

# Maximum explosion pressure of H<sub>2</sub>/O<sub>2</sub>/N<sub>2</sub> mixture at various initial pressures

📅 11.01.2016

**Maximální výbuchový tlak směsi H<sub>2</sub>/O<sub>2</sub>/N<sub>2</sub> pro různé počáteční tlaky**

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výbuchy

tlak

výbuchové charakteristiky

## Abstract

A theoretical study on maximum explosion pressure is presented. The maximum explosion pressures, computed by assuming chemical equilibrium within the explosion front are examined in comparison with the measured explosion pressures. Comparisons of the experimentally measured pressures with the calculated adiabatic pressures indicate the degree of adiabaticity of the explosion. The calculated peak explosion pressures of hydrogen-air mixtures for ambient conditions are examined in comparison with the experimental values and with the calculated adiabatic explosion pressures. In the present contribution we calculated the maximum pressure for hydrogen-air mixtures in a spherical closed volume at different initial temperatures up to 200 °C. The results represent a continuation of numerous efforts by various research groups, where the key underlying problem has been the understanding of results obtained in laboratory tests for predicting the consequences of gas explosion scenarios in industry.

**Keywords:** Maximum Explosion Pressure; Elevated Pressure; Hydrogen

## Abstrakt

V článku je prezentována teoretická studie stanovení maximálního výbuchového tlaku. Maximální výbuchový tlak je vypočítán za předpokladu vzniku chemické rovnováhy na čele výbuchové vlny a srovnán s naměřenými výbuchovými tlaky. Porovnání experimentálně zaměřených tlaků s vypočtenými adiabatickými tlaky demonstruje stupeň adiabaticity exploze. Vypočítaný maximální výbuchový tlak pro různé směsi vodíku se vzduchem pro standardní podmínky je srovnán s experimentálními hodnotami a s vypočtenými adiabatickým výbuchovým tlakem. V tomto příspěvku je vypočítán maximální výbuchový tlak pro směsi vodíku se vzduchem pro případ kulového uzavřeného objemu pro různé počáteční teploty až do hodnoty 200 °C. Výsledky představují pokračování v úsilí různých výzkumných skupin v oblasti porozumění datům získaných v laboratorních testech pro predikci následků scénářů výbuchů plynů v průmyslu.

**Klíčová slova:** Maximální výbuchový tlak; Zvýšený počáteční tlak; Vodík

## 1. Introduction

Hydrogen-air is together with methane-air the most widely used mixture to demonstrate the validity of any new theoretical or experimental approach to determine its combustion or explosion parameters due to availability of many theoretical and experimental results using various techniques (Pekalski, 2005; Movileanu et al., 2011). The characteristic parameter of hydrogen in a closed vessel explosion, so called explosion characteristic, discussed in this contribution is the maximum explosion pressure. The maximum explosion pressure is the highest explosion pressure over the flammable range in a closed volume at a given fuel concentration (Movileanu et al., 2011). According to standards, the maximum explosion pressure is determined experimentally by preparing test mixtures of hydrogen and air as oxidizing gas and conducting ignition tests at ambient conditions. Experiments could be, however, expensive and time consuming, especially at elevated conditions of temperature and pressure, at which many industrial processes occur (Pekalski, 2005). Therefore, approximate calculation methods are being sought with which approximate values of explosion pressure can be calculated in reasonable time. In the field of explosion prevention and for the proper use of this safety characteristic it is necessary to know its transferability to practical non ambient conditions. **The present contribution presents explosion pressures of stoichiometric hydrogen - air mixtures calculated for various initial temperatures. The temperature influence on the maximum explosion pressure was investigated at atmospheric pressure.**

