

NUMERICAL ANALYSIS OF DETONATION PROPENSITY OF HYDROGEN-AIR MIXTURES WITH ADDITION OF METHANE, ETHANE OR PROPANE

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ABSTRACT

The detonation propensity of hydrogen-air mixtures with addition of methane, ethane or propane in wide range of compositions is analyzed. The analysis concerned the detonation cell width, ignition delay time, RSB and χ parameters. Results are presented as a function of hydrogen molar fraction. Computations were performed with the use of three Cantera 2.1.1. scripts in the Matlab R2010b environment. The validated mechanisms of chemical reactions based on data available in the literature were used. Six mechanisms were assessed: GRI-Mech 3.0, LLNL, SanDiego, Wang, POLIMI and AramcoMech. In conclusion, the relation between detonation propensity parameters is discussed.

1.0 INTRODUCTION

Gaseous detonations are self-sustaining shock waves propagating in a combustible mixture, coupled to and sustained by exothermic chemical reactions [1]. These supersonic combustion waves produce substantial increases in gas pressure and temperature. Detonations also induce a velocity in the fluid through which they propagate. A pressure peak that accompanies the detonation front can be particularly destructive for industrial installations, devices, etc. Therefore, assessment of detonation sensitivity of mixtures is crucial nowadays. The multi-dimensional structure of gaseous detonations was experimentally, theoretically and numerically studied by Denisov and Troshin in 1959 and by Voitsekhovskiy in 1963. A detonation develops cellular structure with regular pattern of diamond shapes during the propagation. If the medium is large enough, the detonation cell size depends only on initial conditions. For given fuel it is a function of initial temperature, initial pressure, equivalence ratio, molar composition, type of diluent, etc. If the activation energy is constant, the detonation cell size is proportional to chemical induction zone size (which is depended on temperature in terms of Arrhenius' equation). Based on that, currently detonation cell size is widely used to measure detonation propensity (*detonability*). Many criteria have been developed in order to correlate detonation sensitivity to detonation cell size in given geometry. Most of them are based on empirical measurements and are true only for particular mixtures and initial conditions. It was discovered that dimensions of detonation cells are related to the reaction zone width which can be calculated based on ZND theory for 1D model of detonation wave.

Gavrikov et al. based on analyses of differences in reaction conditions in 1D models and multidimensional detonations, cellular structure, detonation stability and data from numerical modeling of multidimensional detonations, proposed a simple definition of 1D characteristic reaction zone width [2]:

$$\delta = (D_{CJ} - U_{PS}) \cdot \tau_{ad} = (D_{CJ} - U_{PS}) \cdot \frac{RC_v T_{vn}^2}{E_a Q k_0 \rho_{vn}} \cdot \exp\left(\frac{E_a}{RT_{vn}}\right) \quad (1)$$

where: D_{CJ} – Chapman-Jouguet detonation velocity, U_{PS} – postshock gas velocity, τ_{ad} – adiabatic induction time, R – gas constant, C_v – molar specific heat at constant volume, T_{vn} – von Neumann temperature, E_a – activation energy, Q – chemical energy release, k_0 – preexponential factor of reaction rate, ρ_{vn} – von Neumann density.

The assumption is that the reaction begins after the leading shock wave of detonation at *von Neumann* conditions. The analytical formula for adiabatic induction time τ_{ad} is correct for $E_a/RT_{vn} \gg 1$.

Radulescu et al. [3–5] proposed stability parameter χ , which is a combination of other stability parameters—a reduced activation energy E_a/RT_{in} , induction to reaction time ratio τ_i/τ_r and the dimensionless chemical energy release Q/RT . Low values of χ parameter are expected to provide a coherent phenomenon in time and space as a result of overlapping power pulses from neighboring particles. For higher values of χ , these power pulses will not be coherent and can lead to instabilities in the 3D reaction zone structure. Dimensional form of χ is called RSB [4] or a_c and indicates the propensity of different reactive mixtures to develop instabilities, strong internal pressure waves and turbulence in the reaction zone:

$$\chi = \frac{E_a}{RT} \cdot \frac{\tau_i}{\tau_r} \cdot \frac{Q}{RT} \quad (2)$$

$$a_c = \chi \cdot \frac{c}{t_i} = \frac{E_a}{RT} \cdot \frac{1}{t_r} \cdot \frac{Q}{RT} \cdot c \quad (3)$$

where: τ_i — induction time, τ_r — reaction time, c — speed of sound.

