

# BENCHMARK EXERCISES RELATED TO THE SAFETY ANALYSIS OF HYDROGEN/NATURAL GAS MIXTURES TRANSMISSION IN PIPELINES

E. Studer, S. Kudriakov,<sup>1</sup> S. Jallais,<sup>2</sup> V. Blanchetière,<sup>3</sup> J. Hébrard and G. Leroy<sup>4</sup>

<sup>1</sup>CEA/LTMF 91191 Gif-sur-Yvette, France [etienne.studer@cea.fr](mailto:etienne.studer@cea.fr),

<sup>2</sup>Air Liquide BP 126 78350 Jouy-en-Josas, France [simon.jallais@airliquide.com](mailto:simon.jallais@airliquide.com),

<sup>3</sup>GDF SUEZ BP 33 93211 St Denis La Plaine, France

[vincent.blanchetiere@gdfsuez.com](mailto:vincent.blanchetiere@gdfsuez.com),

<sup>4</sup>INERIS BP 2 60150 Verneuil-en-halatte, France [jerome.hebrard@ineris.fr](mailto:jerome.hebrard@ineris.fr).

## ABSTRACT

Future economy based on reduction of hydrocarbon fuels for power generation and transmission may consider hydrogen as possible energy carrier. An extensive and widespread use of hydrogen might require a pipeline network. The alternatives may be the use of the existing network of natural gas or the design of a dedicated network. Whatever the solution, introducing hydrogen in natural gas substantially modify the consequences of accidents. The French National Research Agency (ANR) funded a project called HYDROMEL which focuses on these critical questions. Within this project benchmark exercises have been chosen based on simple and well defined situations in order to share experience related to the two flammable gases and to adapt the available computer tools to the mixture behaviour. Jets, jet fires and explosions have been computed and compared to open literature results. In general, the computer codes tend to be conservative for the different phenomena relevant to safety. However, disparity due to different models can be very important especially for hydrogen. The database for mixtures is not large enough and research work is welcome in that area.

## 1 Introduction

The environmental and economic constraints currently lead different countries to find alternatives to hydrocarbon-based fuels for power generation and transmission. In this context, hydrogen is emerging as a possible new energy carrier. An extensive and widespread use of hydrogen might require a pipeline network: the first and probably the cheapest solution would be to add hydrogen to the existing natural gas network with some improvements to accommodate mixtures. The second solution is the design of a dedicated network for a hydrogen/natural gas mixture with appropriate pressure, size and materials. Whatever the chosen scenario introducing hydrogen in natural gas is likely to modify accident consequences.

The French National Research Agency (ANR) funded a project called HYDROMEL which focuses on these critical questions. The most important of them is the safety impact on gas transmission related to the addition of large hydrogen quantities to natural gas. Hence, the capabilities of the existing simulation codes to predict the behaviour of such mixture during postulated accident should also be investigated. For different consequence analyses, the partners of the project are using different types of computer codes. Most of them are based on phenomenological models while some are CFD codes. Some companies and institutions are familiar only with hydrogen behaviour while others only with natural gas behaviour. Rarely a company has an expertise in the behaviour of both gases and/or their mixture. So,

the present benchmark activity has been organised in order to share experience related to the two combustible gases and to adapt the available computer tools to the mixture behaviour. For that, three situations involved in an accidental release of hydrogen or natural gas from a pressurised pipeline network were selected: under-expanded jet in open atmosphere, ignition of this jet and pressure build-up in an industrial enclosure due to premixed combustion. For the first two scenarios the results of the open literature have been chosen to conduct comparisons on the released mass flow rate, the gas concentration profiles along the axis of the jet, the mass of flammable cloud, the overpressure in case of delayed inflammation, the visible flame length and the radiative fluxes. The latter is studied by making a code-to-code comparison on the development and consequences of premixed combustion.

The following sections include a general description of the computational tools used by the different partners. Then, the benchmark results are presented and discussed. Finally, a section is devoted to the mixture analysis. Conclusions follow.

## 2 Short description of computer tools

In the project, the tools and methods used by GDF SUEZ are included in the platform PERSEE and the FLACS CFD code ([www.gexcon.com](http://www.gexcon.com)). In the former, mass flow rate through the break and depressurisation of the pipeline network are computed by the CALDEIRA 3.0 module. Isothermal behaviour is assumed during depressurisation. Real gas equation of state is used for natural gas and hydrogen is supposed to follow perfect gas behaviour. The combustible gas cloud is computed by the Gaussian integral model developed by Ooms [1] coupled with a pseudo-source model (CATS) in case of pressurised releases. Overpressures are calculated with the model of Deshaies et al.[2] for variable flame speed. Finally, jet fire models in the RAYON module are based on the work of Chamberlain et al. [3]. PERSEE is dedicated and validated to evaluate the consequences of accidental natural gas release. Application to hydrogen and hydrogen/methane mixture is an exploratory work. The FLACS code is used for explosion inside building and overpressure estimation in the surroundings. The turbulence field is calculated with a  $k - \epsilon$  model including extra terms for generation of representative turbulence field along the walls. In far blast simulations, the Euler approximations are used where no combustion is taking place. And FCT algorithm assures optimum shock wave representation with a minimum of numerical diffusion.

