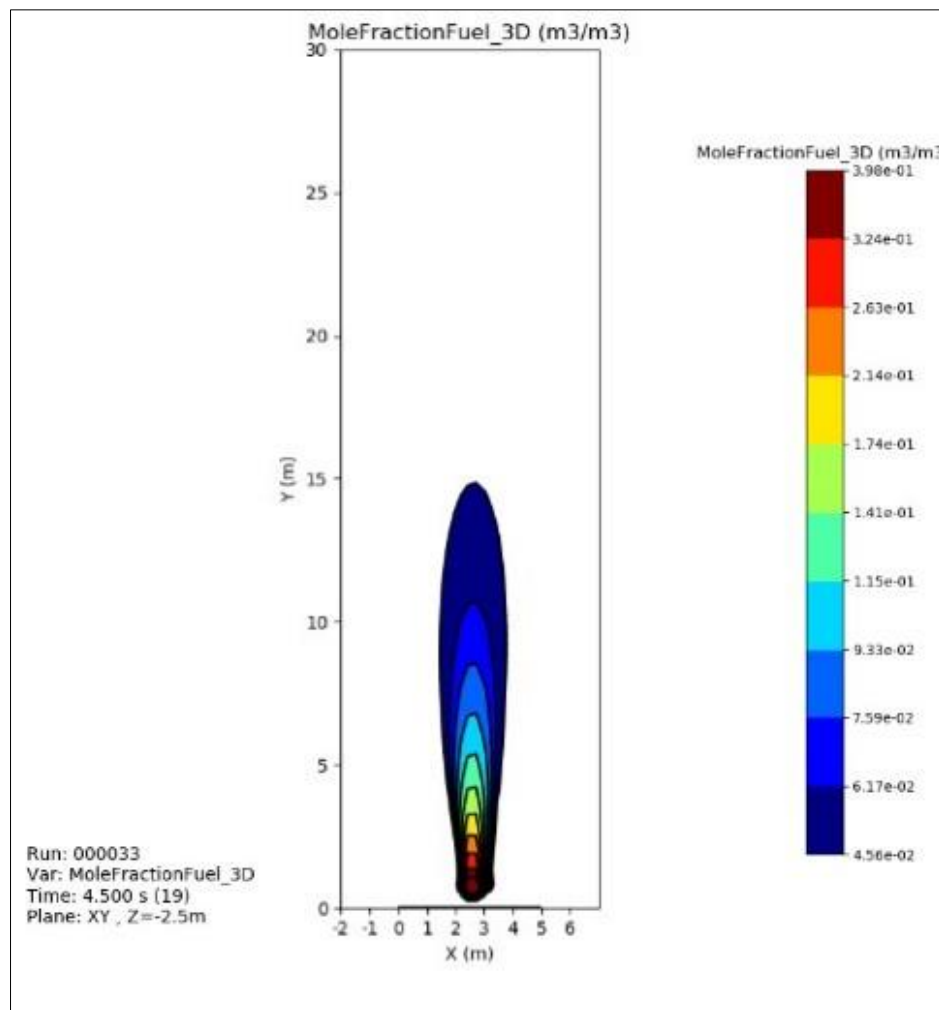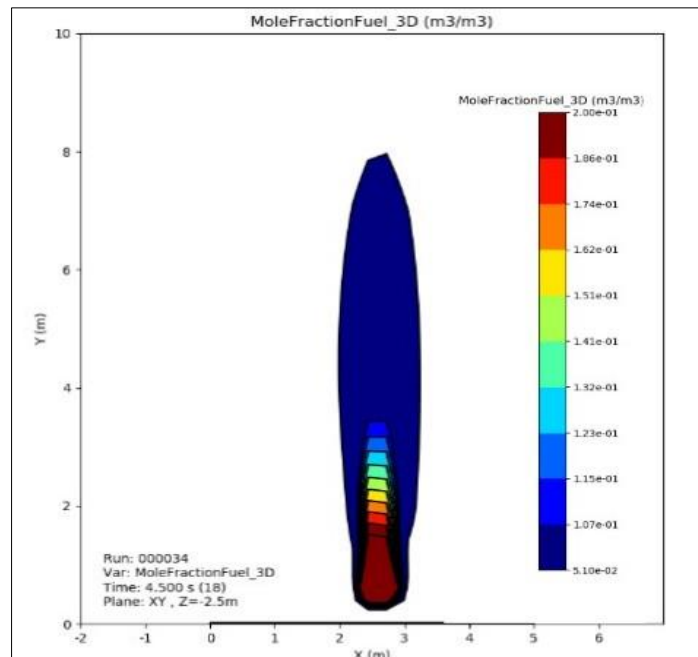

Figure 4. *Large hole, low pressure, hydrogen to methane ratio 50-50%*

With this model simulation, the result of the established 15 meters is much smaller than the calculated 39.71 meters. In *Figure 5*, the volumetric, isosurface