# QUANTIFICATION OF THE UNCERTAINTY OF THE PEAK PRESSURE VALUE IN THE VENTED DEFLAGRATIONS OF AIR-HYDROGEN MIXTURES.

**Gennaro M. Cerchiara , Marco N. Carcassi.**

**Department of Mechanical, Nuclear and Production Engineering (DIMNP) ,
University of Pisa (Italy). E-mail: cerchiara@ing.unipi.it ; carcassi@ing.unipi.it .**

***SESSION : 1.5 - Hydrogen Risk Assessment and Management - Mitigation techniques.***

## ABSTRACT

In the problem of the protection by the consequences of an explosion is actual for many industrial application involving storage of gas like methane or hydrogen, refuelling stations and so on. A simple and economic way to reduce the peak pressure associated to a deflagration is to supply to the confined environment an opportune surface substantially less resistant then the protected structure, typically in stoichiometric conditions, the peak pressure reduction is around the 8 bars for a generic hydrocarbon combustion in an adiabatic system lacking of whichever mitigation system. In general the problem is the forecast of the peak pressure value ($P_{MAX}$) of the explosion. This problem is faced using CFD codes modelling the structure in which the explosion is located and setting the main parameters like concentration of the gas in the mixture, the volume available, the size of vent area and obstacles (if included) and so on. In this work the idea is to start from empirical data to train a Neural Network (NN) in order to find the correlation among the parameters regulating the phenomenon. Associated to this prediction a fuzzy model will provide to quantify the uncertainty of the predicted value.

## INTRODUCTION.

The aim of this work is to build a method able to quantify the uncertainty associated to complex phenomenon like the forecast of the maximum peak pressure ($P_{MAX}$) inside a room, due to the vented explosions of air-hydrogen mixtures in the enclosure. During the deflagration the presence of a vented area reduces the magnitude of its $P_{MAX}$, weakening the explosion [3].The main factors involved are: the $H_2$ concentration in the explosive mixture; the area of the vent system; the pressure of rupture of the vent. The choice of the best procedure to analyse the involved empirical data depends on the number of parameters, the size of the database, the uncertainty sources identification, the kind of feedback to use in order to increase the efficiency of the model.

The empirical data are taken from the experiments done in Scalbatraio Lab of the Department of Mechanical, Nuclear and Production Engineering (DIMNP), University of Pisa (Italy). The experimental facility used is called CVE and it is a cube shaped made in steel and special glass through which it is possible to follow the evolution of the front flame during the explosions.

In general in the modelling the environment in which the explosion evolves, CFD codes are used. The general procedure using those codes is to fix the main parameters like: gas amount, volume involved, opening and obstacles in size and shape and so on. The codes can aid the plan of the industrial installation and it is effective in the most of cases.

Their limits are the slow response calculating the outputs and the bad prediction in very complex cases. The application of NN and these kind of new methods to quantify uncertainty for complex problems and systems it is very important in Risk Assessment Analysis. In fact those methods can aid the decision maker to focus the relevance of certain parameters in confront of others finding the correlation among them.

## 1. PROBLEM STATEMENT.

The problem is the prediction of maximum peak pressure during the explosion and the degree of uncertainty associated with that data. In order to obtain available data the experiments are made in a cubic shaped facility to reproduce a realistic storage room, utilised in a refuelling station for example. As concern the kind analysed explosion they are deflagrations of air-hydrogen mixtures, with homogenous concentration below the DDT concentration limit (Deflagration-Detonation Transition). The main uncertainty sources involved in the phenomenon are the effect of turbulence on the flame speed and the error in the evaluation of the value of pressure with which the vent start to open. In the general case the study of the deflagrations in confined atmospheres, with vent system emergency supply, it has always been complicated from the various typologies of phenomena according to various parameters as:

- the not uniform gas distribution in the environment;
- the volume geometry;
- the ignition point
- the possible presence of multiple ignitions;
- the flame turbulence and the instability.
- the possible presence of mechanisms accelerating the flame;

Considering the confined environments where equipments, systems or ducts inside which it is possible to find of the inflammable material, the risk analysis quantify the deflagration or detonation risk in case of loss of flammable gas and contemporary presence of ignition source.

