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Abstract

The methods implemented by EDF-SEPTEN (Electricité de France – Department of Thermic and Nuclear Studies and Project) of Basic Nuclear Installations (BNI) in Nuclear Electricity Power Stations (NEPS) requires the implementation of pressurized hydrogen.

Within the scope of a study on safety, hypothetical leaks are investigated, leading to the formation of explosive atmosphere (ATEX); the intention here is to evaluate their dangerousness.

The present publication deals with the establishment of a simplified model in order to determine the x_{LEL} [distance on the axis of the leak jet, where a concentration is reached equal to the Lower Explosive Limit (LEL)] and V_{ATEX} (volume of the locus of the spatial points where the concentration is greater than or equal to LEL) parameters for typical H_2-N_2 mixture leaks.

Key-words: ATEX, EXPLOJET software, Explosion, H_2, LEL, PHAST software, V_{ATEX}, x_{LEL}.

1. Introduction

EDF-SEPTEN is confronted with the problem of assessing the risks of ATEX formation during exploitation of various networks of ducts, which convey a pressurized gas (pure hydrogen or hydrogen-nitrogen mixture with known composition) and which are set up in ventilated locals with various volumes of a few hundred cubic meters. Within the scope of studies on safety considering major aggressions (e.g.: earthquake), major leaks of the guillotine rupture type are taken as a hypothesis on these networks, with the goal of controlling their consequences [1].

Under the assumption of loss of the seal of a member of the network, the gas contained in the network would be discharged into the locals through a leak orifice and would mix with air in order to form an ATEX [2], at least in the proximity of this orifice.

EDF-SEPTEN requested INERIS to evaluate the volume of ATEX which would be formed inside these locals [3], [4].

Our study is an integral part of a request from the French Nuclear Safety Authority (NSA) which dealt with various cases of hydrogen leaks, supposed to occur in certain locals and originating from various pressurized ducts, bringing into play pure hydrogen or H_2-N_2 mixtures with a defined H_2 content, C_{H2-N2} (vol. %), in order to evaluate the ATEX volume (V_{ATEX}) and the distance to the LEL (x_{LEL}).

In this study, a simplified model may be established in order to determine for defined H_2-N_2 mixture leaks, the following quantities which characterize the dimensions of the ATEX resulting from the leak :

- the distance to the LEL, x_{LEL} (m),
- the volume of formed ATEX, V_{ATEX} (m^3),

from the following parameters defining a leak :

- the data relating to the leaking duct:
  - its nominal diameter, D (m),
  - its outer diameter, D_{ext} (m),
  - its thickness, e (mm),
- the data relating to the leak orifice supposed to be circular :
  - the diameter of the leak orifice d (m); under the assumption of a guillotine rupture of this duct, d is related to D_{ext} and to e by the relationship $d = (D_{ext} - 2e)$.
  - the diameter of the leak orifice, d (m); under the assumption of a half-guillotine rupture of this duct, d is related to D_{ext} and to e by the relationship $d = (D_{ext} - 2e)/\sqrt{2}$.
- the H_2 concentration of the H_2-N_2 mixture, C_{H2-N2} (%),
- the absolute pressure in the duct, P (absolute bars).

2. Methodology used

2.1 Phenomenology of gas leaks

During a leak on a pressurized network, the compressed gas will mix with ambient air through a most often turbulent jet. The conditions under which the discharged gas and air mix depend on many parameters.

However, if the leak occurs in free air and while it is delivering, it is possible to state that :

- it is always pure gas which is present in the plane of the leak orifice,
- on the contrary, there always exists an area of the space sufficiently away from the leak orifice where the air concentration of discharged gas remains very low or even zero.

The leak therefore generates a concentration field. For this reason and under the assumption that the discharged gas is flammable, there always exists an area of the space where the gas concentration in the air belongs to the explosivity domain and where the air-gas mixture therefore forms an ATEX. Beyond this area, there no longer exists any possibility of ATEX.

If, on the contrary, the leak occurs in a confined medium (for example in locals), a concentration field also appears within the locals by accumulation. Its development over time, as well as the possible increase in the formed ATEX volume depend :

- on the volume of the locals as compared with the gas volume (a priori limited) which is able to be discharged through the leak orifice,
- on the air renewal rate of the locals, regardless of whether it is equipped with mechanical or natural ventilation.

