Cellular structure of detonation wave for hydrogen-methane-air mixtures

Rafal Porowski, Andrzej Teodorczyk

Institute of Heat Engineering, Warsaw University of Technology, 21/25 Nowowiejska str., 00-665 Warsaw, PL

Abstract: *Paper presents a computational study of the fundamental detonation parameters of stoichiometric hydrogen-methane-air mixtures based on Chapman-Jouguet theory, ZND model and detonation wave cell size calculations. Detonation wave of gaseous fuel-air mixture has a multidimensional cellular structure consisting of cellular pattern that could be experimentally determined using smoked foil. The width of detonation cell correlates with several detonation dynamic parameters, e.g. initiation energy or critical tube diameter, and also reflects the stability of detonation wave. Methane-hydrogen mixture is used at different combustion devices like spark ignited engines, gas turbines, different kind of burners with premixed and diffusion flames. Series of calculations on detonation parameters of stoichiometric hydrogen-methane-air mixtures were made with different H2 contents in the mixture, from 10% up to 100% of hydrogen. The effects of the initial composition of the mixtures as well as initial pressure on the detonation velocity and cell size were investigated.*

1. Introduction

An increasing world-wide interest of methane as a fundamental component of natural gas (ca. 90%) concerning alternative fuels is motivated by the demand of reducing exhaust emissions and seems to be the cleanest fuel of all other fossils. But also hydrogen has been investigated as a single fuel in many experimental studies [1]. Unfortunately low density of hydrogen, extremely low boiling point (at 1 atm, 20 K) and wide range of flammability limits make it very difficult to store, handle and transport in large scale for industry all over the world. That is why hydrogen-methane-air mixtures are used at different combustion devices like car engines (e.g. HCCI), gas turbines, some types of burners with both premixed and diffusion flames but also more often in public pipeline transport.

There is almost no infrastructure anywhere in the world for transporting hydrogen. The construction of suitable pipeline networks only for hydrogen comparable to the existing natural gas pipeline network would require a massive investment. As a result of this problem transport of hydrogen can be provided by adding hydrogen to natural gas via existing pipelines.

Hydrogen addition to methane-air mixture increases the flammability limits and stability ranges of flame and the operating conditions can then be shifted towards leaner conditions [2-4]. Hydrogen addition decreases autoignition delay times and emissions of exhaust gases. Furthermore, it makes a change of reaction zone shape and finally creates transport conditions of methane much more fluent. The presence of hydrogen in combustible mixtures extremely increases the risk of explosion and especially detonation hazard because of high overpressures associated with a detonation wave. Although a detonation wave can be initiated directly by the deposition of a large amount of energy in a very small volume of the mixture, typically such ignition sources are not present in most industrial settings. Explosions almost universally start by the ignition of a flame from either an electrical spark or the autoignition of the mixture in contact with very hot surface. Under certain conditions a flame can accelerate and undergo transition to detonation wave, which is also known as the DDT [1] process.

Because of high value of energy required for detonation initiation directly in fuel-air mixtures, the worst case scenario in industrial conditions can be easily excluded in the open air. Sometimes a spontaneous detonation can be associated with DDT and direct initiation given by turbulent jet of combustion products.

Today, hydrogen and methane are the most important energy carriers but their application is determined by safety conditions. Generally speaking, hydrogen is much more dangerous than methane, since the latter is widely used and so far considered as public acceptable [6] of explosion and detonation hazard.

Detonation wave of gaseous fuel-air mixture has a multidimensional cellular structure consisting of cellular pattern that could be experimentally determined using smoked foil. The width of detonation cell correlates with several detonation dynamic parameters, e.g. initiation energy or critical tube diameter, and also reflects the stability of detonation wave.

2. Cellular structure of detonation wave

An actual detonation theory is a three-dimensional shock wave followed by a reaction zone. The leading shock wave consists of curved shock segments. At the detachment lines between these shock segments, the shock wave interacts in a Mach stem configuration. The characterized detonation wave pattern is generated by the triple point (Mach stem) of the shock wave. It is a measure of the reactivity of the mixture representing a length scale determining global reaction in the wave [11,12]. This length λ is often the cell size or the cell width. Generally speaking, the more reactive mixture, the smaller cell size can be obtained. In Explosion Dynamics Laboratory at California Institute of Technology, for many years there was a lot of research provided to build an international database of detonation parameters for various mixtures [13].