In detonation case, that’s consisting in a fast flame front propagation (more the sound speed in air) the shock wave generated cause an high damages. The only way to limit them is to build proper structures resistant to the impulsive force of the pressure wave or to adopt some actions as to use inert gas in the environment (without oxygen the gas cannot burn) or introducing a system of air recirculation able to reduce the gas concentration under the transition deflagration detonation limit. Much more interesting from a technical point of view is the case of the deflagration because it is realistic much more then the detonation; in fact in such circumstances the damages to the interested structures can meaningfully be reduced using the concept of the venting [3].

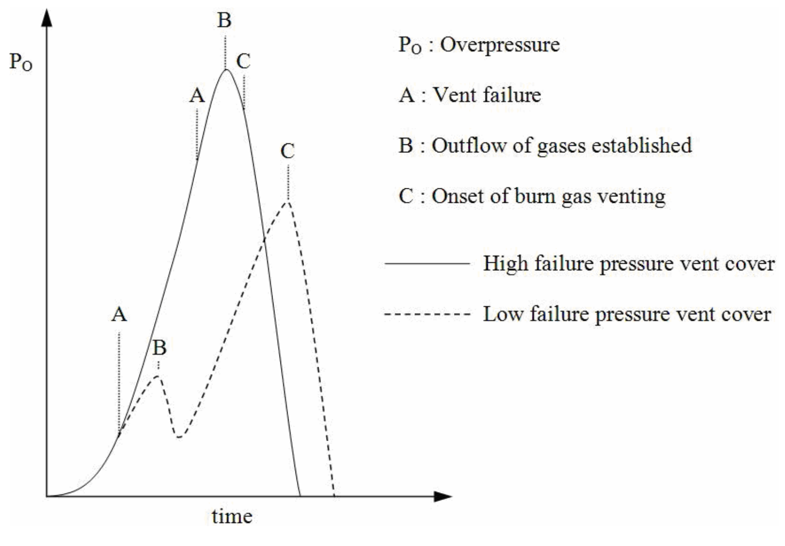


Figure 1. Qualitative Evolution of the pressure in a vented deflagration (the figure is not in scale).

In confront of detonation, a deflagration is sufficiently slow. It does not produce a shock waves but fast enough to produce a consistent peak pressure. Therefore the phenomenological aspect is shown with a substantial increase of pressure and temperature in the confined environment. The possible methods to mitigate the effects of a deflagration substantially belong to two philosophies, the first consist in the prevention (inert environment as said before) and the second in the mitigation of the effect (vent).

Main variables influencing and determining such phenomenon are:

1. the pressure released from the device that normally holds in position the closing vent (for practical reasons it is not normally acceptable to use vent without cover, even if would be favourable in order to reduce the peak pressure on the structure resulting from the deflagration and avoiding the necessary maintenance of such cover);

2. the resistance of the weaker part of the structure that is wanted be protect (it is a planned parameter of the project);

3. the volume and the shape of the enclosure (the shape factor is the ratio between surface and volume of the enclosure), the turbulence or the presence of inducing components as fans, obstacles or aeration systems;

4. the kind of inflammable, gas, powder, fog or mixtures of these;

5. the initial pressure and the temperature of the enclosure; the venting area (planned parameter of the project).

Currently the protection from the deflagrations through emergency venting is represented and reported NFPA68, American guide of the National Fire Protection Association to support the planning of such protection systems. The only limit of this guide is the field of application because the referred concentrations are stoichiometric so the considered explosions are detonations. For such reasons the guide is too prudential for practical purposes. In order to complete the knowledge about deflagration protection systems considering various flammable gas concentrations in different operational conditions its been built an experimental facility by means it is possible to study this kind of problem.