In the project, Air Liquide uses mainly the PHAST software (version 6.53) developed by the company DNV ([www.dnv.com](http://www.dnv.com)). For combustible gas dispersion, the Unified Dispersion Model is applied which is a Gaussian integral model. Jet fires are simulated with the models developed by Chamberlain et al. and Johnson et al. [3, 4]. Overpressures are estimated with the TNO multi energy method. Some other phenomenological models are used to get cross-comparison of the results: ALDEA software which computes the gas dispersion based on the correlations developed by Birch et al.[5] and the jet fire model of Schefer et al.[6]. The FLACS code (hydrogen version) is used for explosion inside and outside of buildings. INERIS uses the same version of the PHAST software. Additional models are also applied such as the EXPLOJET model assuming perfect gas behaviour for mass flow rate calculations and analytical formulas for gas concentration decay (axially and radially). Overpressure are computed by an in-house method that is based on successively a constant volume explosion and an acoustic wave source.

The consequences analyses at CEA are performed by phenomenological models implemented in the CAST3M code ([www.cast3m.fr](http://www.cast3m.fr)). For under-expanded jets, a Gaussian integral model (HyDISP module) is applied based on the work of [7, 8, 9] with the pseudo source model

developed in [5, 10]. Delayed ignition of jets (HyEXPLO module) are computed with the model developed by Dorofeev [11] and jet fires (HyFLAM module) are simulated with the model of Schefer et al.[6, 12, 10]. The CFD part of CAST3M is presently used for the explosion inside a building and the depressurisation of pipelines.

### 3 Benchmark exercises

#### 3.1 General considerations and selections

The industrial case corresponds to a failure of a gas transmission pipeline, for example due to corrosion or excavation by a third party. These pipelines are usually buried or may be in an open atmosphere close to a sectioning point. So, the gas release develops as a vertical or horizontal under-expanded jet that mixes with the surrounding air. For safety considerations, the mass flow rate through the break and the size of the resulting combustible gas cloud are key questions. Then, ignition may occur instantaneously or after a certain delay leading mainly to a jet fire for the former and an explosion prior to the jet fire for the latter. Jet fires produce thermal radiative loads that determine the exclusion distances, while for explosions the criteria are based on the overpressure over the distance from the ignition or release point. Considering these simplified scenarios, it is possible to select from the open literature relevant experimental data in order to validate the different models used by the partners of the project.

After a short exercise which consists of comparison of the mass flow rate through the break, different situations related to consequences analyses have been investigated:

- combustible gas cloud formed from an under expanded jet of methane [13] and hydrogen [14],
- horizontal and vertical methane jet fires [15, 4] and vertical hydrogen jet fires [10],
- delayed ignition of an under expanded jet of hydrogen [16],
- premixed combustion inside an industrial building equipped with vents in a code-to-code comparison.

These conditions cover most of the phenomena involved in consequences analyses. Nevertheless, they only address pure gas behaviour and no mixture effect can be assessed for the moment. The EC NaturalHy project is currently dealing with hydrogen addition up to 50 % v/v in natural gas but only few results have been at present time released to the international community. This important database should be added in the near future. Other experiments mainly related to jet fires have been performed within the HYDROMEL project and some results will be given in the last section of this paper. However the database to address such question of mixture effect is not very large and additional experimental results would certainly be welcome. In all the following computations, the natural gas is supposed to be represented by pure methane.

#### 3.2 Mass flow rate through the break

When the size of the leak is small compared to the diameter of the pipe, the pressure in the latter may be regarded as constant. A common operating condition of the GDF SUEZ natural gas transmission network is about 68.7 bar and the hydrogen transmission network of Air Liquide is operated at about 100 bar. These real operating conditions have been used to compute the mass flow rate for a break size of 25 mm corresponding to a connecting

pipe diameter. The results of this simple exercise are presented in Table 1. The PHAST results (AL and INERIS) are using a calculated discharge coefficient close to 0.86 where the other models does not apply any discharge coefficient which is a conservative approach. For hydrogen, the effect of the real gas equation of state (CEA vs GDF SUEZ) is not so important due to moderate operating pressure. For methane, the effect is much more important but the 13% increase are mainly due to adjusted coefficients in the real gas equation of state related to natural gas behaviour ( $C_2$  and higher hydrocarbon content).