Thus, under the assumption of a hydrogen-nitrogen mixture leak in locals, the problem is therefore not of knowing whether an ATEX will be formed, but rather of knowing whether the volume of this ATEX will be such that its explosion would cause significant damages.

An explosive atmosphere of more than ten liters present in a constant amount in closed locals is always considered as dangerous independently of the dimensions of the locals [5]. It is possible to proceed with an approximate evaluation by applying the empirical rule according to which explosive atmospheres present in closed locals are dangerous when the amounts are greater than one ten thousandth (1/10 000) of its volume. However this does not mean that the whole space should be described as a dangerous location; only the portion of the locals where a dangerous atmosphere is likely to form should be considered as a dangerous location.

Under the assumption of sufficiently ventilated locals where accumulation remains low, the evaluation of the risks of explosion related to the formed ATEX in the case of a leak is therefore directly related to that of the maximum volume of formed ATEX on the jet.

2.2 Approach for evaluating the formed ATEX volume: identification of the influent parameters

In order to evaluate the maximum volume of formed ATEX, all the parameters which have an influence on this volume should be identified first.

2.2.1 Parameters related to the leak conditions

Among the parameters which have a determining influence on the maximum volume of formed ATEX, the conditions of the leak are first found, and in particular the leak flow rate, representative of the rate with which the gas will be discharged into the locals.

For a given gas, the leak flow rate itself only depends on the following parameters :

- the section of the leak orifice,
- the orifice coefficient,
- the internal pressure of the network.

- **Assumption on the section of the leak orifice**

The leak rate first depends on the section of the leak orifice: considering that the question is to evaluate the risks of explosion of an ATEX following a safety approach, EDF-SEPTEN has defined the section of the leak orifice as the one which corresponds to the guillotine rupture of the duct installed in the locals.

Let us note that, for nominal diameters of more than 50 mm, EDF-SEPTEN considers under certain assumptions leak diameters equal to the nominal diameter divided by $\sqrt{2}$, which amounts to stating that the leak section is half of the one which corresponds to the nominal diameter.

In certain locals, it is not only a duct which is installed, but also the capacity which is connected to this duct ; as each capacity is equipped with a manhole, EDF-SEPTEN has contemplated the guillotine rupture of tapping of the manhole and the consecutive discharge of the gas through the totality of the section of the manhole. This is why the diameter of the tapping of the manhole, the thickness of the metal sheet of this tapping and the diameter of the leak orifice appear for these leak conditions.

- **Influence of the network pressure on the leak rate**

For a leak orifice with a given section, the leak rate depends on the value of the pressure of the network relatively to the critical pressure which has the value of 1.89 bars absolute :

- if the pressure of the network is greater than the critical pressure, the leak occurs under supercritical flow conditions,
- if the pressure of the network is less than the critical pressure, the leak occurs under subsonic flow conditions.

INERIS has several leak calculation models for characterizing explosive atmosphere. Taking into account the leak conditions retained in the scenarios considered here, INERIS has envisioned to perform calculations with the computational code of INERIS EXPLOJET 4.0 [6] derived from fluid mechanics and the commercial software package PHAST in its version 6.4 [7].

- ***Case of supercritical flow***

In order to deal with the cases corresponding to supercritical flow, we used the EXPLOJET software package [6] which was developed by INERIS during the nineties, with which supercritical gas jets with densities different from that of air may be simulated.

Developed within the scope of European experimental projects and compared with tests, it is more particularly suitable for simulating supercritical jets. The output data (concentration, rate, flammable mass, distance to LEL) are defined by the dynamics of the jet.

With this software, air overpressures likely to be generated consecutively to the inflammation of free jets of flammable gases may be calculated (pseudo-similarity theory applicable to turbulent jets with variable density).

In its version 4.0, this code consists of three computational modules which allow :

- calculation of the concentration, rate and turbulence fields prevailing in the formed explosible atmosphere (based on the applications of similarity laws, the existence of which has been proved in certain cases during experiments conducted by INERIS),
- calculation of the flame velocities likely to be observed, as a function of the position of the inflammation point (a module designed to be applied to the case of supersonic jets with variable density, however, its design is such that this module may also be applied to the case of subsonic jets with variable density),
- calculation of the air overpressure field generated by the propagation of flames [8], essentially, it should be recalled that this is not strictly applicable if the flame velocities exceed 250 m/s.