and maximum value 3D visualization options are shown for the scenario under consideration.
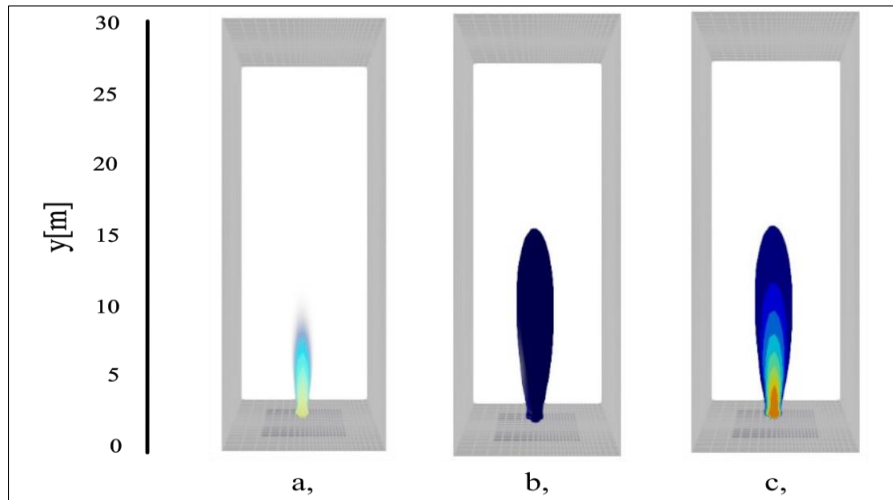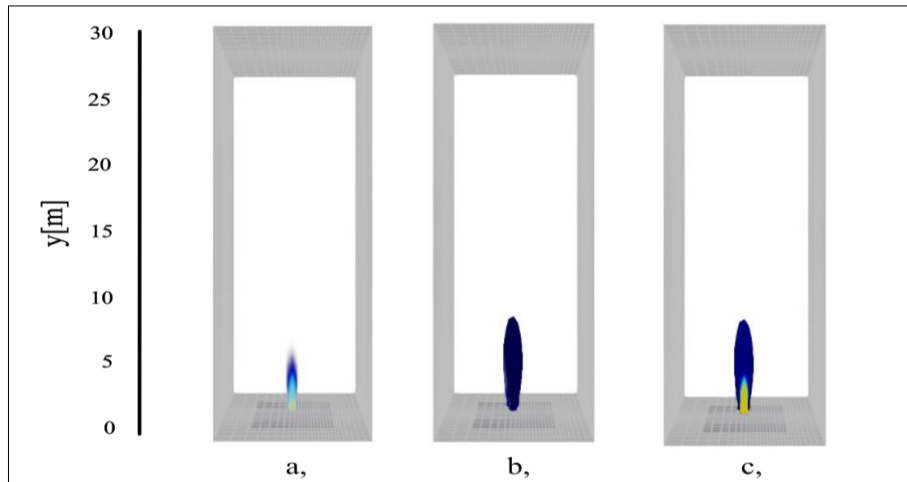
Figure 5. *a, – volumetric, b, – isosurface, c – maximum value*
(large hole, low pressure, hydrogen to methane ratio 50-50%)

