Relevance of PERSEE for the calculation of the consequences of an accidental release of a mix of natural gas and hydrogen

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In the framework of the development of Power to Gas solutions, hydrogen production and injection facilities will be built, and connected to the natural gas network. Operators of gas infrastructures have to ensure safety for employees as well as third parties in the surroundings of equipments; that is the reason why the relevance of codes to simulate the consequences of accidental releases of natural gas and hydrogen mixtures must be studied. PERSEE software has been developed by ENGIE to predict the phenomena associated with a natural gas discharge in a free environment. The impact of the adding of 6% hydrogen in natural gas, which is the maximum concentration expected in transmission networks in France, has been assessed. The predictions of PERSEE software have been confronted to experimental measurements. A slight decrease in the safety distances has been noticed on the typical accidental scenarios considered for safety studies of the French gas transmission network. Further work is still necessary to assess the influence of higher concentrations of hydrogen.

Introduction: the development of Power to Gas raises new challenges for the assessment of the consequences of an accidental gas release

Operators of gas infrastructures such as gas pipelines, gas storages, and regasification terminals have to ensure safety for employees as well as third parties in the surroundings of equipments. In order to comply with this commitment (which is a regulatory requirement in many countries), risk analysis are performed to assess the level of risk for a given installation. The general approach of these analyses is to identify hazardous scenarios and to estimate the risk by quantifying both the frequency of hazardous phenomena, the intensity of the phenomena (for example heat flux for fire and overpressure after ignition) and the vulnerability of nearby people and equipment.

The intensity of physical phenomena is calculated using physical and empirical models available in commercial software such as PHAST developed by DNV GL [1], ORDER developed by DNV GL [2], EFFECT developed by TNO [3] or in-house codes such as FRED developed by SHELL [4], or PERSEE developed by ENGIE [5]. These codes can be used to estimate safety distances in case of leakages of pressurized equipments containing flammable gases. Discharge, dispersion, fire and explosion modelling have to be validated against experimental data to ensure an acceptable level of accuracy in the consequences assessment. Given the cost of performing full scale experiments of fires and explosions, it is difficult to have validation data for each configuration encountered in the industry.

In the framework of the development of Power to Gas solutions, hydrogen production and injection facilities will be built, and connected to the natural gas network, just as biomethane facilities begin to appear. Due to safety concerns, hydrogen may only be present in small proportions in the gas transmission network subjected to safety studies. The relevance of codes aimed to the assessment of the consequences of a gas release must be studied.

Since the development of natural gas in the 1950s, ENGIE (previously GDF SUEZ and Gaz de France) has earned a reputation as a responsible company. ENGIE has, among other, contributed to major experimental and theoretical studies in the framework of safety international partnerships. This work has enabled the gas industry to enhance the knowledge and the modeling of the physical phenomena linked to high pressure natural gas releases.

Thus the Research & Technologies Division has developed many high-performance and easy-to-use tools over the past twenty years for evaluating the risks and the consequences of accidental discharges of natural gas into open fields. These different consequence calculation tools are regularly used by ENGIE and its subsidiaries for evaluating, managing and controlling accidental risks on its industrial installations. This includes drawing up safety studies, and optimizing design and maintenance costs.

Among them, the PERSEE package, developed since 1990 by ENGIE and constantly improved so far, predicts the phenomena associated with a natural gas discharge in a free environment (release flow rate, dispersion plume, thermal radiation…). PERSEE has been validated against more than 100 medium and large scale experiments to ensure the validity of its predictions. It is used as a support for the safety studies carried out on ENGIE and its subsidiaries French transmission network and installations:

- 32000 km of transmission pipelines,
- 12 natural gas underground storages,
- 3 LNG reception terminals (Montoir, Fos Tonkin and Fos Cavaou),
- 26 compressor stations.

This paper aims at studying the relevance of PERSEE to simulate the consequences of accidental releases of natural gas and hydrogen mix for proportions up to 6% of hydrogen, which is the maximum concentration expected in transmission networks in France.

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What are the impacts of adding hydrogen in natural gas?