The experimental equipment CVE (View Explosion Chamber) is conceived to analyze the multi-dependent phenomenon, simulating an environment resembling as much as possible to a real one, (domestic or industrial). The CVE possesses therefore such size to be reasonably able to simulate a storage local of inflammable fuel (in the refuelling stations), or alternatively it could be representative of a domestic room. The intention to simulate an outbreak in a dimensionally consistent environment of civil use, is stimulated from the research of eventual scale laws allowing the forecast of the load on analogous shape structures and various size.

## 2. BRIEF DESCRIPTION OF THE EXPERIMENTAL FACILITY CVE.

The experimental facility CVE (View Explosion Chamber) is conceived for the study of the confined deflagrations evolution considering flammable atmosphere air-hydrogen mixtures or air-methane. The CVE has a volume of approximately 25 $m^3$ and is constituted from a structure of approximately cubical shape. It is realized by means of metallic chassis to which are connected rectangular modules which allow the assembly of the walls with openings for vent (the wall of "test"), metallic emergency panels necessary in case of upset situation they increase the vent area, glass windows to check the evolution of the flame front.

Figure 2. General overview of the CVE.

Therefore, every wall of the machine is constituted from panels connected to the structure and everyone has a specific function; in the detail the equipment is organized (see fig. 3 and fig. 4) as shown below:

Wall (A): test sidewall, it is constituted by a steel panel containing a passage to go inside, this allows the access to the internal part of the equipment, other two panels (steel) constitutes the vent test windows. The shape of these two vents are similar to a door and window for the study of explosion effects in a civil environment. In figure 4 the particular of the test panels assembly in plastic is shown;

Wall (B): equipped with fixed wall of fixed panels;

Wall (C): wall endowed of three constituent steel panels of the emergency vent and fixed from the outside with safe calibrated resistant section screws, in order to aid the detachment from the equipment in case of a peak pressure more then 250 mbar;

Wall (D): equipped sidewall of panels in special glass, fixed on the main structure of the equipment; in this way the possibility is had to observe and to resume the evolution of the deflagration by means of video camera outside of the CVE;

Wall (E): roof, equipped like the D wall with special glasses;

Wall (F): floor, constituted from fixed metallic panels;

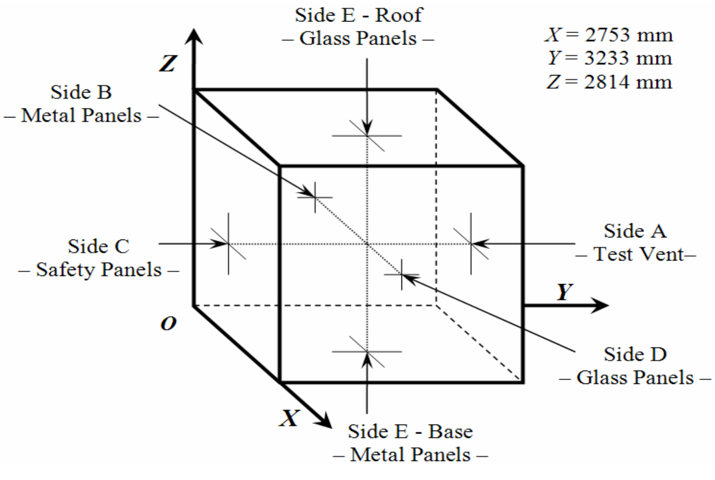


Figure 3. Simplified CVE Schema.

Figure 4. Vent particular CVE wall A.

support Structure of for the transport and handling of the facility is previewed. In figure 3 simplified CVE schema; in figure 4 the vent particular belonged to the CVE test wall provided with the door and the window in plastic material.