Table 1: Mass flow rate through a 25 mm diameter leak for real operating conditions

Network	Hydrogen				Methane			
Operating pressure (bar)	100				67.7			
Organisation	AL	GDF SUEZ	INERIS	CEA	AL	GDF SUEZ	INERIS	CEA
Mass flow rate (kg/s)	2.6	3.0	2.6	3.1	5.5	6.8	5.5	6.0

For large break size compared to the pipe diameter, it is necessary to compute the depressurisation of the pipeline network to take into account this feedback effect. Experiments [17] have been run few years ago by Shell to measure the mass flow rate from a pressurised air pipe suddenly opened at one end. The test conditions are summarised in Table 2. The

Table 2: Shell Canada Resources test 23: test conditions

Data	Test 23 (unit)
Gas	Air
Pipe internal diameter	305 (mm)
Pipe length	3438 (m)
Initial pressure	68.1 (bar)
Initial temperature	278. (K)
Pipe rugosity	107 ( $\mu\text{m}$ )
Duration of the test	180 (seconds)

mass flow rate evolution is plotted in Figure 1. For the first 20 seconds, all models provide similar results, although the results of CAST3M are over-predicting the mass flow rate. For later times, PHAST (long pipeline module) and CAST3M models tend to underestimate it. For consequences analyses mean values over one or two periods are usually considered. If a duration of 60 seconds is assumed, the mean mass flow rate is about 233 kg/s and this corresponds to the mass flow rate computed with an upstream pressure equal to about one fourth the initial one. From these two exercises regarding mass flow rate calculations one can conclude that the different models are equivalent.

### 3.3 Jet release

A hydrogen or methane jet release in the open environment will result in a flammable mixture. Knowledge of the extend of this cloud is an essential part of quantifying the risk associated with high pressure combustible gas transmission. Birch et al. [13, 5] have extensively studied the gas concentration profile resulting from a natural gas under-expanded jet. Recently, Roberts et al. [14] have conducted the same kind of experiments for hydrogen. For the former an upstream pressure of 31 bar was used associated with an exit diameter of 2.7 mm and for the latter, the pressure was 100 bar with a diameter of 3 mm. They both have run the experiments at room temperature. The resulting axial center line gas concentration results

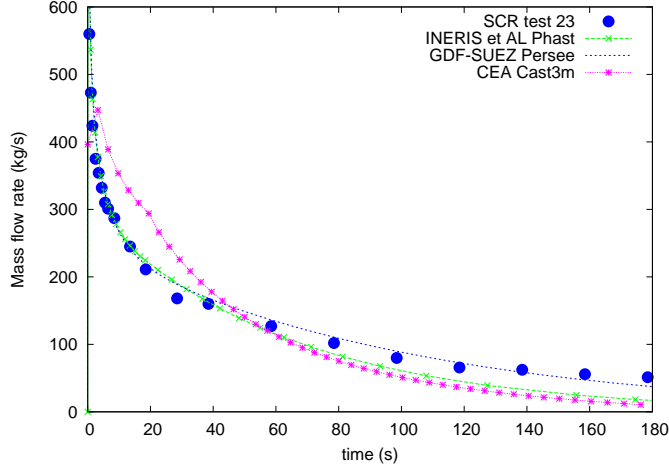


Figure 1: SCR Test 23: Air mass flow rate through the break

are plotted in Figure 2 and compared to the model predictions. The results are generally

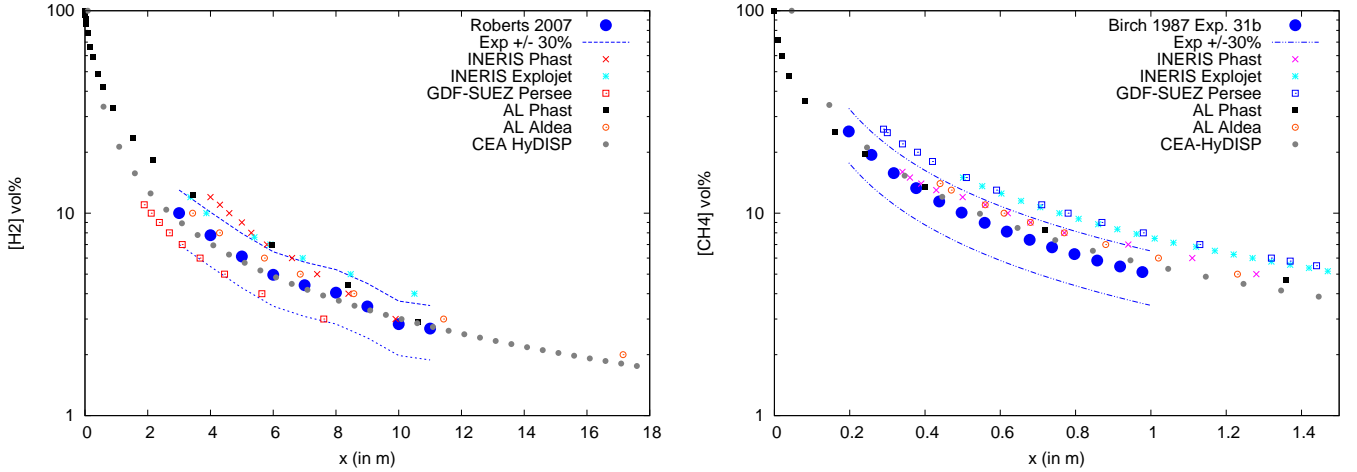


Figure 2: Gas concentration along the center line of the cloud: left - Hydrogen jet [14], right - methane jet [5]

conservative except the PERSEE and the HyDISP ones for the hydrogen case. Nevertheless, this result is within a reasonable accuracy (about 30%) for the modelling of this kind of phenomenon.