Hydrogen properties are different from natural gas properties:

- Density (at atmospheric pressure and 0°C) is 8 times lower,
- Flammability range in air is larger : from 4 to 75% for hydrogen against 5 to 15% for natural gas,
- Flammability energy is lower,
- Laminar flame velocity is higher (up to 8 times),
- Expansion ratio is lower (ratio of density between non burned gas and burned gas),
- A higher flame stability,
- A lower calorific value (LCV) more than three times lower,
- Reverse Joule-Thomson effect,
- An adiabatic flame temperature higher of 100°C.

Impact of release conditions in case of a breach

The empirical correlations which define the flame properties in the module of PERSEE aimed at the calculation of the thermal flux uses density and velocity of the jet [7]. Adding hydrogen in natural gas is going to decrease the molar mass of the mix (decrease of 5% for an adding of 6% hydrogen). Density of gaseous hydrogen is indeed 8 times lower than density of gas natural [6]: 0.08988 kg/m^3 for hydrogen but 0.77 kg/m^3 for natural gas. This adding is going to decrease the mass flow-rate of the release but it will result in an increase of the velocity of the jet. As a consequence, turbulence will increase, which could emphasize the dilution of the mix with air, but it will also increase the overpressure generated when the ignition of the jet plume occurs. Also it could have an influence on the flame detachment.

Impact of flammability range in air

The flammability range of methane in air is 5-15% vol. whereas it is 4-75% vol. for hydrogen. Experimental measurements available in literature on Lower Flammability Limit (LFL) of natural gas and hydrogen mixes are plotted in Figure 1. Important disparities exist between values, however the adding of hydrogen in natural gas seems to have a very low impact on the LFL. The adding of hydrogen seems to show more influence on the Upper Flammability Limit (UFL) as plotted in Figure 2.

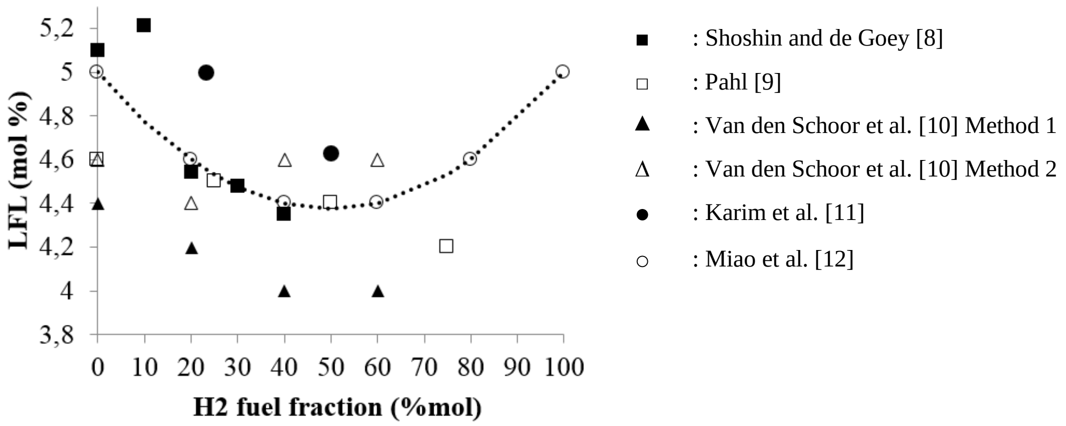

Figure 1. LFL measured on natural gas and hydrogen mixes.

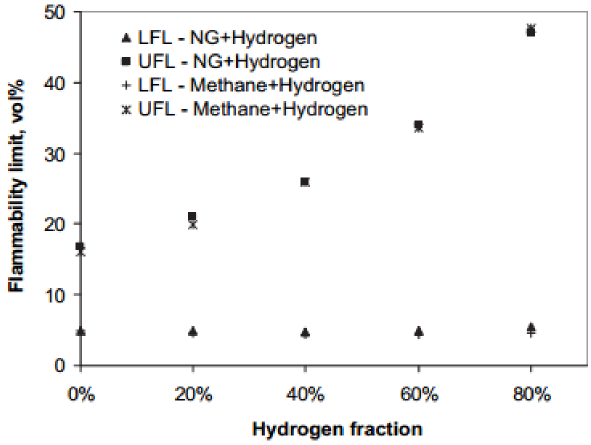

Figure 2. UFL measured experimentally by Miao et al. [12]