The RSB parameter can be used for comparison of the relative stability between mixtures. It does not specify a moment when the stability will be lost. It is an indicator which categorizes the detonability of a given mixture, the propensity for engine knock, the propensity of detonable mixture to undergo the deflagration to detonation transition (DDT) process when a turbulent deflagration is established, the propensity for shocks to amplify in reactive medium and the mode of ignition from shock compression.

Summarizing, the indicators of detonability are: the detonation cell size, the induction time, χ parameter or its dimensional form – the RSB. Using ZND theory or Gavrikov formula, the detonation cell size can be extrapolated for mixtures which were not experimentally examined. Nevertheless, these indicators do not provide the same conclusions.

In this paper numerical analyses of detonation propensity of hydrogen-air mixture with addition of methane, ethane or propane were conducted. For this purpose scripts were written in Cantera 2.1.1 in Matlab 7.11.0 R2010b environment. *Shock & Detonation Toolbox* [6] was used for detonation calculations.

2.0 VALIDATION OF CHEMICAL KINETICS MECHANISM

In order to provide the most reasonable results 6 detailed chemical kinetic reaction mechanisms were validated against experimental shock tube data found in the literature. The object of the comparison was the ignition delay time. Considered mechanism were: GRI-mech 3.0 [7], LLNL [8], SanDiego [9], Wang [10], POLIMI C1-C3 [11], AramcoMech C3 [12] (and H₂ Burke [13], for reference). Table 1 summarizes quantitative characteristic of these mechanisms.

Table 1. Quantitative characteristic of considered mechanisms

Mechanism	Number of reactions	Number of species
GRI-Mech 3.0	325	53
LLNL	689	155
SanDiego	244	50
Wang	614	94
POLIMI C1–C3	2078	114
AramcoMech C3	766	124
H ₂ Burke	27	13

Mechanisms with the smallest number of reactions are H₂ Burke, GRI-Mech 3.0 and SanDiego. The POLIMI C1–C3 requires most computing power.

2.1 Experimental data from shock tubes

The self-ignition of gaseous combustible mixtures can be investigated in the shock tubes. One of the parameters describing this phenomenon is the ignition induction time, which is usually defined as a time from the time of the end of compression of the combustible gas to the moment of temperature rise or appearance of the radiation absorption or emission. In reality all methods provide inconsistent results [14].

The induction time from the shock tube studies is vitiated by imperfect conditions. The reasons are viscosity, heat transfer, boundary layer, flow separation and turbulence. Countermeasure against flow separation is an addition of dilution gas, i.e. argon.

Although the ZND theory describes detonation with very good accuracy, it was decided to use another approach of explosion modeling in shock tubes for the purpose of this study – a constant volume explosion [15]. This simplified model can monitor small constant volume area with chemical reactions. If the volume is constant, the Rayleigh line between the Hugoniot adiabat for products and for reactants is vertical, which leads to infinite burning rate.

In order to calculate the induction times for pressures and temperatures defined by experimental data [16–25], the script was written on the basis of function *explosion_CV()* from *Shock & Detonation Toolbox* [6]. It was assumed that experimental data (pressure and temperature) were the postshock parameters.

Table 2. Summary of experimental data used for a mechanism validation

Mixture	No. of points	Pressure [atm]	Temperature [K]	Delay time [μ s]
H ₂ /O ₂ /N ₂ [16–20]	317	0.211-8.844	808-1937	10.1-14600
C ₃ H ₈ /O ₂ /N ₂ [21]	30	7.12-23.6	1154-1443	11-439
C ₃ H ₈ /O ₂ /Ar [22,23]	181	1-14.184	1089-1701	6.2-3096
CH ₄ /O ₂ /Ar [24]	141	0.24-13.01	909-2597	8.57-1762
C ₂ H ₆ /O ₂ /N ₂ [25]	48	0.24-9.41	1196-1697	3-625