An example picture of cellular structure of detonation wave is shown in Fig. 1. This picture was created by the reflection of detonation wave from glass plate with soot layer. Mechanism of cellular structure imaging on sooted foil is not well-known. Cellular structure from Fig. 1 is the reflection of detonation wave on perpendicular surface to propagation direction. Localization of sooted foil along the direction of detonation wave propagation enables an image of cellular structure. Another example of detonation wave in sooted foil is given in Fig. 2a. Using Schlieren photography it is also possible to observe the structure of waves creating detonation wave, which is given in Fig. 2b. The structure of detonation wave is very complex. As mentioned before this structure is three dimensional and picture is only 2D. It posses many difficulties during analysis such photos.

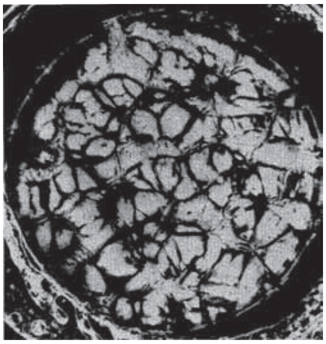
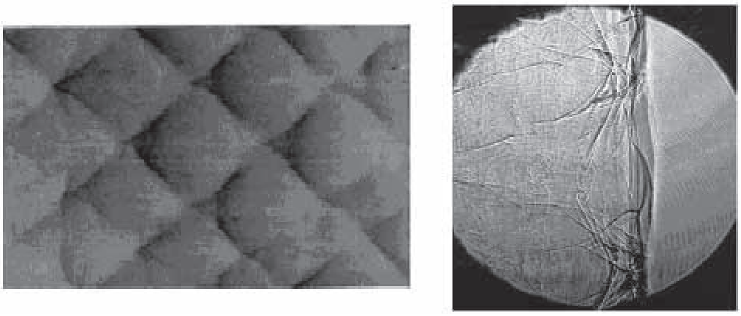


Fig. 1. Cellular wave structure after reflection of detonation wave from glass plate with soot layer [15].



a b

Fig. 2. Cellular structure of detonation wave [16]

The mechanism of cellular structure creation was found and published by Oppenheim and is given in Fig. 3. This picture shows the passage way of detonation wave through the channel of rectangular cross-section.

Part of the side wall in channel was made of transparent materials and provided with soot layer. The X axe shows the distance from initial point, and Y axe includes time at which particular image was taken. Direction of detonation pathway is from left to right.

Tested mixture was hydrogen-oxygen mixture. In Fig. 6 it is shown that behind the detonation wave a cellular structure is visible.

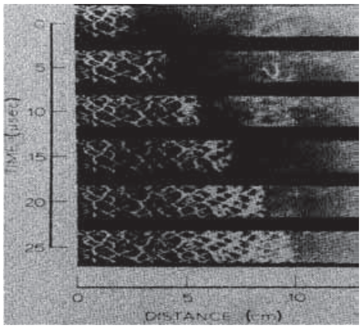


Fig. 3. Pathway of detonation wave with visible cellular structure on sooted foil [17]

The cellular structure of detonation wave is shown in Fig. 4. There are 3 kinds of waves in detonation wave, namely mach stem, incident shock and transverse waves. Mach stem and incident shock waves travel in the same direction as detonation front. Reflected shock waves are transverse to detonation front. Velocity of reflected shock waves is equal to sound speed in combustion gases. Fig. 4 also shows triple points trajectories.

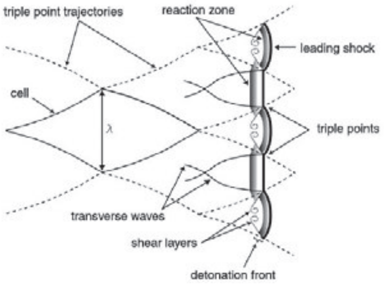


Fig. 4. The cellular structure of detonation wave

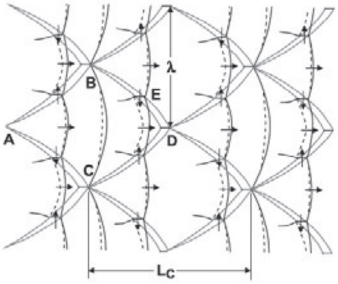


Fig. 5. Schematic of the propagation of a cellular detonation front, showing the trajectories of the triple points (dashed line represent start of exothermic reactions) [15]