The simple law of "le Chatelier" allows to assess the flammability range of a mix of several gases:

$$LFL/UFL_{mix} = \frac{100}{\sum_{i=component} \frac{P_i}{LFL/UFL_i}} \tag{1}$$

For a 6%vol. ratio hydrogen in natural gas, the flammability range of the mix calculated with "Le Chatelier" is given in Table 1. These values are used in the rest of the paper to plot safety distances.

Table 1. The adding of 6%vol. hydrogen has a low impact on the LFL and UFL of the mix

Flammability range in air (standard conditions of pressure and temperature)		
	Natural gas	Natural gas + 6 %.vol hydrogen *(« Le Chatelier »)*
LFL [%.vol]	5	4.92
UFL [%.vol]	15	15.75

Impact of the laminar flame velocity and the expanding coefficient of the mix

Several studies available in the literature deal with the laminar flame velocity of a mix of natural gas (or methane) and hydrogen with different ratios. This laminar flame velocity is involved in the calculation of the velocity of the flame front V_F of the model implemented in PERSEE aimed at the prediction of the overpressure based on Bray [13].

$$V_F = 1.8\beta V_{CL}^{\ 0.784} u'^{0.412} L_t^{\ 0.196} \nu^{-0.196} \tag{2}$$

With β the expanding coefficient (ratio of densities between hot and cold gas), V_{CL} the laminar combustion velocity ($m.s^{-1}$), u' the turbulence of the jet ($m.s^{-1}$), ν cinematic viscosity ($m^2.s^{-1}$), and L_t the turbulence integral scale (m). The value of laminar flame velocity implemented in PERSEE for natural gas has been compared with values proposed by Huang [14] and Burluka [15] for different concentrations of hydrogen in natural gas. The expanding coefficient β of natural gas has also been compared to the one of pure hydrogen (Figure 3). Contrarily to the laminar combustion velocity VCL, the adding of hydrogen in the mix tends to decrease the expanding coefficient.

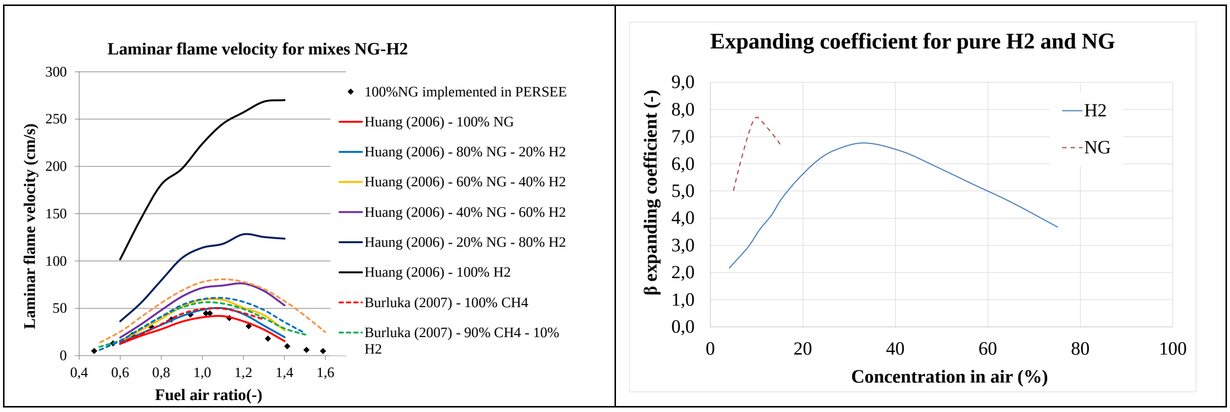

Figure 3. Left : Laminar flame velocity for mixes of natural gas and H_2. Right : expanding coefficient for pure H_2 and natural gas.