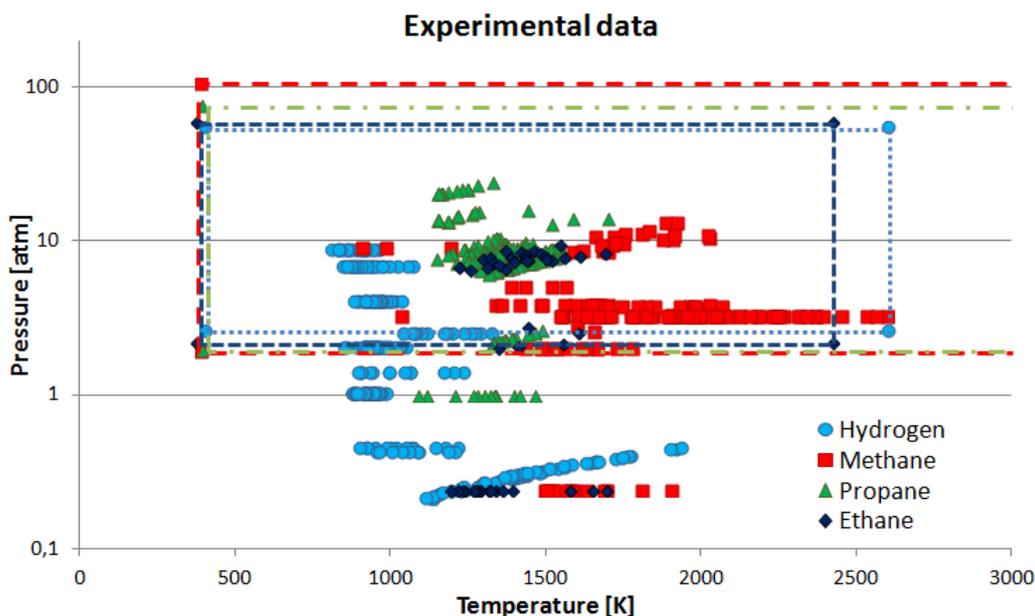


Figure 1. Experimental data – pressure [atm] as a function of temperature [K] [16–25]

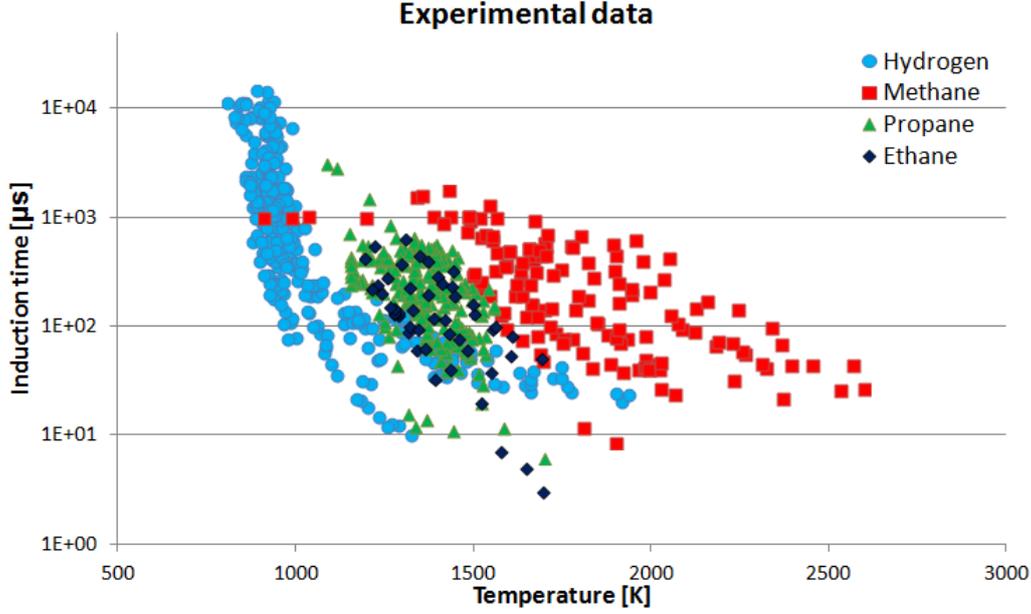


Figure 2. Experimental data – an induction time [μs] as a function of temperature [K] [16–25]