The collision of a pair of neighboring triple points at point A in Fig. 5 results in the formation of a strong leading wave that initiates chemical reactions after a very short induction time. The leading shock wave propagating through the cell from point A to D decays in strength. It is common to use Mach reflection terminology in describing the progression of the leading shock. In the first part of the cell when the strong leading shock is created from the triple-point collision it is referred to as the Mach stem. In the latter part of the cell leading up to the triple-point collision it is referred to as the incident shock. For marginal detonation waves Strelow and Crooker [18] report a centerline shock velocity of roughly 1.6 times the CJ detonation velocity at the start of the cell and 0.6 times the CJ detonation velocity at the end of the cell. The decaying shock wave achieves the CJ velocity in the first 25% of the cell length after which the decay rate is much slower. Experiments performed by Austin et al. [19] suggest that the excursions in the shock strength increase with increased reduced activation energy, in agreement with numerical predictions [20].

In detonation waves the triple point can take on a weak configuration consisting of a single triple point or a strong configuration where there is a secondary triple point at the end of the reflected wave corresponding to the primary triple point, also known as a double Mach configuration. Figure 6 shows details of an ideal weak triple point propagating along the trajectory AC in Fig. 5. Specifically it shows various particle paths crossing the shock front from a reference point relative to the triple point. All the gas particles above the triple point pass through the Mach stem and below the triple point pass through the incident shock. The particles entering just below the triple point pass through the incident wave and then the transverse wave. In general, the induction time for the particles passing through the Mach stem is shorter than those propagating through the incident and transverse waves.

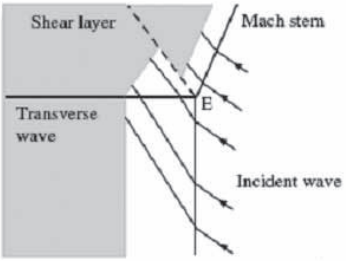


Fig. 6. Schematic showing particle trajectories relative to the triple point for a single Mach stem configuration. The shaded area represents the burned gas region [21].

3. Computational results

Due to a fact that the available literature presents a lack of both experimental and theoretical data on detonation parameters of hydrogen-methane-air mixtures this paper contains some computational results, which are only a part of larger study in this field performed at The Institute of Heat Engineering at Warsaw University of Technology. Detonation parameters of such mixtures should be also investigated because of industrial demand of technical safety measures, an increasing interest in hydrogen as an alternative fuel and of course possibility of pipeline transport.

This computational study on detonation parameters of stoichiometric hydrogen-methane-air mixtures and detonation wave cell size was performed for different hydrogen contents in the mixture. Table 1 shows detailed combustion chemistry for a given H_2 percentage which was further used for calculations of detonation parameters like Chapman-Jouguet pressure, temperature and velocity, ZND parameters and detonation wave cell size based on most adequate codes and tools.

Table 1. Detailed combustion chemistry of particular stoichiometric hydrogen-methane-are mixtures for further calculations.

Content of H_2 [%]	Combustion reactions of hydrogen-methane-air mixtures
10	$0.9\ CH_4 + 0.1\ H_2 + 1.85\ O_2 + 6.89\ N_2 = 0.9\ CO_2 + 1.9\ H_2O + 6{,}89\ N_2$
20	$0.8\ CH_4 + 0.2\ H_2 + 1.7\ O_2 + 6.33\ N_2 = 0.8\ CO_2 + 1.8\ H_2O + 6.33\ N_2$
30	$0.7\ CH_4 + 0.3\ H_2 + 1.55\ O_2 + 5.77\ N_2 = 0.7\ CO_2 + 1.7\ H_2O + 5{,}77\ N_2$
40	$0.6\ CH_4 + 0.4\ H_2 + 1.4\ O_2 + 5.22\ N_2 = 0.6\ CO_2 + 1.6\ H_2O + 5.22\ N_2$
50	$0.5\ CH_4 + 0.5\ H_2 + 1.25\ O_2 + 6.52\ N_2 = 0.5\ CO_2 + 1.5\ H_2O + 6.52\ N_2$
60	$0.4\ CH_4 + 0.6\ H_2 + 1.1\ O_2 + 4.09\ N_2 = 0.4\ CO_2 + 1.4\ H_2O + 4.09\ N_2$
70	$0.3\ CH_4 + 0.7\ H_2 + 0.95\ O_2 + 3.54\ N_2 = 0.3\ CO_2 + 1.3\ H_2O + 3.54\ N_2$
80	$0.2\ CH_4 + 0.8\ H_2 + 0.8\ O_2 + 2.98\ N_2 = 0.2\ CO_2 + 1.2\ H_2O + 2.98\ N_2$
90	$0.1\ CH_4 + 0.9\ H_2 + 0.65\ O_2 + 2.42\ N_2 = 0.1\ CO_2 + 1.1\ H_2O + 2.42\ N_2$
100	$1\ H_2 + 0.5\ O_2 + 1.86\ N_2 = 1\ H_2O + 1.86\ N_2$