Impact on the adiabatic combustion temperature

The adding of hydrogen in the natural gas is going to slightly increase the adiabatic combustion temperature. This parameter is used in the module of PERSEE aimed at the calculation of the thermal flux, and particularly for the flame length in an atmosphere without wind through the following equations:

$$\left(\frac{D_s\gamma}{L_{b0}W}\right)^{2/3} = 0.2 + 0.024\xi(L_{b0}) \tag{3}$$

$$\gamma = \left(\frac{W_{air}T_{comb}}{W_p T_{air}}\right)^{1/2} \tag{4}$$

$$W = \frac{W_g}{(15.916W_g + 39.5)} \tag{5}$$

$$\xi(L_{b0}) = \left(\frac{g}{(D_s u_f)^2}\right)^{1/3} L_{b0} \tag{6}$$

With W_{air} and W_p the molar mass of air and of combustion products, T_{comb} the adiabatic combustion temperature, W the gas mass fraction in stoichiometric proportions, W_g the gas mass molar, ξ the Richardson number and D_s the effective diameter.

Review of the tests performed by NATURALHY project on the consequences of a natural gas and hydrogen mix release

In the framework of the European project NATURALHY, two experimental campaigns have been performed to compare the effects of a fire jet of natural gas and hydrogen mix and of pure natural gas.

Full bore rupture of a 1/6 scaled buried pipeline

Two tests of a full bore rupture of a buried pipeline at the 1/6 scale leading to the formation of a crater have been performed [16]. The first test has been done with 22% of hydrogen whereas the second was with pure natural gas (Figure 4). The main conclusions of this study are :

- The mass flow-rate is lower for the NG-H2 mix than for the pure natural gas, which is explained by the higher density of pure natural gas. The maximum flow-rate reached with the mixture is 175 kg/s whereas it is 215 kg/s with pure natural gas (Figure 5);
- The overpressure measured due to the rupture of the pipeline is about two times higher than the overpressure due to the ignition;
- The height of the fireball is the same in both cases: about 40-55 m;
- The shape of the flames and their sizes are nearly the same;
- There is no significant difference on the thermal flux measured (Figure 6).

These tests show that there is no risk increase linked to the adding of hydrogen in natural gas. Only slight gain in the distances of the thermal dose may have been observed during these tests. The presence of hydrogen decreases the mixture density, which allows a faster decrease of the pressure in the pipeline.