Experimental data [16–25] were collected for mixtures of interest: pure hydrogen, methane, ethane and propane. Summary of data collected is presented in Table 2, Figure 1 and Figure 2. In Figure 1 ranges of $D_{CJ} = 60\%–140\%$ [14] were marked for each mixture. Only data inside of these rectangles were used for validation of mechanisms.

2.2 Calculations

For mechanism assessment the average deviation [14] was calculated:

$$\sigma = \frac{1}{N} \sum_{i=1}^N \log \left(\frac{\tau_{s,i}}{\tau_{e,i}} \right) \quad (4)$$

In order to describe a dispersion of the average deviation following parameter was used:

$$\sigma_{abs} = \frac{1}{N} \sum_{i=1}^N \left| \log \left(\frac{\tau_{s,i}}{\tau_{e,i}} \right) \right| \quad (5)$$

where N is the total number of experimental points θ or simulations \mathcal{S} and τ is the induction time. Figures 3 and 4 show the average deviation σ for all of mixtures. For $\sigma = 0$ an experimental induction time overlaps with this from simulations, for $\sigma = 1$ or $\sigma = -1$ a difference between both times is an order of magnitude.

A computational results were not obtained for all of the experimental points, therefore a percentage of successfully computed results N_{cs} was used for a mechanism assessment. Table 3 summarizes all parameters (σ , σ_{abs} , N_{cs}). The best mechanism would fulfill following criteria: $\sigma \rightarrow 0$, $\sigma_{abs} \rightarrow 0$ and a percentage of computed results $\rightarrow 100\%$. It should be consider whether an insignificant benefit of better simulated reality is not related with much longer computational time, what is a direct result of the amount of reactions in mechanism.

Based on these results for hydrogen mixtures the best is Wang mechanism, for methane SanDiego and Wang, for ethane and propane GRI-Mech 3.0. It was decided to use GRI-Mech 3.0 mechanism for all mixtures.