The hydrogen gas feeds the CVE through stainless steel pipes from four 200 bar cylinders (there is a pressure reducer over the hydrogen bottles manifold). Before the inlet phase an aerosol stream is injected in the CVE internal volume in order to see the hydrogen flame (the aerosol NaCl in water makes the flame red). A five channels hydrogen concentration analysers samples the internal atmosphere during and after the inlet in order to stop that phase at a predetermined value of concentration. Two pressure transducers located inside the CVE measure and register the explosion overpressure; other three pressure transducers located outside the CVE and arranged in front of the vent area measure the pressure outside the vent discharge cone.

## 3. DATA SET AND QUANTIFICATION OF THE UNCERTAINTY.

In the studied case the attention is focused on the behaviour of the deflagration respect to the volume geometry and the presence of factors as the turbulence, accelerating the flame. The experimental acquired data include the concentration of hydrogen in the mixture, the size of the venting area, the pressure of rupture of the vent and the maximum pressure reached during the deflagration with the final maximum value of the temperature inside the experimental facility.

The experimental work is finalised to find and to quantify the main sources of uncertainty calculating the error involved. The successive theoretical step consists in the training of the predictive Neural Network on the interested output (i.e. the maximum peak pressure) and the last step is the modelling the uncertainty associated to the prediction of the network realised by a Fuzzy Model. In this way the final result of this kind of analysis is a set of predicted values of the peak pressure ($P_{MAX}$) associated with the uncertainty $U(P_{MAX})$ to obtain $P_{MAX} \pm U(P_{MAX})$, a discrete function of values [7]. The considered data for the construction of the Fuzzy model are:

- H2 Concentration inside the CVE volume, $H_2$% [6%vol – 14%vol];
- vent Area , Av [0.35 $m^2$ – 2.5 $m^2$];
- Peak Pressure vent rupture, Pstat [20 mbar - 80 mbar];
- Max Peak Pressure with venting, $P_{MAX}$ [5 mbar – 250 mbar].

Table 1. Partial data set from experimental deflagrations.

| TEST | Av ($m^2$) | Pstat (mbar) | H2% (%vol) | P MAX experimental (mbar) | P MAX Neural Network (mbar) | Error (mbar) | Error % |
|---|---|---|---|---|---|---|---|
| CR07 | 0,35 | 20 | 13 | 151 | 146,66 | -4,34 | -3% |
| CR09 | 0,35 | 20 | 11,2 | 143 | 143,88 | 0,88 | 1% |
| CR28 | 0,7 | 20 | 11,7 | 92 | 90,48 | -1,52 | -2% |
| CR29 | 0,7 | 18 | 11,7 | 155 | 133,13 | -21,57 | -14% |
| CR31 | 0,7 | 21 | 11,7 | 98 | 77,12 | -20,48 | -21% |
| … | … | … | … | … | … | … | … |

Other data regarding the initial temperature, the atmospheric pressure before the ignition and the humidity do not influence on max peak pressure. Therefore the Fuzzy model will be structured with the first four factors previously seen as inputs and the $P_{MAX}$ as output. It would be interesting to add the output "duration of the deflagration maximum peak" and/or the "number of peaks generates" but the first approach can be thought constructing a model of base and then to add ulterior useful information where it is necessary.

One of the advantages to work with an instrument based on Fuzzy Logic is in fact the possibility to enrich the knowledge of the model without losing the job previously done.

From the statistical analysis, the main sources of uncertainty is detectable on the measure of Pstat and statistically it is quantifiable as (PP is peak pressure):

- Up to 5-10 mbar for weak cover of the vent, every range of the PP;
- Up to 10-25 mbar for both weak and strong cover of the vent, every range of the PP;
- Up to 25-30 mbar for strong cover of the vent, for high PP.