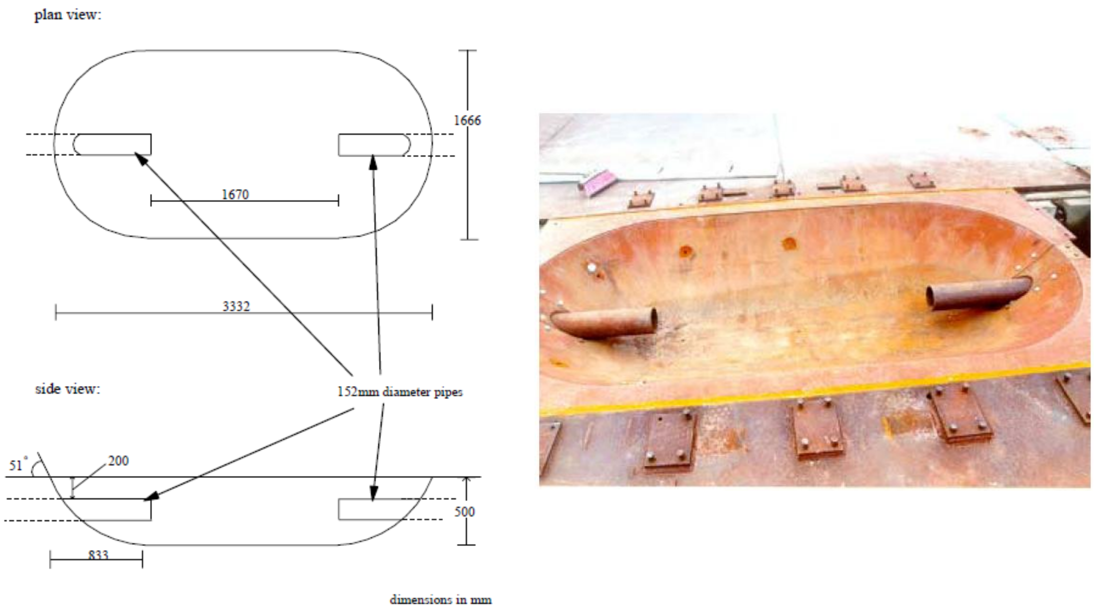

Figure 4. Experimental test configuration for the rupture of a 1/6 scale buried pipeline.

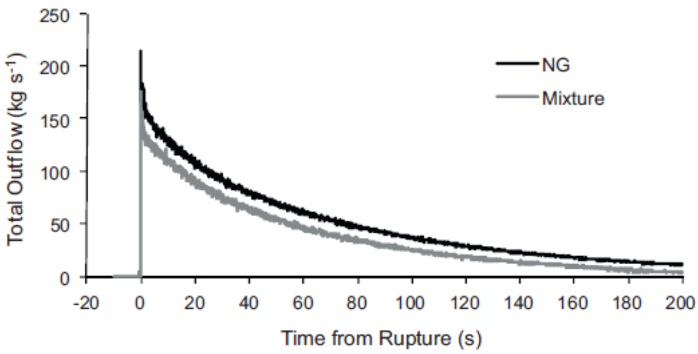

Figure 5. Comparison between mass flow-rates: the adding of hydrogen decreases the mass flow-rate.

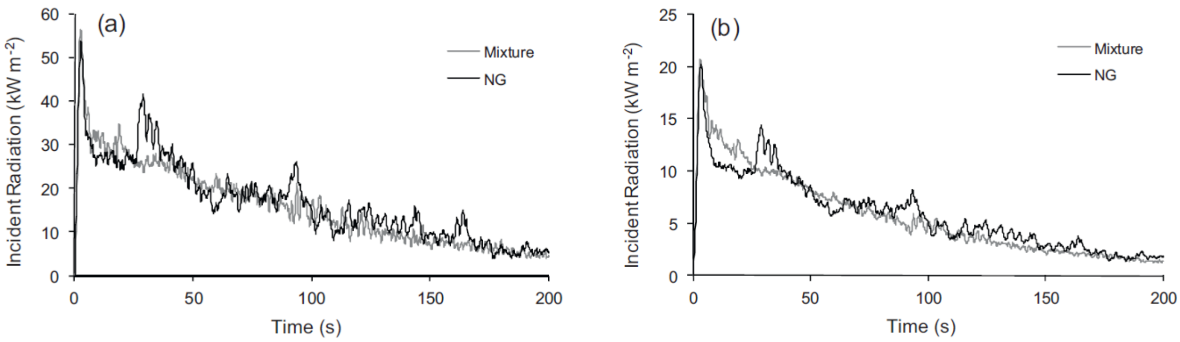

Figure 6. Comparison between the thermal flux obtained with mixture and with pure natural gas at 40 m (a) and 76 m (b).

Jet fires from a small leak at 60 bar

Another experimental campaign [17] has been performed to compare the effects of three 60 bar jet fires for three different leak size: 20, 35 and 50 mm diameter. The concentration of hydrogen in the mixture is about 24% vol. The mass flow-rates obtained on these releases vary from 3 to 20 kg/s. The main conclusions of these tests are:

- The mass flow-rates are lower for NG-H2 mixtures than for pure natural gas as noticed previously (Table 2);
- The flame length are nearly the same (Table 2) but the flame is slightly smaller for NG-H2 mixtures (but the wind velocity could have an impact on the stretch of the flame);
- There is no significant difference on the thermal flux emitted by the flame;

- A difference on the thermal flux in the flame has been noticed: the maximum flux is about 15% higher for NG-H2 mixtures and may exceed 350 kW/m^2. It may have a strong impact on the elements held in the flame.