## 2. Previous studies

Results of explosion experiments depend on many different parameters of the investigated process, such as the energy and type of ignition source, size and shape of explosion chamber, initial temperature, initial pressure and composition of the flammable mixture. To ensure the compatibility of data we selected the results for experiments that are in agreement with EN 13673-1 with the only exception that is volume of the testing vessel. (Holtappels et al., 2002) reports measurement of explosion pressures of hydrogen-air mixtures, at various initial concentrations close to stoichiometric (9.5-10.5 vol.%), in closed vessels of different volumes. The results have shown a similar behavior of investigated system. The maximum explosion pressures are  $(7.9 \pm 0.3)$  bar(a) for measurements made in the standard  $20.0 \times 10^{-3}$  m<sup>3</sup> spherical vessel. Higher deviations from these values are observed, however, when using smaller or larger size vessels, where radiative and convective heat losses to the walls could be neglected. (Cashdollar et al., 2000) reports different value of maximum explosion pressures for hydrogen-air mixtures, depending on the volume of the explosion vessel: 8.1 bar(a) in a  $120.0 \times 10^{-3}$  m<sup>3</sup> explosion vessel. The reported results from  $6.0 \times 10^{-3}$  are identical to those results obtained in the  $20.0 \times 10^{-3}$  m<sup>3</sup> and  $120.0 \times 10^{-3}$  m<sup>3</sup> despite the great difference in volume. There are not reported experimental studies for 1 m<sup>3</sup>.

## 3. Analysis

Mathematical model used in this study computes adiabatic flame temperatures and constant volume adiabatic explosion pressures at various initial temperatures and pressures, taking into account 26 species. It has been shown (Skrinsky et al., 2015) that the model is able to predict, with a reasonable accuracy in different fuel-enriched conditions, for different types of gaseous mixtures explosions.

Element balanced equation:

$$a_j = \sum_{i=1}^I n_i A_{i,j} \quad (1)$$

where  $a_j$  are moles of j-th element (atom);  $n_i$  are moles of i-th species;  $A_{i,j}$  number of j-th element in i-th species;  $I$  is the number of elements;  $J$  is the number of species.

The free energy (Helmholtz function) of the system  $F$  equation:

$$a_j = \sum_{i=1}^I n_i A_{i,j} \quad (2)$$

where  $F$  is the free energy (Helmholtz function) of the system;  $n_i$  are moles of i-th species;  $f_i$  is free energy of i-th species.

$$a_j = \sum_{i=1}^I n_i A_{i,j} \quad (3)$$

where  $f_i$  is free energy of i-th species;  $\lambda_j$  are the Lagrangian multipliers for each element ( $j=1$  to  $J$ );  $A_{i,j}$  number of j-th element in i-th species.

$$a_j = \sum_{i=1}^I n_i A_{i,j} \quad (4)$$

where  $g_i$  is the Gibbs free energy for single i-th species;  $\Delta H_f^i$  is the enthalpy of formation of the i-th species at standard conditions;

$$a_j = \sum_{i=1}^I n_i A_{i,j} \quad (5)$$

where  $g_i$  is the Gibbs free energy for single i-th species;  $R$  is the universal gas constant;  $T$  is temperature;  $n_i$  is the number of moles of every species;  $V$  is the volume.

$$a_j = \sum_{i=1}^I n_i A_{i,j} \quad (6)$$

where  $a_j$  are moles of j-th element (atom);  $n_i$  are moles of i-th species;  $A_{i,j}$  number of j-th element in i-th species;  $I$  is the number of elements;  $J$  is the number of species;  $g_i$  is the Gibbs free energy for single i-th species;  $\lambda_j$  are the Lagrangian multipliers for each element ( $j=1$  to  $J$ );  $R$  is the universal gas constant;  $T$  is temperature;  $n_i$  is the number of moles of every species;  $V$  is the volume.

$$a_j = \sum_{i=1}^I n_i A_{i,j} \quad (7)$$

where  $g_i$  is the Gibbs free energy for single i-th species;  $A_{i,j}$  number of j-th element in i-th species;  $I$  is the number of elements;  $\lambda_j$  are the Lagrangian multipliers for each element ( $j=1$  to  $J$ );  $R$  is the universal gas constant;  $T$  is temperature;  $n_i$  is the number of moles of every species;  $V$  is the volume.

The equations 1-7 were used to investigate and quantify the role of initial temperature and pressure in affecting the explosion behaviour of  $H_2/O_2/N_2$  mixtures.

#### 4. Results and discussions

### A) Adiabatic temperatures and explosion pressures for H<sub>2</sub>/O<sub>2</sub>/N<sub>2</sub>

Calculated adiabatic temperatures,  $T_{ad}$ , and explosion pressures,  $P_{ex}$ , for H<sub>2</sub>/O<sub>2</sub>/N<sub>2</sub> were determined at various initial temperatures and ambient initial pressure. The results of calculations are given in Table 1.