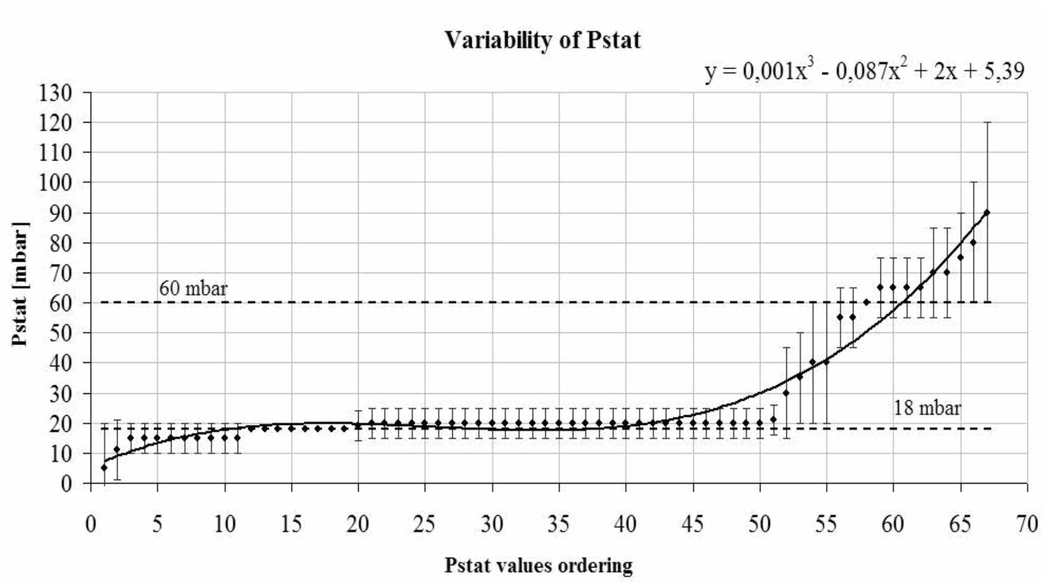


Figure 5. Variability of Pstat in increasing order.

The variability of the Pstat is described in the figure 5, data are ordered in increasing value and the interpolation line is indicated. The two values 18 mbar and 60 mbar are the Pstat value of breakdown of the plastic material of the vent cover (dotted lines). If the rupture of the vent was without uncertainty the graph should be constituted from two plateaus (of 18 and 60 mbar) instead of the trend in the figure 5.

The error bars in red have a variability from 5-10 mbar up to 25-30 in the field of high resistance plastic and high peak pressure. The peak pressure values are not reported in the graph because only the Pstat variability confronted with the material of the vent has been taken into account.

However the points belonged to the last part of the graph are representative of experiments in which the peak pressure value was high (i.e. from 150 mbar up to 250 mbar), as shown in figure 6.

The other sources of uncertainty are localised in the measurements of the H2%vol concentration and of the peak pressure from the transducers. However the error involved in these measures is very small, 0.1% of the value, typically 0.1% of 12%vol of hydrogen in the mixture equivalent to ~ 20 liters of $H_2$ on 3000 liters ) and 2 mbar - 3 mbar for the pressure transducers confronted with the uncertainty introduced by the vent rupture before considered.

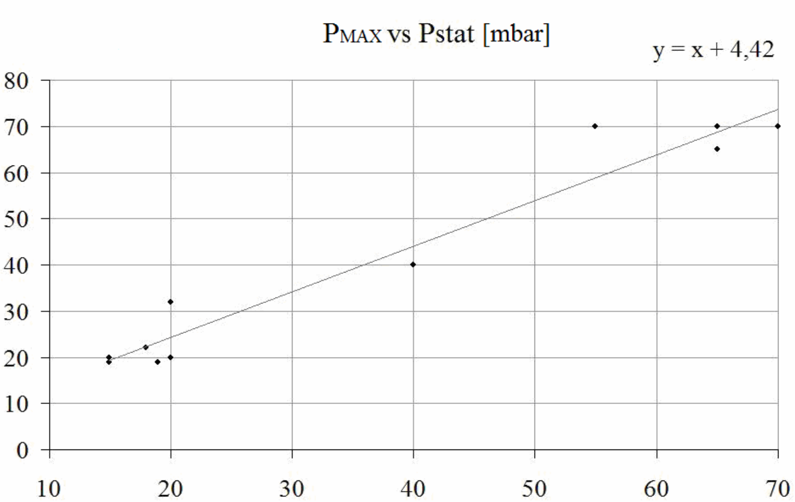


Figure 6. The overpressure $P_{MAX}$ versus Pstat for high concentration of $H_2$ (from 10% to 12,5%).