Assuming that the gas is discharged in the form of a free leak jet and without any obstacle, and also supposing that the jet is stationary, i.e. fed under the initial pressure of the network, assumed to be constant, with EXPLOJET, it is possible to calculate the following quantities :

- the volume flow rate of the discharged gas (in Nm^3/h),
- the distance from the point of the axis of the jet where the discharged gas content exactly reaches the LEL, (x_{LEL} (m)),
- the volume of the formed ATEX, V_{ATEX} (m^3),
- the mass of hydrogen contained in the formed ATEX (m_{H2} (kg)).

In order to reach these results, the EXPLOJET software mainly needs the following data :

- Data relating to the ambient air :
- its temperature,
- the atmospheric pressure.

- Data relating to the discharge gas :
  - its pressure in the network,
  - the kinematics viscosity and the γ ratio of the specific heats,
  - its temperature,
  - its LEL in air.
- Data relating to the leak orifice supposed to be circular :
  - its diameter,
  - the orifice coefficient C_D (for all the cases, the assumption of a guillotine duct rupture has led us to consider a single value equal to 0.77). Generally, the influence of the shape of the orifice in a capacity is expressed by a discharge coefficient ($0 < C_D < 1$). In order to provide assistance in determining the value of the discharge coefficient C_D, an INERIS report [9] specifies values of C_D, depending on the shape of the orifice for turbulent flows of homogeneous fluids (either totally liquid or totally gaseous).

The assumption of a stationary jet is of course not verified in the investigated cases here and it amounts to increasing the maximum volume of the ATEX likely to be formed; indeed the diameters of the leak orifices are often large and would allow rapid decrease of the network pressure, so that the maximum volume of the formed ATEX would necessarily be less than the volume calculated by EXPLOJET.

Further, in order to express the final result, in reality, the maximum amount of H_2-N_2 mixture likely to be contained in the formed ATEX should be taken into account. Of course, we must ensured that the volume provided by EXPLOJET does not exceed the amount of H_2-N_2 mixture initially contained in the network.

- ***Case of subsonic flow***

In order to deal with the cases corresponding to subsonic flow, we used the software package PHAST [7] version 6.4 developed by DNV Software. The versions 6.0 and 6.1 of the software package were subject to full evaluation by INERIS, the version 6.4 being placed in the continuity of the evaluated versions.

The PHAST software is based on the UDM (Unified Dispersion Model) method which combines models of jets, of dispersion of dense or lightweight gases and of passive dispersion. PHAST in particular allows simulation of gas jets, with variable density in their inertial phase and beyond in the entrainment phase in which inertial forces are dominated by atmospheric dispersion and gravity forces.

The complexity of this type of software is intermediate between Gaussian type dispersion calculations and three-dimensional software packages proceeding with finite volumes or elements.

The version 6.1 of the PHAST software was the subject of an evaluation of its capability of determining the consequences of accidents according to a strict methodology. An evaluation report has been established [10] and is available on the INERIS internet site (http://www.ineris.fr).

Like EXPLOJET, this software leads to the mass leakage flow rate and to the distance to the LEL on the axis of the jet, but it does not allow direct access to the volume of the ATEX or to the hydrogen mass contained in the ATEX.

It essentially requires the same data as EXPLOJET; let us note however that it has several limitations as to the amounts of discharged gas; moreover, it is basically reserved for calculations of atmospheric dispersion of gases, i.e. outdoors (in particular, stability characteristics of the atmosphere and wind speed are required), and dispersion in confined locals is treated with significant uncertainty. To be more specific, in order to limit this uncertainty, the software should be used with the maximum stability index of the atmosphere.

2.2.2 Parameters related to the amount of discharged hydrogen-nitrogen mixture

The maximum volume of ATEX which would be formed in the case of a leak, first depends on the total amount of H_2-N_2 mixture (insofar that it is limited) which is contained in the network and which is therefore capable of being discharged into the locals through the leak orifice; this amount itself depends on the following parameters :

- the proportion of H_2 in the H_2-N_2 mixture contained in the network, as well as the explosivity limits in the air of this mixture,
- the internal volume of the network,
- the pressure of the H_2-N_2 mixture contained in the network.

- ***Flammability characteristics and H_2 content of the H_2-N_2 mixture contained in the network***

In the case when the gas of the network is not pure hydrogen, this is a hydrogen-nitrogen mixture, the hydrogen volume content of which is comprised between 3.2 and 43.1 %.