Important safety information recorded from this exercise is the distance from the jet exit where the mean concentration decays below the lower flammability limit (LFL). For hydrogen the generally accepted value for the upward propagation in air is 4 vol%. The different results for the hydrogen jet are displayed in Table 3. This distance varies between 5.6 to more than 9 meters depending on the model. Houf et al.[10] use this length scale to compare with the distance where the jet fire radiative flux is equal to  $1.5 \text{ kW/m}^2$  corresponding to exposure limit at property line in US.

Another interesting information for safety is the mass of fuel that is mixed with air within the flammable range of concentration ( $M_{EX}$ ). From this quantity, the total energy that could be released after ignition of the combustible gas cloud can be estimated and used to estimate the blast and as a consequence the damage produced by the explosion. The set of equations (1 and 2) derived by [5, 18] can be used and integrated between the upper and the

lower flammability limits to produce this “explosive” mass.

$$X_{cl} = 5.4\sqrt{\rho_{\infty}/\rho_{gas}d_{eq}}/(z - z_0) \quad (1)$$

$$X(r, z)/X_{cl,z} = \exp\left[-57\left(\frac{r}{z}\right)^2\right] \quad (2)$$

where  $X$  - mass fraction;  $r, z$  - radial and axial coordinates, m;  $\rho$  - density, kg/m<sup>3</sup>;  $d_{eq}$  - equivalent diameter, m.

The results for the hydrogen jet are given in Table 3 based on the value of 75 vol% for the upper flammability in air. This explosive mass varies by a factor of five depending on

Table 3: HSL hydrogen jet experiment: EX mass and LFL distance - P: means PHAST A: ALDEA and E: EXPLOJET

Source	$M_{EX}$ (g)	$z_{LFL}$ (m)
Experiment	-	7.79
[5, 18]	25.1	9.3
Air Liquide	30. (P) 18.8 (A)	8.7 (P) 8.7 (A)
CEA	11.1	7.07
GDF SUEZ	6.	5.64
INERIS	30. (P) 37.4 (E)	8.7 (P) 10.5 (E)

a contribution. But the associated overpressures are proportional to the cubic root of this quantity and as a result, a factor less than two is expected for the overpressure at a certain distance from the ignition point.

The same results are obtained for the methane jet except that all contributions lead to conservative values. This is the general trend for most of the models used in the present exercise.

### 3.4 Overpressure due to jet ignition

The simple explosion analysis described in the previous paragraph can be supported by a benchmark exercise regarding delayed ignition of high pressure jet release. Natural gas experiments reported by Hoff et al. [19] have shown very low overpressures. So it has been concluded that thermal radiation is the relevant parameter for exclusion distance calculation. For hydrogen gas higher flame velocities are expected and as a consequence higher overpressure levels. Unfortunately there are only few experiments dedicated to this question in the literature especially if we consider the experimental conditions with constant upstream pressure in order to have well defined boundary conditions for models. Constant pressure releases and ignitions of high momentum hydrogen jet are reported by Takeno et al.[16] and we have selected the case described in Table 4 for benchmarking the different models. The overpressures versus the distance from the released point are plotted in Figure 3 and

Table 4: Characteristic of the hydrogen jet [16]

Data	Value (unit)
Diameter of the orifice	5 (mm)
Upstream pressure	400 (bar)
Initial upstream temperature	288 (K)

integral values are given in Table 5. The spreading of the results is very wide and generally conservative. Close to the explosion point, the overpressure are mainly driven by the flame velocity computed by the different correlations. Far from the ignition point, the multi energy method with an explosion index of 4 (AL contribution) maximises the safety distance at the threshold value of 20 mbar.

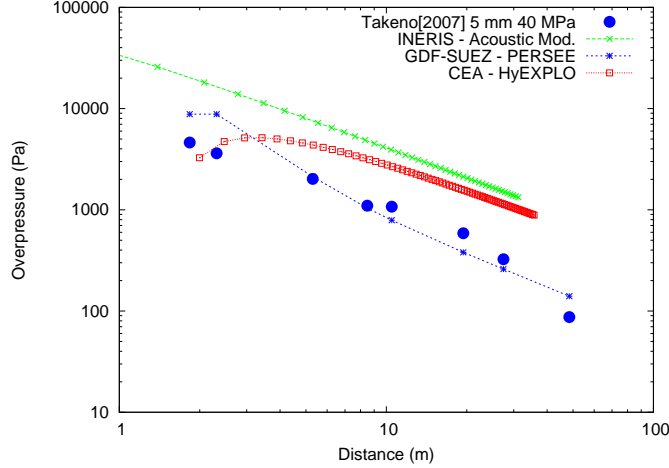


Figure 3: Overpressure versus distance from the released point for the test of [16] - 5 mm leak at 40 MPa