In general another important uncertainty source is the possible inhomogeneous distribution inside the CVE, this factor can influence the turbulence and the flame speed but in the considered case study the experiments are planned including a mixing phase (using a fan) and a sampling from five different points of suction inside the facility. This procedures guarantee an high degree of knowledge about the uniformity of the distribution of the explosive mixture.

## 4. THE PREDICTIVE NEURAL NETWORK AND THE FUZZY SYSTEM QUANTIFYING THE UNCERTAINTY.

The neural network (NN) is an useful tool used to reproduce a multifunctional phenomenon starting from historical knowledge (data). The flexibility and the fast time of response of the NN are its main advantages; the difficulty to translate the structure of the network in an analytical function (for example $y\ (o_1, o_2, \ldots, o_m) = f\ (i_1, i_2, \ldots, i_n)$ , with $i_n$ = generic input, $o_m$ = generic output) is its main weak point.

The predictive NN for the present case study accepts three inputs and one output. The inputs are: the $H_2$%vol concentration in the explosive mixture; the vent area (in $m^2$); the pressure of breakdown of the vent (Pstat in mbar). The output is the maximum peak pressure of the deflagration. The available data consist in 57 deflagration recorded during 3 experimental assets.

The NN architecture is a Back-propagation 3 × 11 × 1 layers (3 inputs, 11 neurons in the hidden layer, 1 output) developed with NeuroShell 2.0 release 3. The NN is trained using 90% of available data (50 points) and tested with the remaining 10% data (7 points), the results of the correlation between experimental data versus predicted are shown in the figure 7.

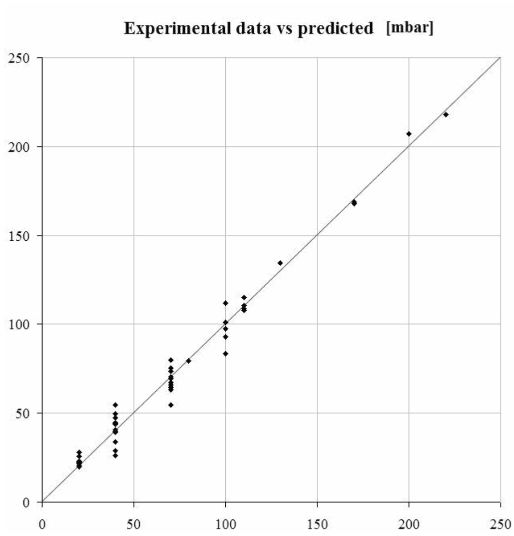


Figure 7. The correlation between the experimental data and the NN predicted data.

The Fuzzy model [4] (developed with Matlab 6.0 R.12) gets four input parameters and a single output consisting in the value of the maximum peak pressure in the CVE (fig. 8).