For having a hydrogen-nitrogen mixture form an ATEX in the presence of air, it is required that the content in the hydrogen-nitrogen mixture belong to the explosivity domain of this mixture, comprised between the lower and upper explosivity limits [LEL and UEL (Upper Explosive limit) respectively] :

- in the case of a mixture without any nitrogen (pure hydrogen case), the LEL of hydrogen is equal to 4 %,
- in the case of ternary air-hydrogen-nitrogen mixtures, the LEL of each mixture may be obtained from a ternary diagram such as the one in the following Fig. 1.

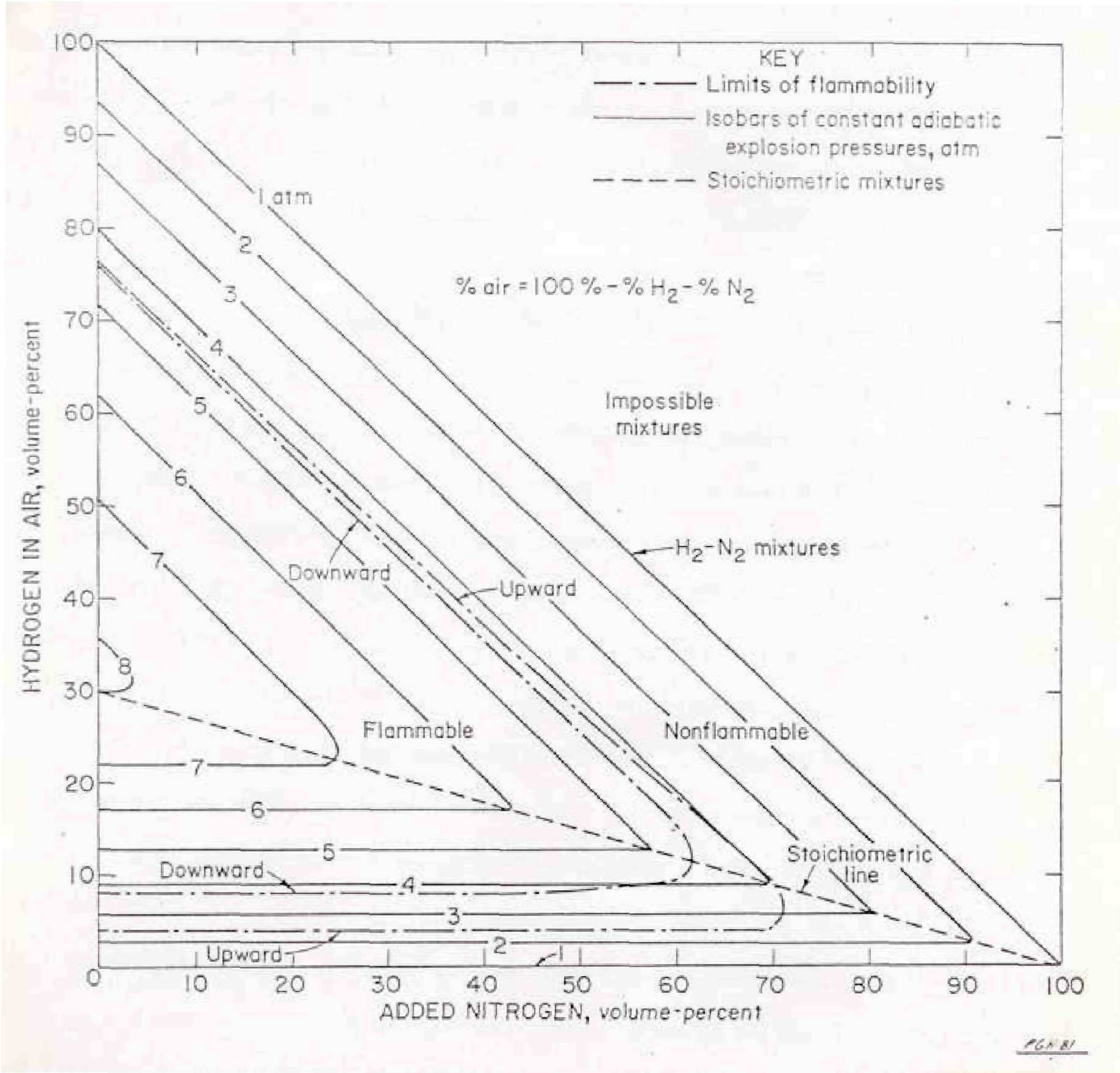

Fig. 1 : Ternary hydrogen-nitrogen-air diagram

Source : Flammability limits and pressure development in H_2-air mixtures, PRC Report No. 4305, M. Hertzberg, US Bureau of Mines, 1981.