3.1. CJ theory

Chapman-Jouguet (CJ) model gives simple solutions for the steady detonation wave. Equation 1 is the basis of the CJ model and equation 2 is an alternative form for ideal gases [7]:

$$h_2 - h_1 - q = \frac{1}{2}(p_2 - p_1)(v_1 + v_2)\,, \tag{1}$$

$$\frac{\gamma}{\gamma - 1}(p_1 v_1 - p_2 v_2) - q = \frac{1}{2}(p_2 - p_1)(v_1 + v_2)\,, \tag{2}$$

where: q is the energy addition per unit mass, or specific energy input, in the flow behind the shock front; h is a specific enthalpy of the gas; p is the pressure, and; υ is the specific volume.

The CJ theory treats the detonation wave as a discontinuity with infinite reaction rate. The conservation equations for mass, momentum and energy across the one-dimensional wave give unique solution for the detonation velocity and the state of combustion products immediately behind the detonation wave [7]. Based on CJ theory it is possible to calculate detonation velocity, detonation pressure, etc. The basic assumption in this theory is that there is no information required about the chemical kinetics.

All computational studies concerning CJ parameters of stoichiometric hydrogen-methane-air mixtures have been performed at initial pressure of 1 atm and temperature of 300 K. As outlined in Table 2, the preliminary computational work was first made with the application of STANJAN tool which is well suitable for thermodynamic calculations and gas dynamics. CJ parameters were calculated for stoichiometric hydrogen-methane-air mixtures beginning from the 10% H_2 contents in the mixture up to pure hydrogen-air.

Table 2. CJ parameters for stoichiometric hydrogen-methane-air mixtures at initial P = 1 atm and T = 300 K with different H_2 content in the mixture, given by STANJAN.

Content of H_2 in the mixture [%]	P_{CJ} [bar]	T_{CJ} [K]	V_{CJ} [m s^{-1}]
10	18.892	3002.45	1875.4
20	18.816	3007.03	1880.6
30	18.727	3012.42	1886.7
40	18.607	3016.77	1893.3
50	18.517	3026.81	1909.6
60	18.333	3036.16	1914.7
70	18.113	3045.38	1928.7
80	17.846	3060.73	1949.0
90	17.482	3081.60	1978.4
100	16.955	3111.55	2024.8

Calculated results for CJ parameters were firstly compared with theoretical values taken from the literature [7,8] (for similar initial conditions) both for CJ velocities and CJ pressures of stoichiometric hydrogen-air and methane-air mixtures. Literature value of CJ velocity for hydrogen-air mixture is 1968 m/s and for methane-air mixture is 1802 m/s [8]. These values were lower than those calculated by STANJAN concerning H2 content in the mixture. The 10% of H_2 in hydrogen-methane-air mixture gives the CJ velocity of ca. 1875 m/s which is higher than in pure methane-air. The same is that 90% of H_2 in the mixture gives CJ velocity of c.a. 1978 m/s which is quite comparable with theoretical one for H_2-air.

The similar evaluation was provided with CJ pressures. Theoretical value from the literature of CJ pressure for hydrogen-air mixture is 15.8 bar and for methane-air mixture is 17.4 bar [7,8]. These values were lower than those calculated by STANJAN concerning H_2 contents in the mixture. The 10% of H_2 in hydrogen-methane-air mixture gives the CJ pressure of ca. 18.9 bar which is higher than in pure methane-air. The same is that 90% of H_2 in the mixture gives CJ pressure of c.a. 17.5 bar which is also higher than theoretical one for H_2-air.

Using the opensource CANTERA [9] and MATLAB software the same CJ parameters of stoichiometric hydrogen-methane-air mixtures were computed for H_2% in the mixture from 10% of H_2 up to 100% in the mixture and for initial conditions of P1 = 1 atm and T1 = 300 K. As one can see in Fig. 7 for particular contents of H_2 in hydrogen-methane-air mixtures a dynamic increase of the CJ velocities and decrease of CJ pressures can be observed. In the Fig. 7 values 0.1, 0.2 up to 1.0 equal to 10%, 20% to 100% of hydrogen in the stoichiometric hydrogen-methane-air mixture.