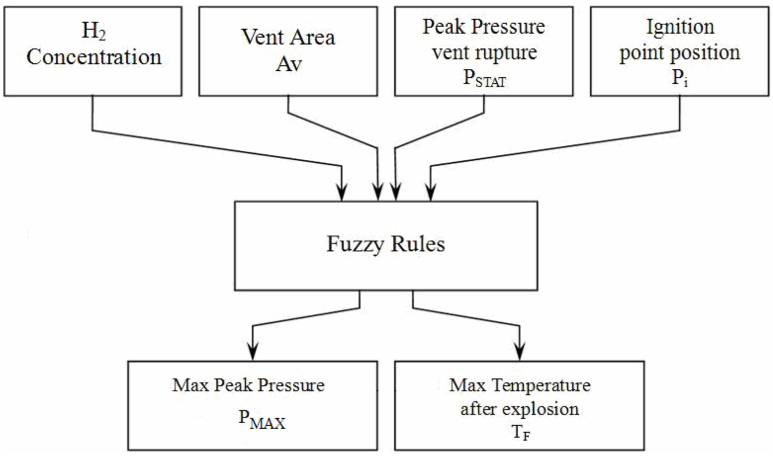


Figure 8. Schema of the Fuzzy Model for vented deflagrations.

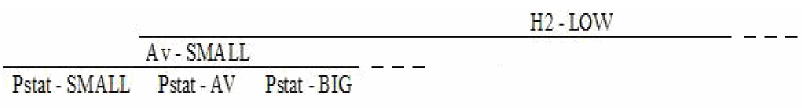


Figure 9. Part of the Fuzzy Model Event Tree, case of H2-LOW / Av-SMALL.

The logical linguistic rules which regulate the model are determined from the statistic analysis in terms of frequencies of occurrence of all the possible events from the connections of the inputs with the output. These events can be visualized through a event tree (fig. 9) that contains the linguistic variable with which the input are defined, for example:

IF H2-LOW ***AND*** Av-SMALL ***AND*** Pstat-SMALL ***THEN*** OUTPUT.

The OUTPUT is the value of $P_{MAX}$ from the statistic analysis previously said. Referring to a limited number of experiences the preliminary model for the uncertainty appraisal associated to the vented explosions with relative forecast and calculus of the maximum peak pressure is constituted from three inputs (H2; Av; PSTAT) ignition point position is fixed and one output $P_{MAX}$. The fuzzy model properties are:

Membership Functions → Mamdani (triangular);
AND method → min;
OR method → max;
Implication → min;
Aggregation → max;
Defuzzification → centroid.

Using the fuzzy model the obtained results are shown in the following figures 10-11.

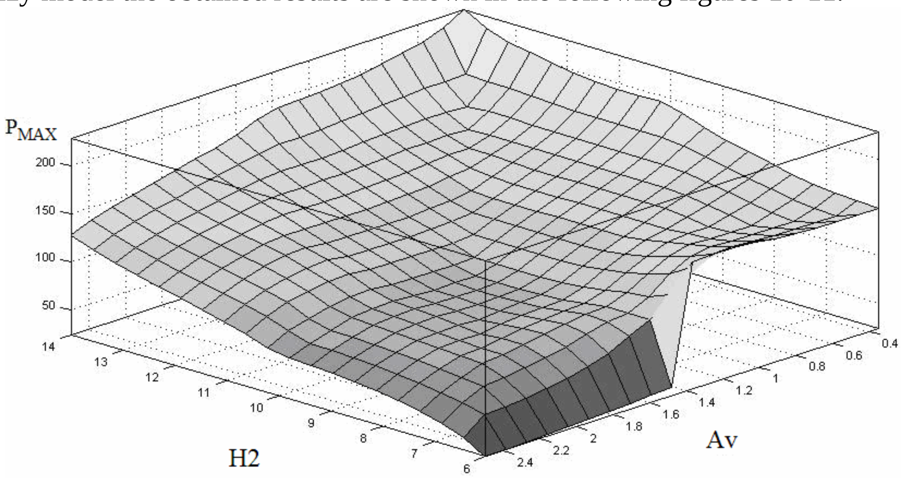


Figure 10. Results with Pstat = 60 mbar.