Table 2. The adding of hydrogen in the mixtures leads to smaller flow-rates and flames (but wind velocity could have an effect in these measurements)

Leak diameter [mm]	Mass flow-rate [kg/s]			Flame length [m]			Flame separation [m]		
	NG	NG + 24%.vol H_2	Deviation	NG	NG + 24%.vol H_2	Deviation	NG	NG + 24%.vol H_2	Deviation
20	2.9	2.7	-7%	19.8	17.6	-11%	6	5.8	-3%
35	9.6	7.2	-25%	37.8	30.7	-19%	7.5	6.8	-9%
50	19.5	16.9	-13%	49.9	45.2	-9%	8.7	7.2	-17%

Properties of the NG-H2 mixture in PERSEE

The user variables which characterize the natural gas declared in PERSEE are showed in Table 3. A proposition for values with a 6% adding of hydrogen is also given. It can be noticed that the changings are not significant.

Table 3. Properties of natural gas declared as default in PERSEE, and proposition of values for a mixture with 6% hydrogen

Gas composition [%.vol]	NG (PERSEE as default)	NG + 6 %.vol H_2
Methane	91.15	85.68
Ethane	5.35	5.03
Propane	1.1	1.03
Butane	0.35	0.33
Nitrogen	1.65	1.55
Carbon dioxyde	0.4	0.38
Hydrogen	0	6
Mixture properties		
Mass molar [g/mol]	17.57	16.63
Critical pressure [bar]	49	44*
Critical temperature [K]	191	189*
c_p/c_v [-] at 15°C	1.296	1.298*
Lower Calorific Value [J/kmol]	8.39795 10^8	8.03868 10^8
Lower Calorific Value [MJ/m^3] *(ideal gas assumption : V_{mol} constant = 22,414 L/mol)*	37.6	35.8*
Specific heat c_p [J/kg/K]	2096	2200*
** value obtained with PHAST software using the value as default in PERSEE*		

Other values directly coded in the source programs must be modified to take into account the adding of hydrogen, as the combustion velocity or the expanding coefficient. If the existing expanding coefficient is conserved, it leads to conservative results for the ignition overpressure. However, the laminar flame velocity must be adapted for a mixture of natural gas and hydrogen (Table 4).

Table 4. Laminar combustion velocity implemented in PERSEE for pure Natural Gas and modified values for a mixture with 20% hydrogen.

Fuel concentration (%.vol)	Laminar Combustion Velocity V_{CL} (m/s)	
	Natural Gas	Natural Gas + 20 %.vol H_2 [15]
5.00	0.05	0.05
5.91	0.13	0.13
6.83	0.22	0.22
7.73	0.3	0.3
8.62	0.383	0.39
9.48	0.434	0.46
10.16	0.448	0.5
10.33	0.447	0.505
11.17	0.398	0.49
11.99	0.312	0.4
12.79	0.18	0.3
13.58	0.10	0.18
14.35	0.061	0.061
15.00	0.047	0.048

In the framework of the HYDROMEL project [18], a specific study has been performed by CNRS to determine the fundamental flame velocity for mixtures of methane and hydrogen. The comparison between these experimental data and mixture laws concludes that the use of a weight by mass fraction is the most relevant. As a consequence, for a mixture with 6% hydrogen, the following weight ratio must be considered : f_{NG}=0.993 and f_{H2}=0.007. The maximal laminar flame velocity of a 6% hydrogen mixture should thus not exceed 47,2 cm/s if laminar flame velocities of 45 and 350 cm/s are respectively considered for natural gas and hydrogen.

Fire jets: comparisons between PERSEE results and NATURALHY tests

Results given by PERSEE have been compared to the experimental data obtained on jet fires by the NATURALHY project described previously [17]. The exact composition of the natural gas used in the tests is not known. As a consequence, pure methane has been considered, with an adding of 24% vol hydrogen. The crosswind incident radiations have been plotted in Figure 7. Results given by PERSEE are consistent with the experimental measurements. The adding of hydrogen and the changings in the properties of the mixtures have a law influence on the predictions of PERSEE. The flame characteristics have also been compared in Table 5.