Both STANJAN and CANTERA provided the computation of CJ detonation parameters of stoichiometric hydrogen-methane-air mixtures. Calculated CJ velocities and CJ pressures are slightly lower in case of CANTERA results than STANJAN results. This is due to the fact that two tools do not take into account the same free radical species during calculations and this may induce slightly different values.

An increase of hydrogen contents in the mixture is responsible for higher value of CJ velocities and lower for CJ pressures.

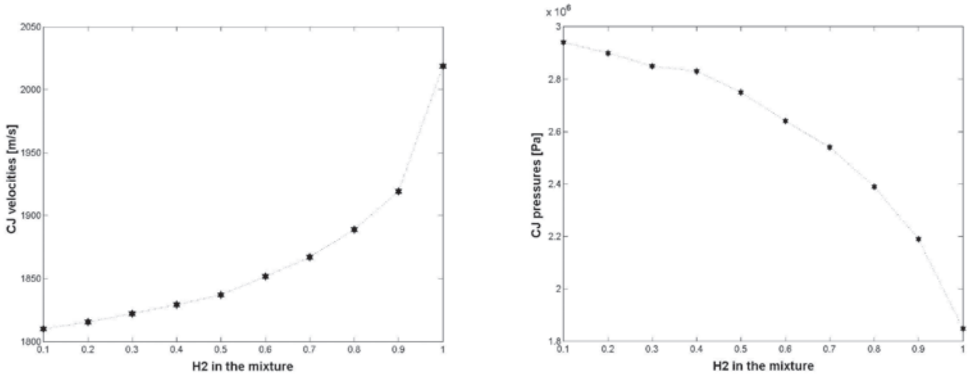


Fig. 7. CJ velocities and pressures versus H_2 % in hydrogen-methane-air mixture at initial P = 1 atm and T = 300 K.

Figure 7 presents the CJ pressure and temperature as a function of H2 content, calculated for stoichiometric hydrogen-methane-air mixture, at initial P = 1 atm and T = 300 K.

3.2. ZND theory

A weakness of the CJ model is the assumption that the chemical reaction which is the source of the heat release is infinitely fast. A further advance came with the development of a model which takes account of the finite rate of reaction and of heat release. The model was formulated independently by Zeldovich (1940), von Neumann (1942) and Doring (1943), and is known as the ZND model. In this model there is no reaction immediately behind the shock wave and there is an incubation period before the reaction begins [7]. The fractional completion of the reaction is characterized by the parameter ξ, and there is therefore a family of R-H curves for values of ξ between 0 and 1as shown in Figure 9.

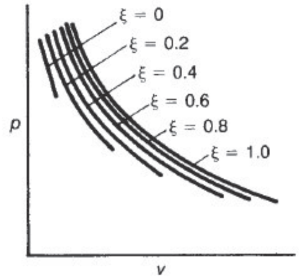


Fig. 8. Rankin-Hugoniot curves for different fractions of completion reaction [7]

The ZND model is more realistic and provides a firmer basis for the development of uni-dimensional models. One particular use is in predicting the pressure-time profile of the detonation, including the von Neumann spike. Considerable effort was expended from 1950 to 1970 to test the validity of the ZND model. While ZND corrected values were most frequently below the CJ value, they were occasionally larger [7].

The ZND theory gives the same detonation velocities and pressures as CJ theory, the only difference between the two models is the thickness of the wave.

After the calculation of the CJ parameters that have been performed, the ZND parameters were also computed with the same initial conditions (P = 1 atm, T = 300 K) of hydrogen-methane-air mixtures.

Calculations were made with two existing chemical kinetics mechanisms, namely:

- GRI-MECH v. 3.0 developed by Gas Research Institute which considers 53 species and 325 reactions,
- KONNOV v. 1.5 developed by A.A. Konnov which takes into account 127 species and 1027 reactions.

Adding hydrogen to methane-air mixture is responsible for a decrease of P_{ZND} both in computations using GRI-MECH and KONNOV mechanisms. For hydrogen contents in the mixture from 70% to 100% a rapid P_{ZND} decrease was observed.

Table 3. ZND parameters for hydrogen-methane-air mixtures at initial P = 1 atm and T = 300 K with different H_2 content in the mixture, calculated by CANTERA with GRI-MECH v.3.0 mechanism.