FUEL FRACTION [VOL.%]	INITIAL TEMPERATURE (K)							
	300		350		410		470	
	$P_{EX}$	$T_{AD}$	$P_{EX}$	$T_{AD}$	$P_{EX}$	$T_{AD}$	$P_{EX}$	$T_{AD}$
4.50	2.62	798	2.33	852	2.12	905	1.96	958
27.5	7.84	2679	6.58	2696	5.68	2712	5.01	2729
50.5	4.14	2334	5.95	2372	5.17	2408	4.59	2444
75.0	4.60	1426	3.96	1477	3.51	1527	3.17	1578

Table 1: Computed explosion pressures for H<sub>2</sub>/O<sub>2</sub>/N<sub>2</sub> mixtures at  $p_0 = 1$  bar(a)

From the numerical results of Table 1 it is possible to identify that the increase in the initial temperature lowers the maximum explosion pressure, and increases the flammability range. The value of the explosion pressure with varying H<sub>2</sub>/O<sub>2</sub>/N<sub>2</sub> concentration is similar at all investigated initial temperatures. The maximum value of the explosion pressure is found close to 30 vol. % of H<sub>2</sub> for all conditions. Further, in Table 2, we reported simulations on the explosion properties of H<sub>2</sub>/O<sub>2</sub>/N<sub>2</sub> mixtures at various initial pressure and ambient initial temperature.

FUEL FRACTION [VOL.%]	INITIAL PRESSURE (BAR(A))							
	1		5		10		15	
	$P_{EX}$	$T_{AD}$	$P_{EX}$	$T_{AD}$	$P_{EX}$	$T_{AD}$	$P_{EX}$	$T_{AD}$
4.50	2.62	798	13.10	798	26.19	798	39.29	798
27.5	7.84	2679	39.94	2740	80.36	2761	120.91	2771
50.5	7.03	2334	35.28	2345	70.62	2348	105.97	2349
75.0	4.54	1426	22.70	1427	45.40	1428	68.10	1428

Table 2: Computed explosion pressures for H<sub>2</sub>/O<sub>2</sub>/N<sub>2</sub> mixtures at  $T_0 = 298$  K

From the data performed in Table 2, it is clear that the increase of initial pressure has significant effect on explosion temperatures i.e. up to 500 K, but we may say that the chemistry is faster, but the fraction of

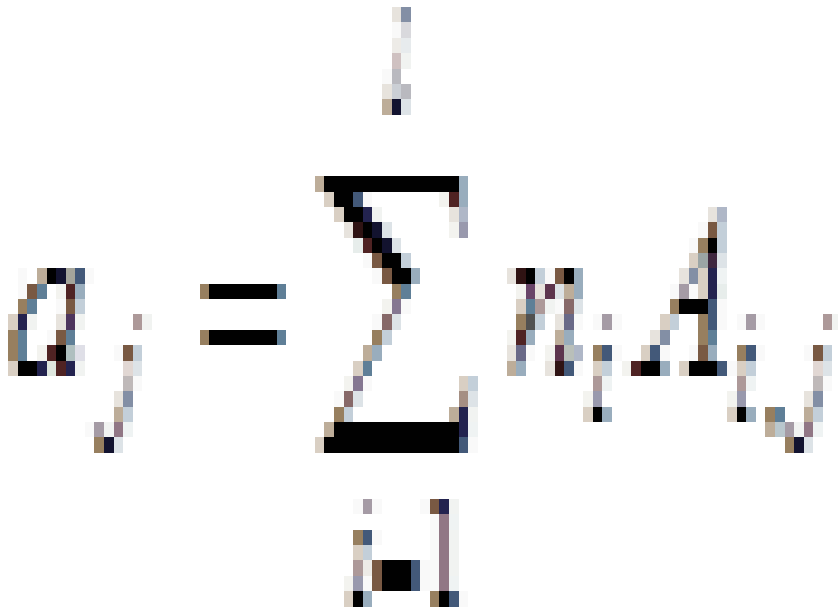
$$p_j = \sum_i n_i A_i$$

a)