The comparison between the predictions of PERSEE and the results of the NATURALHY experiments, with and without the adding of 24% vol. hydrogen, confirms the relevance of PERSEE to model the thermal radiations of such scenarios. The low influence of hydrogen on the distances to critical incident flux does not justify to specifically modify the variables which characterize the gas for mixtures up to 6% hydrogen.

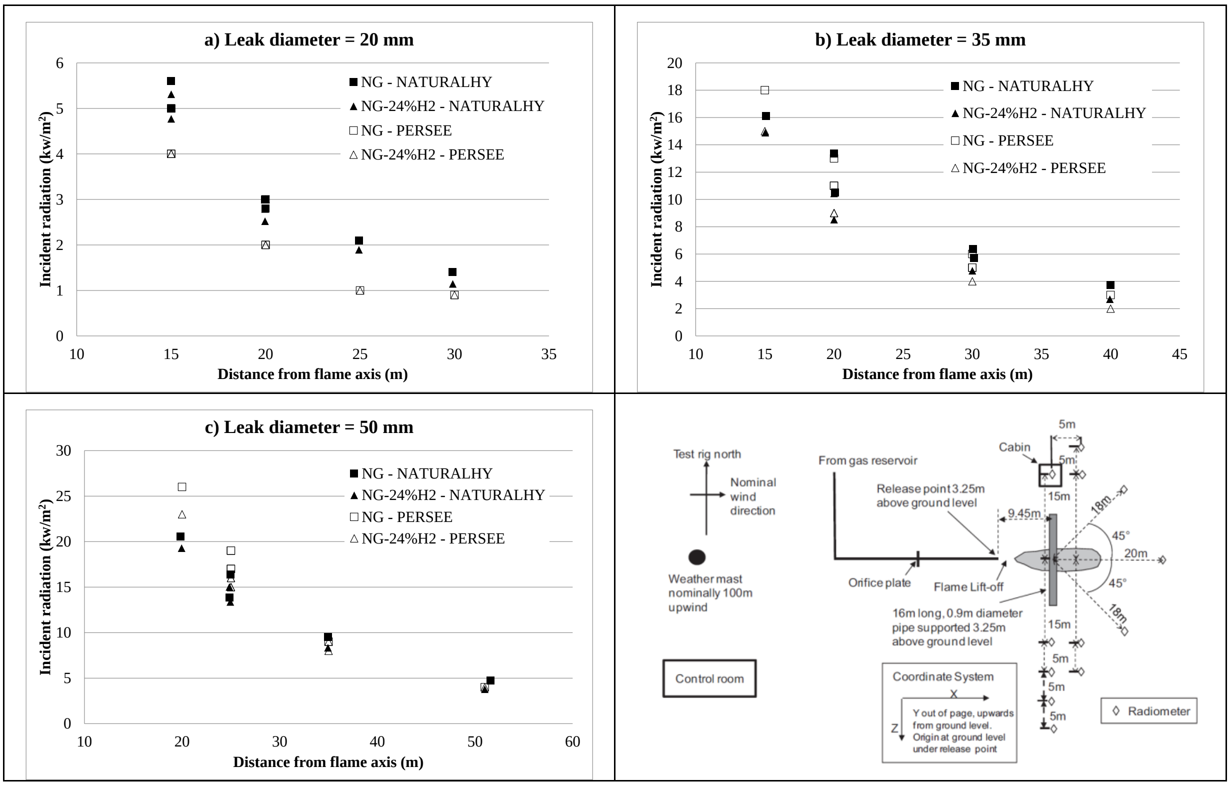

Figure 7. Comparisons between experimental results from NATURALHY [17] and PERSEE predictions of incident radiation.

Table 5. Comparisons between experimental results from NATURALHY [17] and PERSEE predictions of flame geometry.