Content of H_2 in the mixture [%]	P_{ZND} [bar]	T_{ZND} [K]	Density [kg m^{-3}]
10	29.83	3032.66	3.15
20	29.42	3033.10	3.09
30	28.94	3033.59	3.03
40	28.39	3033.49	2.98
50	29.03	3032.53	3.31
60	26.81	3035.45	2.75
70	25.73	3035.16	2.61
80	24.27	3035.22	2.42
90	22.19	3033.30	2.17
100	20.74	3028.63	2.07

Table 4. ZND parameters for hydrogen-methane-air mixtures at initial P = 1 atm and T = 300 K with different H_2 content in the mixture, calculated by CANTERA with KONNOV v. 1.5 mechanism.

%H_2 in the mixture	P_{ZND} [bar]	T_{ZND} [K]	Density [kg m^{-3}]
10	19.63	3004.33	2.75
20	19.25	3004.10	2.69
30	18.72	3004.27	2.63
40	18.19	3004.38	1.98
50	19.03	3003.46	2.25
60	16.81	3005.25	1.97
70	15.56	3005.16	1.84
80	14.38	3005.32	1.75
90	12.26	3003.20	1.53
100	10.89	2928.84	1.48

Assessing T_{ZND} values for a given hydrogen-methane-air mixtures it was also smooth decrease through particular H_2 contents both for GRI-MECH and KONNOV mechanisms.

The reason of such differences in calculated values of ZND parameters, especially P_{ZND} for hydrogen-methane-air mixtures between these two mechanisms is that they do not take into account the same species and chemical reactions which directly influence on various results.

3.3. Detonation cell size

An actual detonation theory is a three-dimensional shock wave followed by a reaction zone. The leading shock wave consists of curved shock segments. At the detachment lines between these shock segments, the shock wave interacts in a Mach stem configuration. The characterized detonation wave pattern is generated by the triple point (Mach stem) of the shock wave. It is a measure of the reactivity of the mixture representing a length scale determining global reaction in the wave [11,12]. This length λ is often the cell size or the cell width. Generally speaking, the more reactive mixture, the smaller cell size can be obtained.

The cell size λ is a parameter which is of practical importance. The transition from deflagration to detonation, flame acceleration in certain conditions can be evaluated based on the knowledge of the cell size for particular mixture [14].

The main goal of the present work was to combine the detonation cell width λ with the ignition induction zone length Δ for detonation in hydrogen-methane-air mixtures. The detonation cell width λ is the characteristic feature of the mixture as well as the information about their reactivity. If the value of the detonation cell width is known it becomes possible to determine detonation limits and energy required for direct initiation of the detonation. Up to now numerical simulations of detonation propagation do not allow to compute the three dimensional cellular structure of the detonation wave properly and in consequence do not allow determining the value of the detonation cell width λ with sufficient accuracy. The best way to determine the value of λ is the experimental study, which is the second part of this study.

Numerous analyses have shown, that the detonation cell width λ can be related to ignition induction zone length Δ for detonation process. In this work linear correlation $\lambda = A * \Delta$ was used, where A is a proportionality parameter. Using a model of the propagation of the detonation wave proposed by Zeldovich, von Neumann and Döring, it becomes possible to compute ignition induction zone length Δ with good accuracy. If the values of the ignition induction zone length and the proportionality parameter A are known, the value of detonation cell width λ can be calculated. The ignition induction zone lengths Δ were computed using ZND program.

Computations with ZND program are based on the detailed chemical kinetics mechanisms. However, up to now there is no detailed chemical kinetics mechanism available especially for hydrogen and methane as fuels.

Accuracy of the detonation cell width prediction using constant proportionality parameter A has also been checked. The possibilities to improve accuracy of the cell width prediction using proportionality parameter as a function of selected detonation parameters have been analyzed. Brief review of others relationships between λ and ignition induction zone length Δ has also been performed.

Using the Cantera program the detonation cell width was computed as a function of initial pressure and molar methane fraction in fuel for stoichiometric methane-hydrogen-air mixture at initial temperature 295 K. Results of computations will be compared with experimental results obtained in laboratory for the same mixture and initial conditions. Comparison will enable validation of the computational model.

Furthermore, the basic theory of detonation process as well as review of studies of burning hydrogen-methane fuel mixtures, with emphasis on detonation, has been presented. Cellular structure of detonation, mechanism of their formation and relationships between detonation cell width λ and dynamic parameters of detonation have been also discussed.