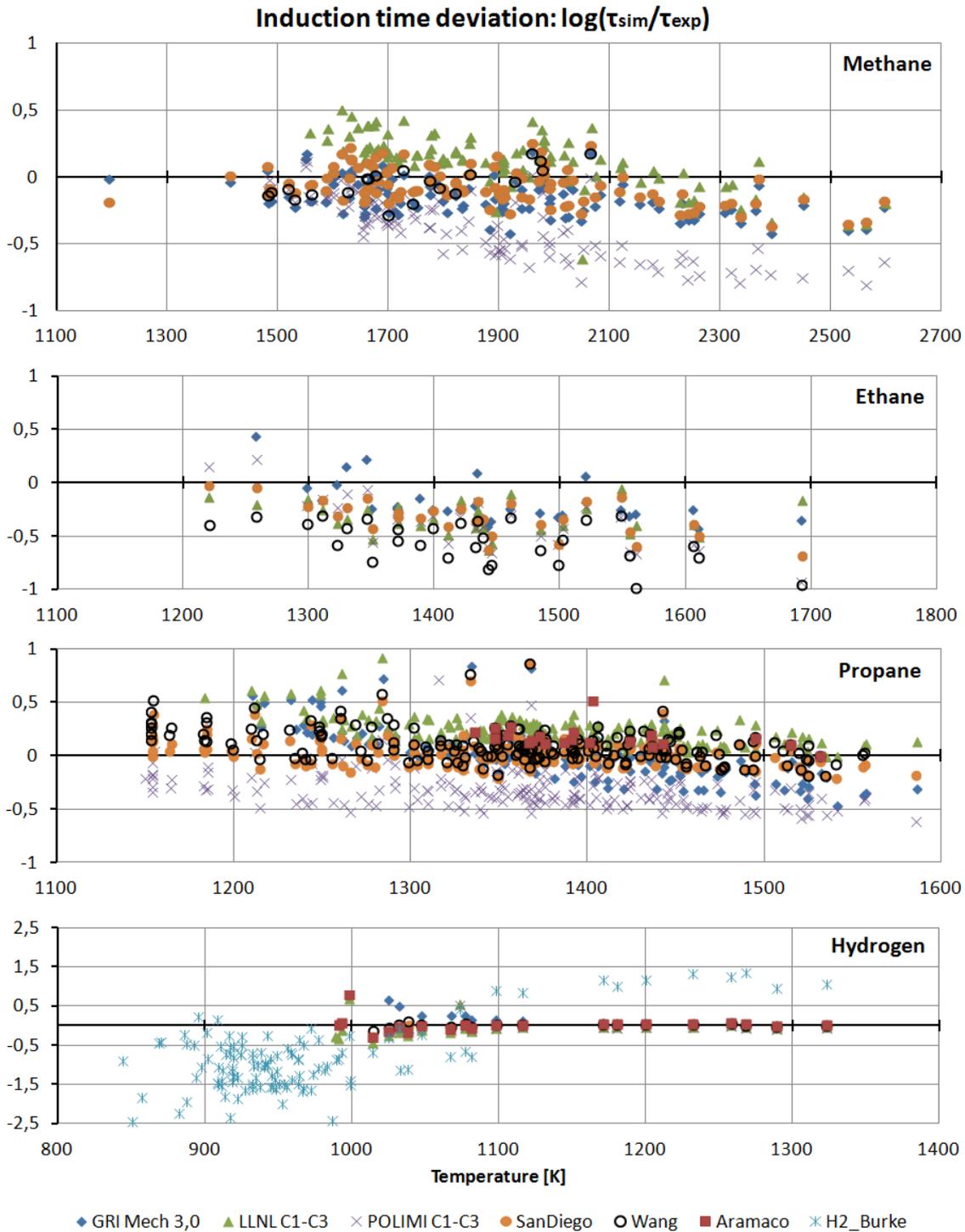


Figure 4. Induction time deviation for methane, ethane, propane or hydrogen mixtures

3.0 CALCULATION OF χ PARAMETER

Dimensionless χ parameter and its dimensional form a_c [3–5] were calculated assuming that initial state is the *von Neumann state* and a detonation wave propagates with *Chapman-Jouguet velocity*.

The *von Neumann state* was calculated using $znd()$ function from *S&D Toolbox* [6], *CJ* velocity $CJ_speed()$. Mixture composition was unchanged across detonation wave (*frozen Hugoniot*, *PostShock_fr()*).

Equation 2 can be written as:

$$\chi = \frac{t_l}{t_r} \frac{E_a}{RT_{vn}} \frac{Q}{RT_0} \left(\frac{T_{vn}}{T_0} \right)^{-1} \quad (6)$$

Dimensionless activation energy E_a/RT_{VN} was assessed based on reaction times behind shocks τ and τ_+ with two different speed D and D_+ . The difference in these times is an effect of different corresponding temperatures T_{vn} and T_{vn+} .

$$\frac{E_a}{RT_{vn}} = \frac{1}{T_{vn}} \frac{\ln(\tau_+) - \ln(\tau)}{\frac{1}{T_{vn+}} - \frac{1}{T_{vn}}} \quad (7)$$

Next equations [26] origin from CJ theory. The adiabatic exponent γ and molar masses remain the same across the shock (*frozen Hugoniot*) and $M_{CJ} \gg 1$.

$$\frac{Q}{RT_0} = \frac{\gamma}{2(\gamma^2 - 1)} \left(M_{CJ} - \frac{1}{M_{CJ}} \right)^2 \quad (8)$$

$$\frac{T_{vn}}{T_0} = 1 + \frac{2(\gamma - 1)\gamma M_0^2 + 1}{(\gamma + 1)^2 M_0^2} (M_0^2 - 1) \quad (9)$$