Table 5: Experiment of Takeno et al [16]: integral values (Air Liquide: multienergy method with explosion index of 4, CEA: correlations assuming homogeneous mixture at rest and a flame velocity equal to the maximum, GDF SUEZ: variable flame velocity model taking into account the turbulence, INERIS: acoustic module with in-house flame velocity correlation)

Source	$Q$ (kg/s)	$M_{EX}$ of $H_2$ (g)	$V_{F,max}$ (m/s)	$z(50mb)$ (m)	$z(20mb)$ (m)
Experiment	-	-	-	<1.8	5.3
Air Liquide	0.42 (A) 0.39 (P)	679. (A) 560. (P)	- -	13.0 (A) 12.2 (P)	31.8 (A) 29.8 (P)
CEA	0.47	366.	75	3.9	14.8
GDF SUEZ	0.49	360.*	429	3.	5.4
INERIS	0.42	1400.	500.	8.1	20.6

\* computed mass was 240 g and a corrected value has been taken into account for comparison

### 3.5 Jet fires

When a flammable gas is released from a container immediate ignition leads to a jet fire. Then, it is important to be able to predict the thermal radiation transferred to persons or objects outside this jet fire. As we have already said, this phenomenon is considered as the design case for determining the exclusion distances for natural gas transmission networks. Large scale natural gas jet fires have been performed by Shell in the British Gas Spadeadam test site [15, 4]. We have selected the test 1089 described in Table 6. The radiometers were located radially at about 15 meters downstream the released point. The comparison between experiment and computations is plotted in Figure 4. The computed results are very close to the experimental ones. Some models (Phast and HyFLAM) gives slightly conservative results.

Table 6: Natural gas jet fire performed by SHELL: conditions of test 1089

Data	Value (unit)
Release Height	3 (m)
Release direction	horizontal
Wind velocity	9 (m/s)
Angle wind/release	-25 (degrees)
Temperature	12.7 (Celsius)
Humidity	91 (%)
Pressure	727.3 (mm Hg)
Release diameter	20 (mm)
Upstream pressure	66.8 (bar)
Mass flow rate	3.7 (kg/s)

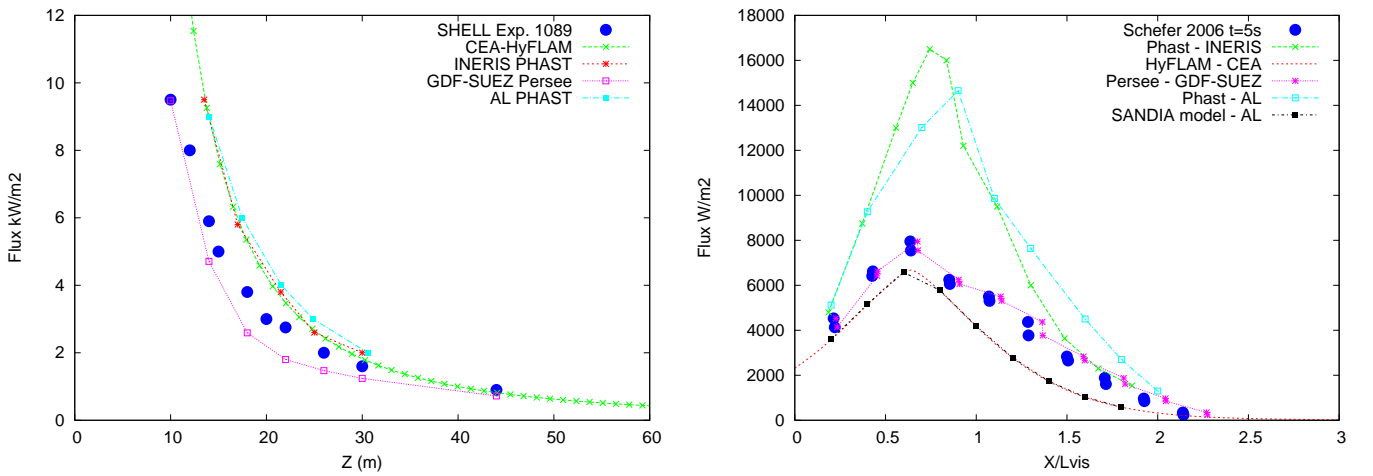


Figure 4: Jet fires : left Test SHELL 1089, thermal radiation heat flux measured radially 15 meters downstream the released point [15], right Profile of the radiative heat flux along the centerline [6] at  $t = 5$  seconds - the experimental visible flame length  $L_{vis}$  is about 4 m