The result of this diagram is that a hydrogen-nitrogen mixture, for which the hydrogen content is less than or equal to 5.2 % by Vol. is not flammable in air at ambient pressure and temperature and therefore cannot form any ATEX.

Table 1 hereafter indicates the LEL value of the other hydrogen-nitrogen mixtures considered here.

Hydrogen content of the H_2-N_2 mixture (% vol.)	LEL (% vol.)
43.1	9.3
42.6	9.3
23.5	16.4
18.8	20.0

Table 1: Values of LEL for the applied hydrogen-nitrogen mixtures

The curve of Fig. 2 allows determination of the value of the LEL of an H_2-N_2 mixture depending on its H_2 content $C_{H2\text{-}N2}$.

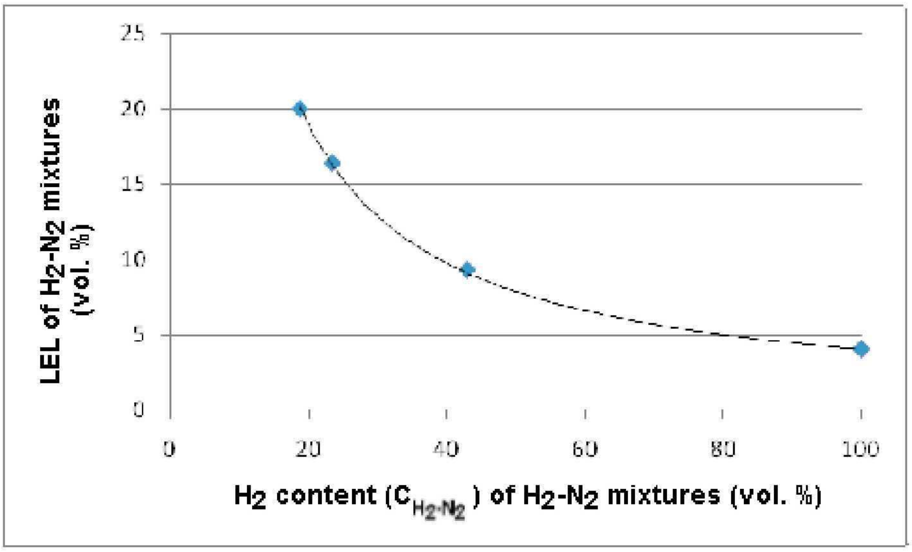

Fig. 2 : LEL variation of H_2-N_2 mixtures versus their H_2 content $C_{H2\text{-}N2}$

- ***Internal volume of the networks***

Each network consists of several duct sections defined by their inner diameter and their length, and the internal volume of which may be calculated; however this volume is always much smaller than the internal volume of the capacity(ies) to which the relevant networks here are connected, so that the internal volume of the network may be considered as equal to the sole volume of this or these capacities.

The value of the internal volume of the networks considered here (inclusive capacity(ies)) is comprised between 1 m^3 and 60 m^3. The networks connected to the compressed gas supply frames are generally assumed to have infinite capacity (permanent operating conditions) in the case of the absence of any cut-off system.

- ***Internal pressure of the gas of the networks***

In the present report, all the internal pressure values are expressed in bars absolute. For a few locals, this pressure has a value of 155 bars absolute; for the whole of the other locals, it is comprised between 1.3 and 7 bars absolute.

- ***Calculation of the maximum amount of discharged hydrogen***

The amount of H_2-N_2 mixture which would be discharged may be calculated by performing the product of the 2 following parameters :

- the volume of the capacity connected to the faulty member of the network,
- the relative gas pressure in this network,

As for the amount of hydrogen contained in the network, it may be obtained by multiplying the amount of H_2-N_2 mixture contained in the network by the proportion of H_2 in this mixture.