For a computation of λ value of the detonation wave cell size for hydrogen-methane-air mixtures a chemical kinetics mechanism called LUTZ88 was chosen. The mechanism involves 39 species and 154 reactions. Calculations were made with CANTERA and SDT toolbox module. Using ZND model an ignition induction zone length Δ was computed. Particular detonation wave cell sizes were determined by the equation:

$$\lambda = A \cdot \Delta$$

where the factor A equals to 19. Figures 9 and 10 present computational results with initial T = 295 K, where x means mole fraction of methane in the mixture.

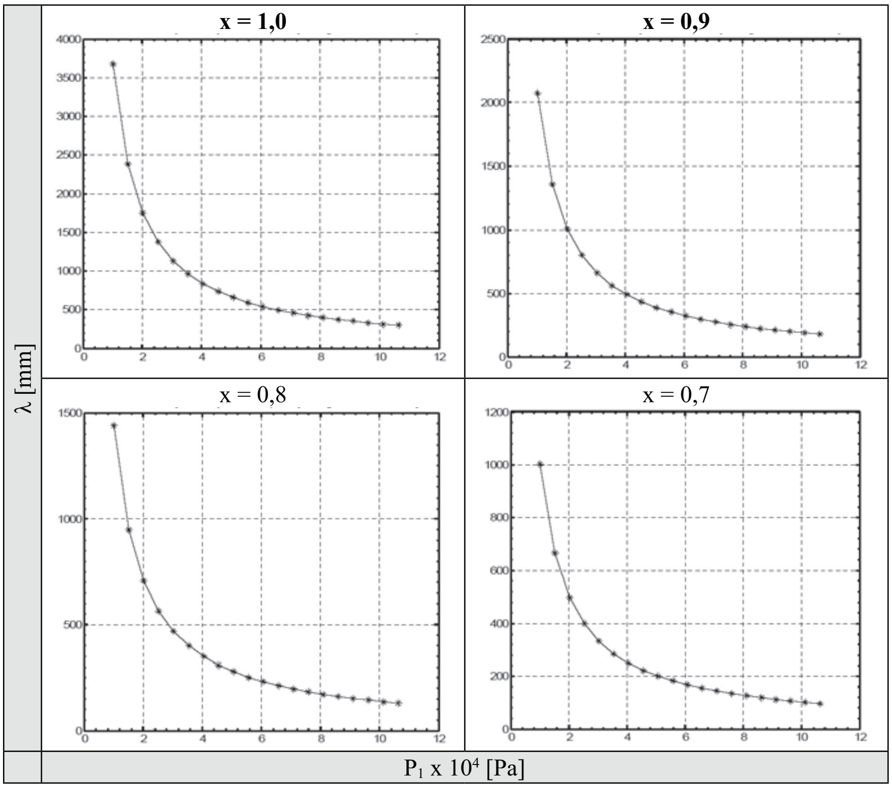


Fig. 9. Detonation wave cell size as a function of initial pressure of hydrogen-methane-air mixtures for CH_4 mole fraction in the mixture from 1.0 to 0.7.

For the mole fraction of CH_4 in the mixture from 1.0 to 0.7 at initial pressure of 0.1 atm the detonation wave cell size λ varies from c.a. (3700 to 1000) mm and is much more smaller for increasing values of initial pressures up to more than 1 atm, where λ is ca. (300 ÷ 100) mm.