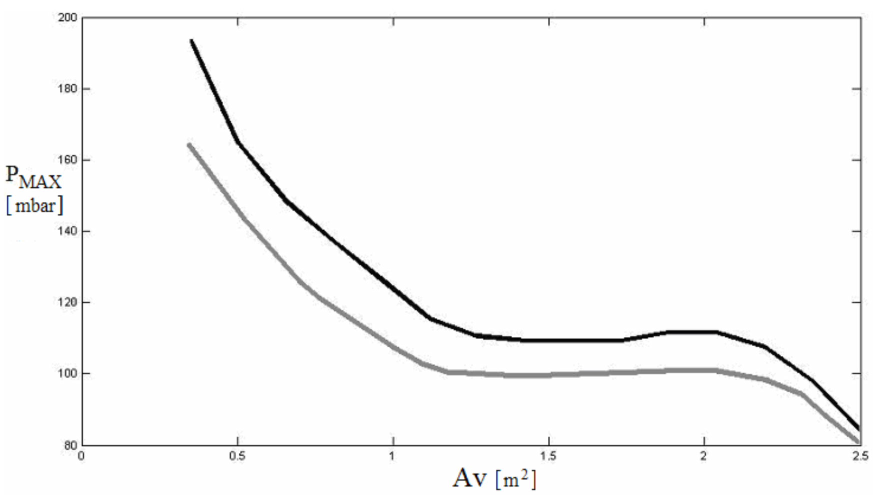


Figure 11. Results with Pstat = 60 mbar and Hydrogen $H_2$ = 11%vol. The line in black is the upper limit of $P_{MAX}$.

## 5. CONCLUSIONS.

From preliminary obtained results it can be noticed the influence that the inputs have on the final value of the maximum pressure (fig. 11). Such system brings to the definition of the laws previously said, the model does not need of calibration or validation because it reproduces the phenomenon statistics elaborated through fuzzy logic.

At this point the attention can be focused on the general characteristics of the method, the prediction of the NN is the most credible result $P_{MAX}$, the forecast from the fuzzy system is the upper limit of $P_{MAX}$ (see fig. 11 the line in black) [6] and the range of the main uncertainty source (Pstat) gives the range of variability on $P_{MAX}$ value [5].

It is possible calculate the lower limit for $P_{MAX}$ using probability boxes [2] constructing Belief measures starting from experimental data. This kind of technique is a powerful tool to quantify the uncertainty. In the present work has not used because for risk assessment purposes it is meaningful the upper limit of $P_{MAX}$ value. On the other hand the greater number of experiences is necessary to build this kind of model.

The NN and Fuzzy system integration promptitude and handling flexibility constitute its greater points of force, the limited applicability to the single deflagrating phenomenon and not detonating or of transition one, its main weak point. In order to upgrade the model it is necessary to acquire new experimental data and to opportunely train it. The previous train is always useful and new information are simply added to the old one completing the set of knowledge.

## REFERENCES.


1. Dubois Didier, Prade Henri, "Possibility Theory, an Approach to Computerized Processing of Uncertainty" Plenum Press, 1988.
2. Ferson S. et al., "Constructing Probability Boxes and Dempster-Shafer Structures", Sandia Laboratories Albuquerque NM, SAND2002-4015, January 2003.
3. Harris R.J. "Gas Explosions in Buildings and Heating Plant" E&FN Spon USA NY10017 isbn 0419132201 – 1983.
4. Ross T.J., "Fuzzy logic with engineering applications", McGraw-Hill, New York, 1995.
5. Yager R. "An Approach to Ordinal Decision Making", International Journal of Approximate Reasoning, 1995; 12:237–261, Elsevier.
6. Yager R., Detynieki M., Bouchon-Meunier B., "A Context-Dependent Method for Ordering Fuzzy Numbers Using Probability " Information Science 138 - 2001 (237-255) Elsevier.
7. Zadeh L.A. "Fuzzy Sets as the Basis for a Theory of Possibility", Fuzzy Sets and Systems (FSS) 1:3-28, 1978. (Reprinted in FSS 100 (Supplement): 9-34, 1999.).