For hydrogen jet fires, the available database is not so important especially for large scale experiments. Radiative properties of large scale hydrogen jet fires were recently published by Schefer et al. [6, 10]. These tests were run with high pressure cylinders of hydrogen and as a consequence the released gas led to a decreasing upstream pressure. At time 5 seconds, this upstream pressure has been reconstructed by the use of the mass flow rate given in [6]. The

Table 7: Characteristics of hydrogen jet fire performed by [10] - 5 seconds after the beginning of the release

Data	Value (unit)
Release diameter	7.94 (mm)
Estimated upstream pressure	18.4 (bar)
Mass flow rate	57.3 (g/s)

comparison for the radiative flux along the centerline between experiment and computation is given in Figure 4. The SANDIA model underestimates this flux as reported in [10], but 10% corresponds to the scatter of the data used to derived correlations for dimensionless flame length and radiant power. Phast software overestimates the peak flux by a factor of about three. These experiences are perhaps at the lower limit of validity of Phast correlations



and also not adequate for hydrogen behaviour. Publication of larger scale experiments would certainly be welcome to reinforce that conclusion.

### 3.6 Explosion in enclosure

Normally, along a gas transmission network only few buildings are present. For hydrogen, the compression stage is performed close to the production unit. In the case of natural gas, some compression unit or decompression stage are located along the gas transmission network. The latter has been selected for the present benchmark. The building depicted in Figure 5 is an industrial enclosure equipped with various openings: door, windows and two large sky domes located on the roof. Simplification of this geometry has been performed for the exercise and the inner obstacles have been removed due to the low blockage ratio, and the vents are limited to the two sky domes with an opening pressure of 60 mbar and no delay for full size venting. The latter assumption has been made to compare these tools. In a real case, it would be particularly important for hydrogen to fully take into account the kinetics of opening of the vent. Finally, this volume is filled with stoichiometric mixture of flammable gas and air and ignition is located at the center of the enclosure. Various results have been

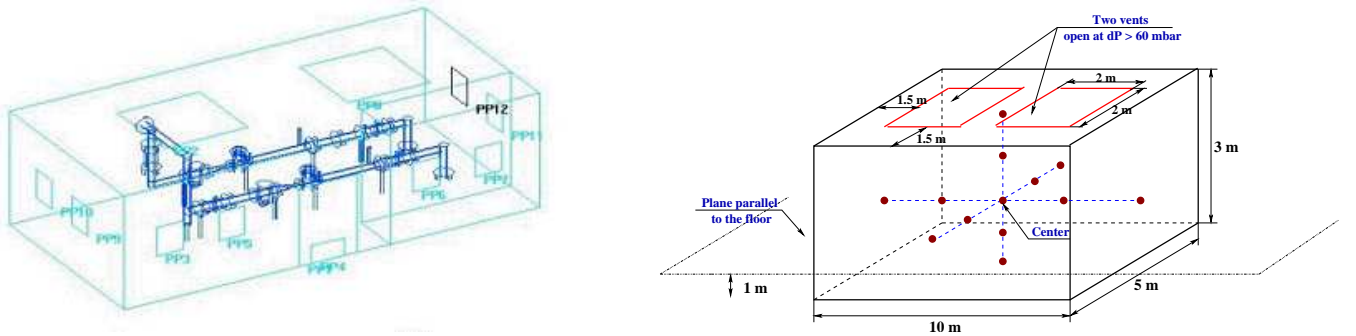


Figure 5: Decompression Building design: left - real, right - simplified

produced and compared during the exercise and only some are highlighted in this document. For example, Table 8 shows the time of opening of the sky domes ( $T_{vent}$ ) and the maximum overpressure ( $\Delta P_{max}$ ) inside the building in the different computations. The opening time of the vents are similar for each gas mixture. It occurs when only a few percent of the mixture is burned. For maximum overpressure, the results depend on flame acceleration process if we assume that the vent opens instantly. For hydrogen, the differences between models can be very large and reach a factor of 5. As against, for hydrogen due to faster flame, if the vent takes some time to open, the overpressure can be significantly increased (about 1 bar). An example of the produced CFD results is the overpressure field outside the building

Table 8: Explosion inside building: Global results

Partner	Hydrogen			Methane		
	GDF SUEZ	AL	CEA	GDF SUEZ	AL	CEA
$T_{vent}$ (ms)	60	45	35	350	-	137*
$\Delta P_{max}$ (mbar)	623	883	160	93	-	70*

\* computed with coarse grid only

at about 1 meter high (Figure 6). The isolines are very similar in the both cases and the overpressures are below the threshold value of 20 mbar used in France. Comparison with

experimental data will be welcome but the lack of reliable data is especially noticeable for hydrogen mixtures in large scale vented geometry.