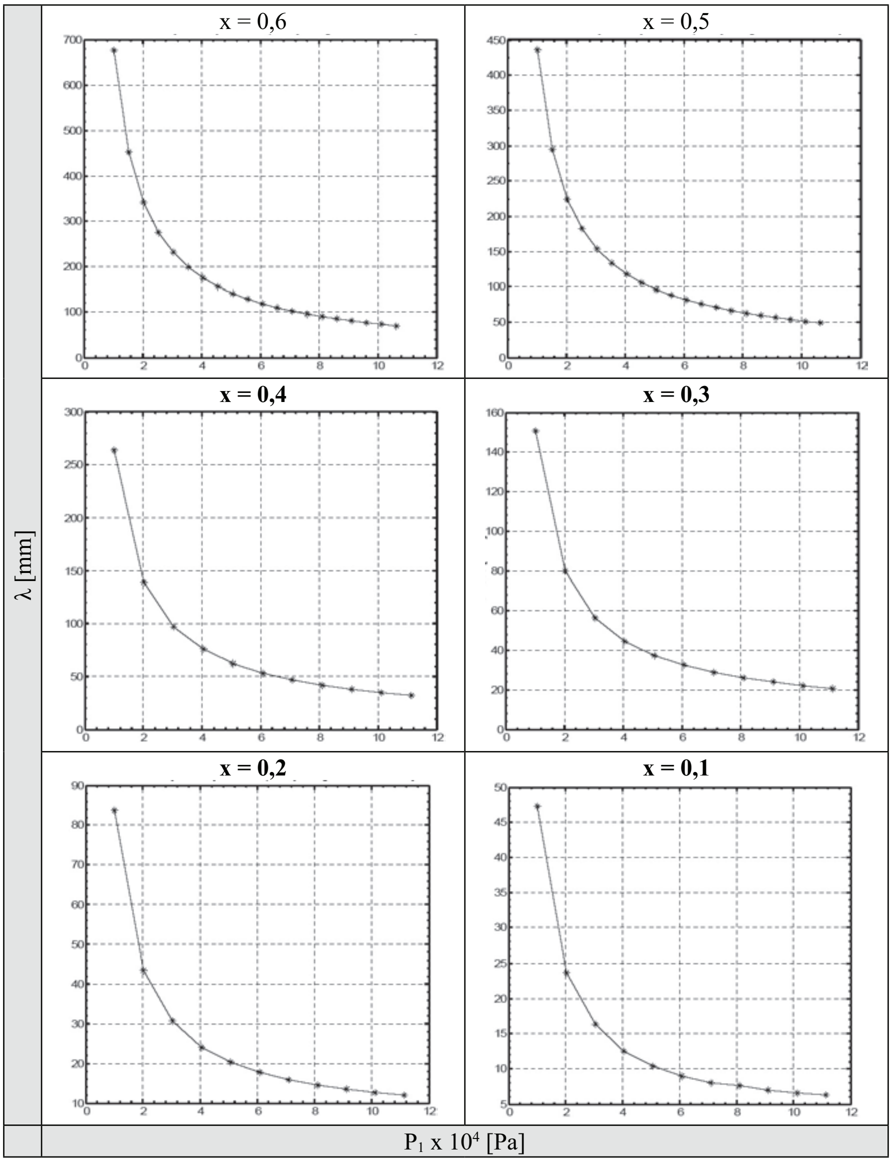


Fig. 10. Detonation wave cell size as a function of initial pressure of hydrogen-methane-air mixtures for CH_4 mole fraction in the mixture from 0.6 to 0.1.

For the mole fraction of CH4 in the mixture from 0.6 to 0.1 at initial pressure of 0.1 atm the detonation wave cell size λ varies from c.a. 680 to 47 mm and is much more smaller for increasing values of initial pressures up to more than 1 atm, where λ is ca. (80 – 7) mm.

4. Future works

To find the cellular detonation wave structure for hydrogen-methane-air mixtures an experimental study is now performed in a 6 m circular cross section channel with inner diameter of 140 mm (full diameter of 170 mm).

Experimental channel consists of four sections (2 x 2 m and 2 x 1 m) jointed together. Driver section of 0.8 m long tube with stoichiometric acetylene-oxygen mixture was applied to initiate a test mixture by the shock wave. The initial conditions of stoichiometric hydrogen-methane-air mixtures are 0.1 MPa and 293 K with different hydrogen content. The flame propagation and pressure wave are monitored by pressure transducers and ion probes. Pressure transducers are positioned at different locations along the channel to collect data concerning detonation development.

5. Conclusions

Computed detonation parameters such as CJ velocity, pressure, temperature and detonation wave cell size for hydrogen-methane-air mixtures give an overall review of potential risks and hazards which could be made during pipeline transport of such mixtures. One can be said that hydrogen addition to existing natural gas pipelines results in an increase of safety rather than pure hydrogen transport, especially in the context of detonation parameters. Furthermore, such mixtures can make hydrogen as an energy carrier all over the world where due to storage and transport problems in large industrial scale it seems to be a long future.

For better understanding of dynamics of detonation phenomena for hydrogen-methane-air mixtures, the second stage of this study is to perform experiments. An experimental study is now being performed at the Institute of Heat Engineering (Warsaw University of Technology) regarding detonation parameters, flame propagation and acceleration and DDT of hydrogen-methane-air mixtures in 6 m circular cross section channel with inner diameter of 140 mm.

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