- ***Parameters related to the ventilation conditions of the locals***

In the case of leakage on a network, it is conceivable that the maximum volume of the formed ATEX as well as the period during which this ATEX would persist, depend on the relative extent of the ventilation flow rate of the locals (i.e. the rate with which the atmosphere of the locals is renewed with fresh air) with respect to the leak rate (i.e. relatively to the rate with which the air of the locals is loaded with hydrogen).

3. Results and interpretation

We indicated earlier that the case of leaks under supercritical flow conditions which correspond to P > 1.9 bars absolute, and the case of leaks under subsonic flow conditions, which correspond to $P \leq 1.9$ bars absolute, should be considered separately.

3.1 Case of leaks under supercritical flow conditions

Establishing the simplified model consisted of clarifying the functions which each relate the following quantities :

- x_{LEL},
- V_{ATEX},

as a function of the following parameters :

- P,
- d,
- C_{H2-N2}.

In order to specify the quantities x_{LEL} and V_{ATEX}, with the EXPLOJET model, we calculated the values of each quantity for various pairs of d and P values.

For each pair, we imposed fictitious values of the LEL of hydrogen, which amounts to studying the influence of the H_2 content of the H_2-N_2 mixtures, designated as C_{H2-N2}.

The values of the LEL of the H_2-N_2 mixture versus their H_2 content (C_{H2-N2}) are grouped in Table 1 and shown in Fig. 2.

Let us add that in order to take into account the assumption of a guillotine rupture of the duct, the orifice coefficient C_d was taken in every case to be equal to the value proposed by the PHAST model, i.e. 0.77, as well as for the calculations performed with EXPLOJET.

The calculations led to the following relationships :

$$x_{LEL} = P^{0.5} \times d \times C^{1.3}{}_{H2-N2} \quad (1)$$

and

$$V_{ATEX} = P^{1.5} \times d^3 \times C^{2.68}{}_{H2-N2} \quad (2)$$

wherein the quantities and parameters have the definitions and units as indicated above.

As regards the leaks under supercritical flow conditions, the relationships (1) and (2) show :

- the exponent 0.5 in how the quantity x_{LEL} varies with P,
- the exponent 1 in how the quantity x_{LEL} varies with d,
- the exponent 1.5 in how the quantity V_{ATEX} varies with P,
- the exponent 3 in how the quantity V_{ATEX} varies with d.

These correlations were established in the domain of validity of EXPLOJET and are therefore reliable.

As regards how the quantities x_{LEL} and V_{ATEX} vary with C_{H2-N2}, the values of the exponents [1.3 for relationship (1) and 2.68 for relationship (2)] are approximate values.

3.2 Case of leaks under subsonic flow conditions

As in the case of leaks under supercritical flow conditions, establishing the simplified model consisted of specifying the functions which relate x_{LEL} and V_{ATEX} to P, d and C_{H2-N2}.

But this time, we calculated the values of the first two quantities for different pairs of d and P values with the PHAST model.

In order to study the influence of the H_2 content of H_2-N_2 mixtures (C_{H2-N2}), we again imposed here fictitious LEL values for hydrogen, by using the values of Table 1 and as shown in Fig. 2.

The calculations led to the following relationships :

$$x_{LEL} = P^{0.38} \times d \times C_{H2-N2} \qquad (3)$$

and

$$V_{ATEX} = 0.004 \times x^3{}_{LEL} = 0.004 \times P^{1.14} \times d^3 \times C^3{}_{H2-N2} \qquad (4)$$

wherein the quantities and parameters have the definitions and units as indicated above.

As regards the leaks under subsonic flow conditions, the relationship (3) shows :

- the exponent 0.38 in how the quantity x_{LEL} varies with P,
- the exponent 1 in how the quantity x_{LEL} varies with d,
- the exponent 1 in how the quantity V_{ATEX} varies with C_{H2-N2}.

Unlike the EXPLOJET model which directly provides the volume of the ATEX by integrating the function (integral of (c(x, y, z)dxdydz), the PHAST model only considers the extension of the ATEX on the axis of the jet, i.e. $x_{LEL.}$

Consequently, the volume of the ATEX is calculated in a relatively inaccurate way by assimilating it to that of an ellipsoid for which the major axis and the minor axis are estimated from the value of x_{LEL}. This is why the relationship (4) shows that the quantity V_{ATEX} varies as to the power 3 of x_{LEL}.