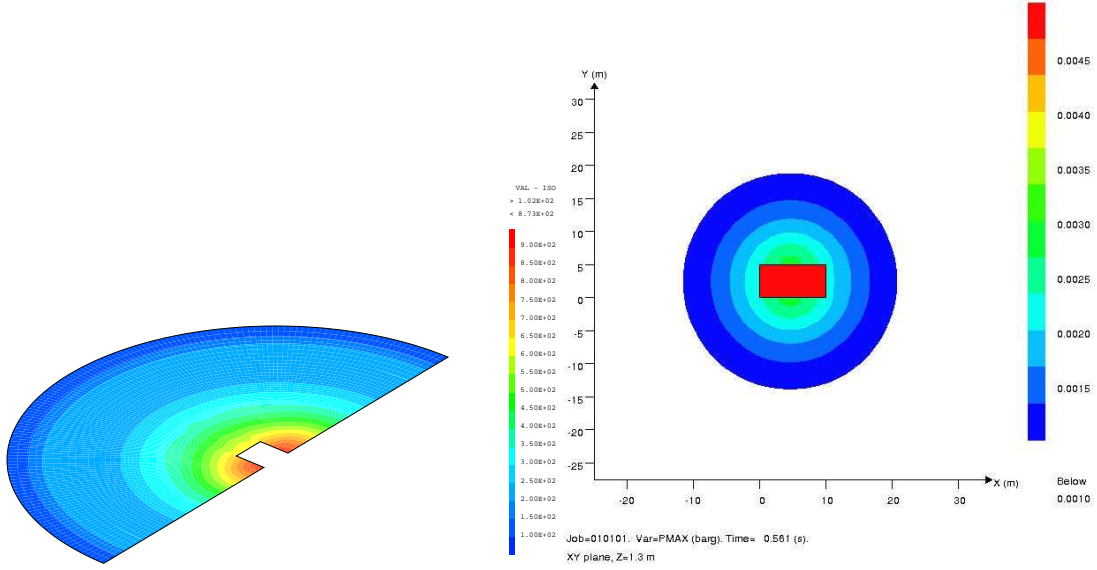


Figure 6: Maximal Overpressure in the surrounding of the building at 1 meter high: left Hydrogen CEA (red colour corresponds to 9 mbar), right Methane GDF SUEZ

## 4 Mixture effect

All previous benchmark exercises have involved pure flammable gases: methane or hydrogen. The HYDROMEL project deals with gas mixtures and in this paper we will only consider a few points related to some properties of the gaseous mixture. When a property  $\Phi_i$  for pure gases is known it is interesting from an engineering point of view to derive simple laws to obtain the equivalent property for the mixture of the two gases. Ideal mixing rules are rather simple  $\Phi_m = \sum_i^N f_i \Phi_i$  where  $f_i$  represents mass or molar fractions. Sometimes, interaction coefficients  $k_{ij}$  may be introduced to derive non-ideal mixing rules  $\Phi_m = \sum_i^N \sum_j^N f_i f_j k_{ij} \Phi_i$ . Finally, Le Châtelier type laws may also be envisaged  $1/\Phi_m = \sum_i^N f_i/\Phi_i$  for the flammability limits calculation when the molecular weight of the different species are not so different. The first studied property refers to the equation of state for a mixture of gases. If perfect gas hypothesis is used the mixing rule is very simple, while for Abel-Noble type EOS (Eq.3) the mixing rule is not so evident.

$$P = \frac{\rho RT}{1 - b\rho} \quad (3)$$

where  $P$  is the pressure,  $\rho$  the density,  $R$  a gas constant,  $T$  the temperature and  $b$  a coefficient that has no relation to the critical state and has been adjusted to follow the EOS for a certain domain of validity. Figure 7 demonstrates that for our conditions the mass fraction weighted perfect mixing rule is close to the reference data.

The second property is the radiative fraction for jet fire  $F_s$ . In the model of Chamberlain et al. [3], this fraction is an empirical function of molecular weight of the released gas  $W$  in  $g/mol$  and the velocity at the equivalent diameter  $u_{eq}$  in  $m/s$ :

$$F_s = f(W) [0.21 \exp(-0.00323 u_{eq}) + 0.11] \quad (4)$$

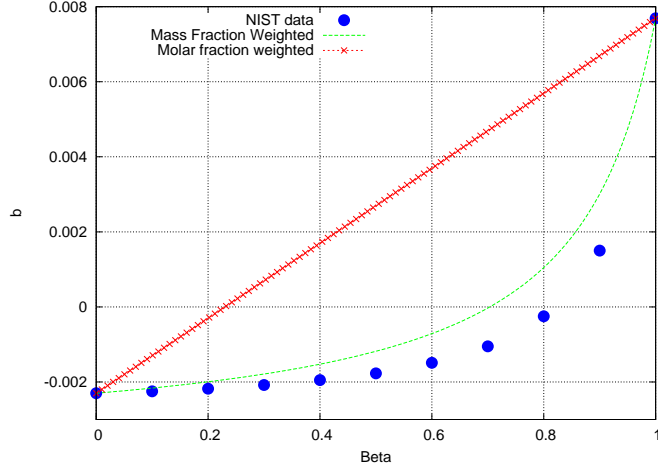


Figure 7:  $b$  coefficient of the Abel-Noble type Equation Of State for mixture of hydrogen and methane (reference data are from NIST database ([www.nist.gov](http://www.nist.gov)) at room temperature and pressure between 1 and 100 bar) and  $\beta$  represents the percentage of hydrogen in the mixture