In the case where the proportion of hydrogen methane is 10–90%, the simulation gives an explosive region of approximately 8 m, which is shown in *Figure 6*.
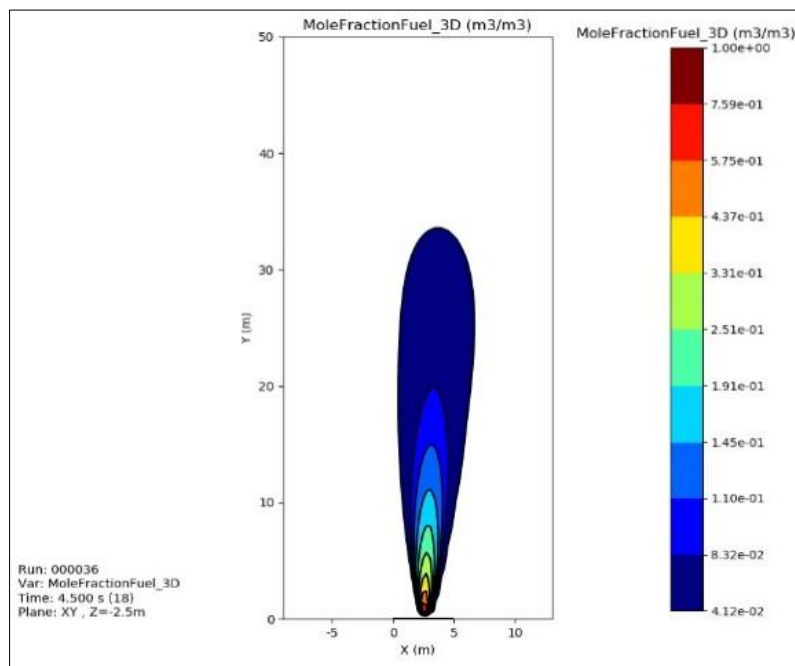

Figure 6. *Large hole, low pressure, hydrogen to methane ratio 10–90%*

At this mixing ratio, the simulation yielded a zone width of 8 metres, again much smaller than the calculated 34.32 metres. *Figure 7* shows the volumetric, isosurface and maximum value results for the scenario under study.
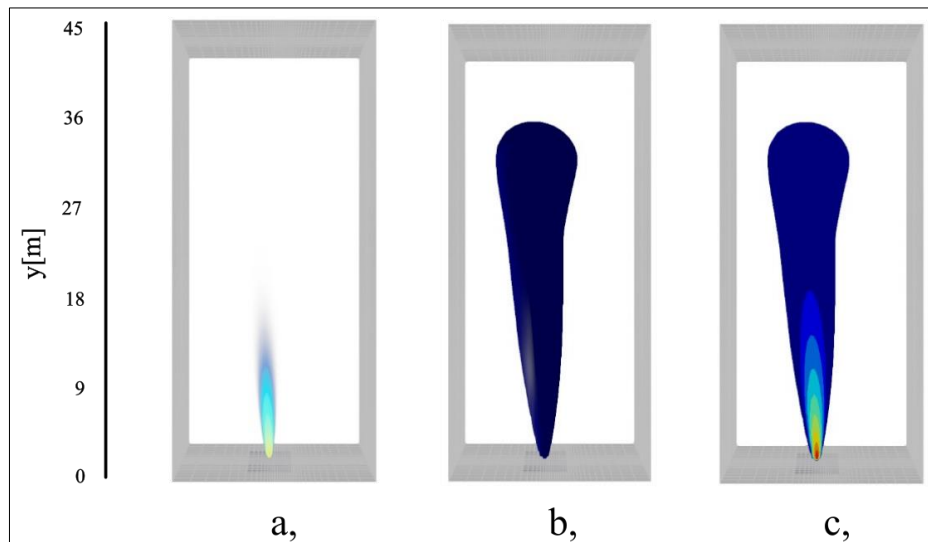
Figure 7. *a, – volumetric, b, – isosurface, c – maximum value*
(large hole, low pressure, hydrogen to methane ratio 10-90%)

When hydrogen is significantly present in the mixture, i.e. 90–10% relative to methane, the simulation gives an explosive region of the order of 35 metres, as shown in *Figure 8*.

Figure 8. *Large hole, low pressure, hydrogen to methane ratio 90–10%*

For this mixture, the simulation showed a zone extent of 35 m, which is still significantly different from the calculated 54.52 m, but the smallest difference is only 19 m. *Figure 9* shows the volumetric, isosurface and maximum value results for the scenario under study.

Figure 9. *a, – volumetric, b, – isosurface, c – maximum value*
(large hole, low pressure, hydrogen to methane ratio 90–10%)

7. Summary

From the derived relationship and the computational results of the tested mixture, it can be seen that the possible sizes of the zones between the two 100% concentrations, varying the magnitude of the concentrations, are proportional. Although the results of the simulations with FLACS-CFD give a smaller zone, but this is confirmed by our own and other research, the zone values are also proportional. As described in the introduction, none of the standards provide an approach to the extent of the potential explosive atmospheres of mixtures. According to EN IEC 60079-10-1:2020, the method can be adapted to be applicable to multiple component gases. More accurate results could be obtained, which could result in lower costs from an EHS point of view, with positive economic benefits when selecting explosion-proof products. The potential for failure is low because the standard calculation is still considered conservative.

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