4. Conclusion

The INERIS study for EDF-SEPTEN basically consisted of establishing a simplified computational model for determining the parameters V_{ATEX} and x_{LEL}, for defined H_2-N_2 mixture leaks.

From the moment that a flammable H_2-N_2 mixture is discharged into the air of locals, through a leak orifice, it is established that :

- an ATEX is always present at the leak orifice,
- the volume of this ATEX depends on the section of the leak orifice and on the network pressure upstream from the leak,
- depending on whether this pressure is greater or less than the critical pressure, i.e. a little less than 2 bars absolute, the leak will occur under the conditions of a respectively supercritical or subsonic jet,
- regardless of the flow conditions, the leak is characterized by its flow rate,
- depending on the values of this flow rate and of the ventilation flow rate of the locals, an ATEX may form in the locals and may accumulate there, further away from the leak orifice,
- the dangerousness of each of the ATEX which form in the locals is all the more significant since their volume is greater.

Let us add that as the present evaluation is conducted within the scope of a safety step, the dangerousness of an ATEX is appreciated with regard to the effects which its explosion would produce on sensitive pieces of equipment. The tolerance on this account is greater than in terms of protecting workers for example.

In the case of a leak under supercritical flow conditions, the formed volume of ATEX at the leak orifice may be calculated by means of the EXPLOJET software developed by INERIS, assuming the jet to be stationary, free and without any obstacle, which amounts to obtaining an upper bound value of the actual volume.

In the case of a leak under subsonic flow conditions, we evaluated the volume of the ATEX formed at the leak orifice by using the PHAST software but the obtained results are marred with significant uncertainty, because above all this is an atmospheric dispersion software which we therefore used at the limits of its capabilities.

Finally, we compared the results obtained with those resulting from the application of the homogeneous approach, a method which consists of :

- assuming that the discharged H_2-N_2 mixture homogeneously mixes with the atmosphere of the locals,
- comparing the content of this mixture with its LEL,
- deducing the possibility of formation of a dangerous ATEX in the locals.

In the case of freely developing jets, the evaluation of the ATEX volumes and distances on the jet is a useful addition to the approach by homogeneous dilution. In the first case, the instantaneous ATEX is characterized, in the second case the ATEX is characterized by accumulation. In the investigations conducted by EDF-SEPTEN, they were able to ascertain that the first type may become sensitive in the case of large size locals where accumulation does not necessarily lead to a notable rise in the average values.

References

1. B. Gautier EDF-SEPTEN "Reference Base for safety requirements concerning protection against the risk of internal explosion for the EPR" ENGSIN080356 A 2009.
2. European Directive ATEX 1999/92/EC relating to minimum prescriptions directed to improving protection as regards the safety and health of workers likely to be exposed to the risk of explosive atmospheres (Official Journal of the European Communities).
3. Studies of hydrogen leaks in large locals (INERIS – DRA -06 – P71922).
4. Study of dimensioning of the formed ATEX in the case of H_2-N_2 mixture leaks from pressurized ducts (INERIS DRA-07-89258-08949A).
5. Guide of good practices with no restriction for implementing the ATEX 1999/92/EC Directive (January 2003).
6. Explojet: Code for calculating explosions in turbulent flammable gas jets. Summary of research work and evaluation of version 4.0 (INERIS EMA-YMo-ERu/YMo-98-16FA26).
7. Evaluation of PHAST versions 6.0 and 6.1, summary report (INERIS DRA- 2002-29576 - SDu/Jco/Ebe, Nov 2002).
8. Deshaies B., Clavin P. (1979). Dynamic effects generated by a spherical flame at constant velocity (Journal de mécanique, Vol 18, n°2, pp 213-223).
   Deshaies B., Leyer J.C. (1981). Flow field induced by unconfined spherical accelerating flames (Combustion and Flame, Vol 40, pp 145-153).
   Cleaver R.P, Robinson C.G. (1996). An analysis of the mechanisms of overpressures generation in vapour cloud explosions (Journal of Hazardous Materials, Vol 45, pp 27-44).
9. INERIS Ω–19 Report « Determination of characteristic quantities of the source term required for using a model for atmospheric dispersion of accidental emissions » (INERIS-DRA-2005-P46055-C51076).
10. Duplantier et al., 2002: Evaluation of PHAST versions 6.0 and 6.1 (INERIS-DRA-2002-29576 report).