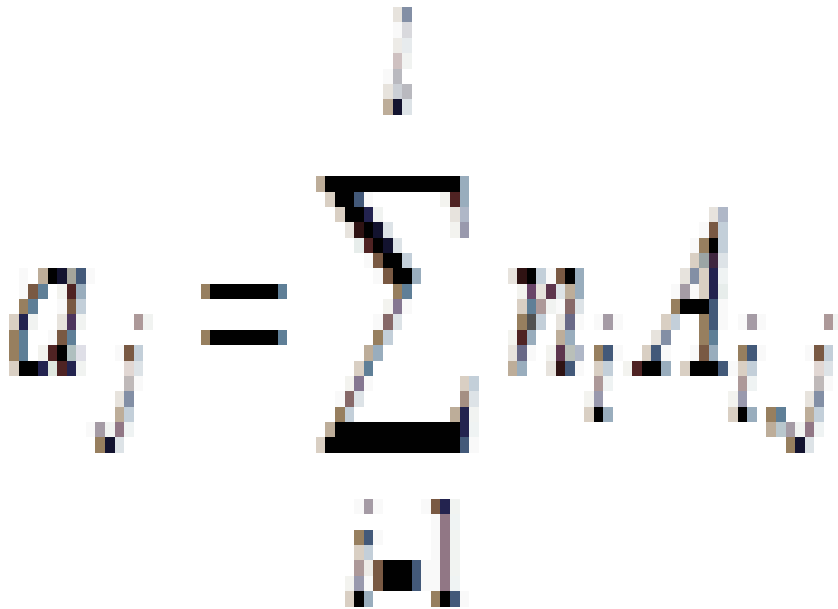
$$p_j = \sum_i n_i A_i$$

b)

Figure 1: Calculated explosion pressure vs fuel fraction for explosions of a) H<sub>2</sub>/O<sub>2</sub>/N<sub>2</sub> mixture at 298 K (top), 358 K (upper middle), 418 K (lower middle), and 478 K (bottom); b) H<sub>2</sub>/O<sub>2</sub>/N<sub>2</sub> mixture at 1 bar(a) (top), 5 bar(a) (upper middle), 10 bar(a) (lower middle), and 15 bar(a) (bottom)



a)



b)

Figure 2: Calculated explosion pressure vs initial temperature for explosions of a)  $H_2/O_2/N_2$  mixture at 27.50 vol. % (top), 50.50 vol. % (upper middle), 75.50 vol. % (lower middle), and 4.50 vol. % (bottom); b)  $H_2/O_2/N_2$  mixture at 1 bar(a) (top), 5 bar(a) (upper middle), 10 bar(a) (lower middle), and 15 bar(a) (bottom)

## 5. Conclusion

Adiabatic explosion pressures of hydrogen-air mixtures at various initial temperatures were calculated. The influences of initial temperature are compared with the experimental results and with the equilibrium calculations. Although the results from the evaluation indicate that presented theoretical simulations can become a valuable tool for rough estimation, the modeling requires further improvements to be useful for consequence modeling and design of

industrial facilities. Thus, at the first stage, the equilibrium calculations can be used as a rough calculation of a worst case scenario. At the same time, these values will be used as approximate initial values for explosion experiments carried out in heated 1 m<sup>3</sup> explosion apparatus built by OZM Research s.r.o. at Energy Research Centre, VŠB - Technical University of Ostrava.

## 6. Acknowledgement

This work would not have been possible without the financial support of two grants: (1) Innovation for Efficiency and Environment, reg. no. ED0036/01/01 supported by Operation Program Research and development for Innovation and financed by the Ministry of Education, Youth and Sports; (2) Innovation for Efficiency and Environment - Growth, reg. no. LO1403 supported by National Programme for Sustainability and financed by the Ministry of Education, Youth and Sports. J.V. is thankful for the financial support of the project "Support research and development in the Moravian-Silesian Region 2014 DT 1-International research teams" 02722/2014/RRC, financed from the budget of the Moravian-Silesian Region. J.S. is thankful to his advisor Ing. Jan Koloničný, Ph.D. and mentor RNDr. Prof. Pavel Danihelka, CSc. for their knowledge support in the area of decision process, industrial explosion safety and enthusiasm for a team work.

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SKŘÍNSKÝ, J. ...[et al.]. explosion characteristics of syngas mixtures at elevated temperatures and pressures. *Časopis výzkumu a aplikací v profesionální bezpečnosti* [online], 2015, roč. 8, č. 4. Dostupný z WWW: <<http://www.bozpinfo.cz/josra/josra-04-2015/maximum-explosion.html>>. ISSN 1803-3687.

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