Leak diam. [mm]	Flame length [m]						Flame separation [m]					
	NG			NG + 24%.vol H_2			NG			NG + 24%.vol H_2		
	Exp.	PERSEE	Dev.	Exp.	PERSEE	Dev.	Exp.	PERSEE	Dev.	Exp.	PERSEE	Dev.
20	19.8	18	-9%	19.8	17	-14%	6	7	17%	5.8	7	21%
35	37.8	31	-18%	37.8	28	-26%	7.5	8	7%	6.8	8	18%
50	49.9	40	-20%	49.9	38	-24%	8.7	9	3%	7.2	9	25%

Influence on the safety distances for the gas transmission network

The classical assumptions considered for the French gas transmission network in safety studies are:

- For a buried pipeline: vertical release with leak diameters of 12 mm, 70 mm and full bore rupture;
- For an above ground pipeline : horizontal release with leak diameters of 5, 12 and 25 mm.

A mixture with 6% hydrogen in natural gas has been considered. Characteristics of this gas mixture are presented in Table 3. The thermodynamic properties have been calculated using the Soave-Redlich-Kwong (SRK) model implemented in PHAST 7.11. For the calculation of the ignition overpressure, the expanding coefficient is the same as the natural gas one. This approach is conservative. Only the values of the laminar combustion velocity (Table 4) have been modified for these calculations. The adiabatic combustion temperature is kept constant at 1976.85°C. There is no specific change of this value for the mixture and the use of a mixture law only gives an increase of 2°C, which has been considered as negligible. The LFL has been fixed to 5% for pure natural gas and 4.9% for the 6% hydrogen mixture.

A pipeline of 20 km length with a diameter of 400 mm has been considered. For these accidental scenarios, the adding of 6% hydrogen in natural gas tends to decrease the safety distances predicted by PERSEE (Table 6). Models currently used in PERSEE are therefore relevant and conservative to model the hazardous phenomena following an accidental gas release with 6% hydrogen, without any changings in the models.

Table 6. Comparison between safety distances with and without 6% hydrogen for typical accidental scenarios

[H2] (%.vol)	Pressure (barg)	Leak diameter (mm)	Mass flow-rate (kg/s) at 120 s	LFL distance (m)	Max overpress. when ignition (mbar) at 1 m above ground	Distances (m)								Horizontal projection of the flame (m)
						Thermal doses* (TDU)			Incident radiation (kW/m^2) at t=120 sec					
						600	1000	1800	3	5	8	16	20	
Buried pipeline of 400 mm diameter and 20 km length – Vertical release														
0	67.7	12	1.6	2	26	4	3	2	18	14	11	7	6	4
6			1.6	2	25	4	3	2	18	14	11	7	6	4
0		70	53	11	37	35	24	14	99	76	59	38	32	13
6			52	11	33	34	23	13	96	74	57	37	31	13
0		400	339	27	51	182	142	100	242	187	146	96	82	28
6			328	28	47	177	138	97	238	184	143	94	80	27
Above ground pipeline of 400 mm diameter and 20 km length – Horizontal release														
0	67.7	5	0.28	4	58	-	-	-	6	5	-	-	-	6
6			0.27	4	54	-	-	-	6	5	-	-	-	6
0		12	1.6	10	80	-	-	-	18	15	13	10	9	13
6			1.6	10	77	-	-	-	18	15	13	10	9	13
0		25	7	38	105	24	22	20	45	37	32	27	26	25
6			7	37	100	23	21	19	44	37	32	27	26	25

** thermal doses calculated with the assumption of a reactive time of 3 s, then move with a velocity of 2.5 m/s*

Conclusion: safety distances slightly lower with 6% vol. hydrogen

Taking into account the presence of 6% hydrogen in natural gas does not increase the safety distances calculated by PERSEE A slight decrease in these distances has even been noticed on the typical accidental scenarios considered for safety studies of the French gas transmission network.

For higher concentrations of hydrogen, further work is necessary to assess the influence on the flammability range, combustion velocity, expanding coefficient, etc. that could modify the empirical correlations used in PERSEE. Work is also necessary to assess the stability of a flame with hydrogen. Indeed, if some configurations with pure natural gas lead to unstable flames, it could be different with high concentrations of hydrogen, particularly due to the minimal ignition energy which is much lower for hydrogen.

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