In our cases  $f(W)$  is equal to 1 and so the mixture effect is taken into account in the velocity at the equivalent diameter. For the model of Schefer et al.[6, 12], the radiant fraction is a product of three terms: the flame residence time, the Planck mean absorption coefficient  $a_p$  and the adiabatic flame temperature. This absorption coefficient may be calculated by the use of regression laws provided by Barlow et al.[20] and equilibrium calculations or approximated by a Le Châtelier type law weighted by the mass fraction of each flammable gas as shown in Figure 8.

Finally, the fundamental flame velocity  $S_L^0$  in  $m/s$  is examined. A literature survey has shown that only few data are available for mixture of methane and hydrogen. Most of these values have been obtained for hydrogen content below 50%. Additional experiments have been performed within the HYDROMEL project by the French ICARE Laboratory using a spherical bomb. Figure 8 shows that ideal mixing rule with mass fraction seems the best fitting law for the fundamental flame velocity at stoichiometric composition.

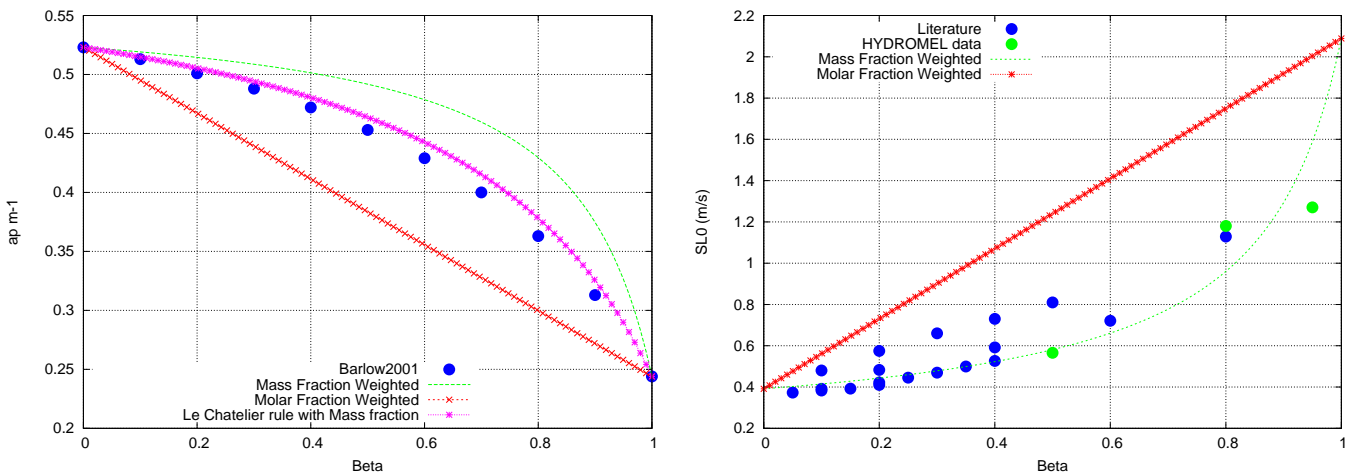


Figure 8: Left: Mean Planck absorption coefficient for a stoichiometric hydrogen/methane flame. Right: fundamental flame velocity for a stoichiometric mixture of hydrogen and methane -  $\beta$  represents the hydrogen content

Within the HYDROMEL project, some other experiments have been performed regarding

flame acceleration in a tube equipped with internal obstacles and jet fire for mixture. Verification of the above mixing rules is under progress against these experimental results.

## 5 Conclusions

Benchmark activities have been organised in order to share experience related to the two combustible gases and to adapt the available computer tools to the mixture behaviour. Mass flow rate calculations are dependent on the discharge coefficient and during depressurisation the different models are equivalent. Size and explosive mass inside the flammable cloud are generally conservative. Overpressures in case of delayed ignition of an under-expanded jet is a difficult task and only few results have been reported in the literature. Models provide large discrepancies depending on several parameters. Jet fire exercises have shown that the models are relatively conservative compared to the experimental data. The spreading of the results is higher for the hydrogen case compared to the methane one. There is a lack of experimental data regarding a large scale hydrogen jet fires and vented explosions. Some simplified mixing rules have been proposed for some properties relevant for safety such as fundamental flame velocity, radiant fraction for jet fire or Abel-Noble type equation of state. In the next future, they will be applied to validate models against experimental results obtained within the HYDROMEL project.

## Acknowledgments

This work has been supported by French Research National Agency (ANR) through Plan d'Action National sur l'Hydrogène et les piles à combustible program (project HYDROMEL n°ANR-06-PANH-001).

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