3.1 Results

Figure 4 shows obtained χ parameter. Taking into account ranges given by Radulescu [3] (Table 4) it is possible to assess the detonation structure of mixtures of interest. Three ranges of cell structure regularity were distinguished – regular, irregular with substructure and very irregular with substructure. Propane mixture in a wide range of hydrogen molar fraction $X_{H_2} = 20\% - 100\%$ exhibits an irregular structure. With increase of H_2 composition the structure is more regular. Ethane mixture has similar behavior with slightly more irregular cellularity. For both mixtures the diagrams are quite flat beginning from $\chi \approx 425$. Methane mixture behaves significantly different – for small dose of hydrogen it exhibits very irregular structure ($\chi \approx 2500$). With increasing H_2 fraction the regularity instantly increases, what results in more regular detonation cell structure for methane mixture than for ethane and propane in a range $X_{H_2} = 50\% - 100\%$. However, in reality this difference could be not visible, such as χ values are similar. All diagrams meet in $X_{H_2} = 100\%$, $\chi = 65$.

Table 4. The variation of the parameter χ computed for a wide range of mixtures and comparison with the regularity of the detonation cellular structure [3]

Mixture	χ	Cellular regularity
H ₂ /O ₂ + 70% Ar	2	Very regular
C ₂ H ₂ /O ₂ + 75% Ar	20	Regular
H ₂ /Air	60	Irregular
C ₂ H ₂ /Air	110	Irregular
C ₂ H ₂ /O ₂	310	Irregular
C ₃ H ₈ /Air	370	Irregular with substructure
CH ₄ /Air	2800	Very irregular with substructure
H ₂ /Air, $\phi = 0.5$	3300	Very irregular with substructure

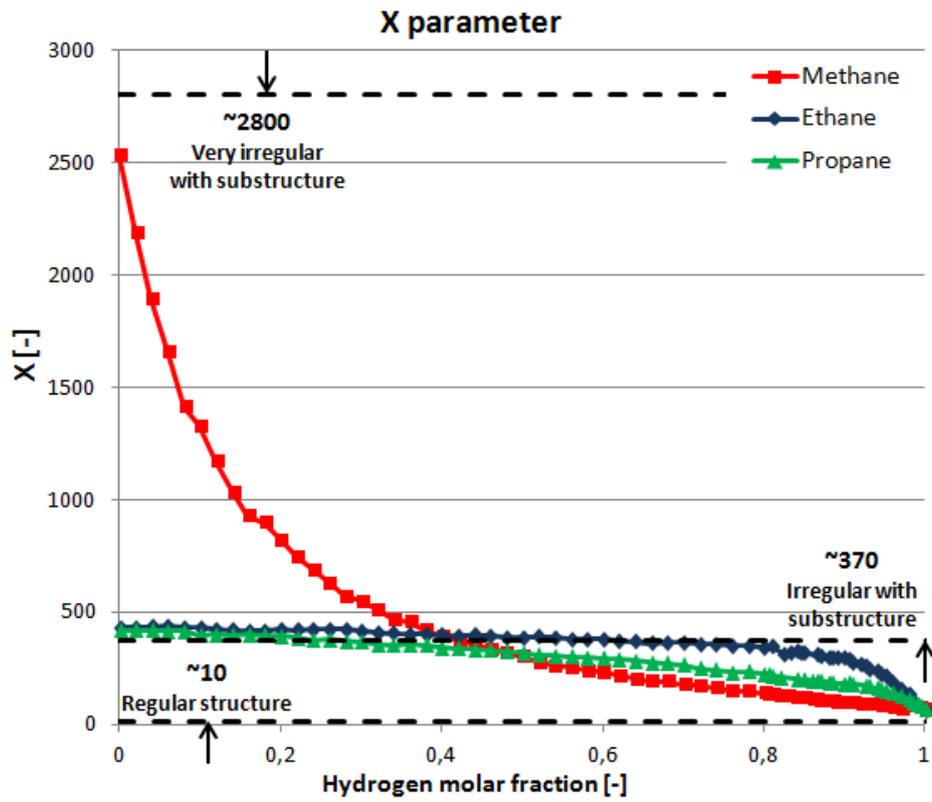


Figure 4. χ parameter [-] as a function of hydrogen molar fraction in fuel [-] with ranges of structure regularity proposed by Radulescu [3].

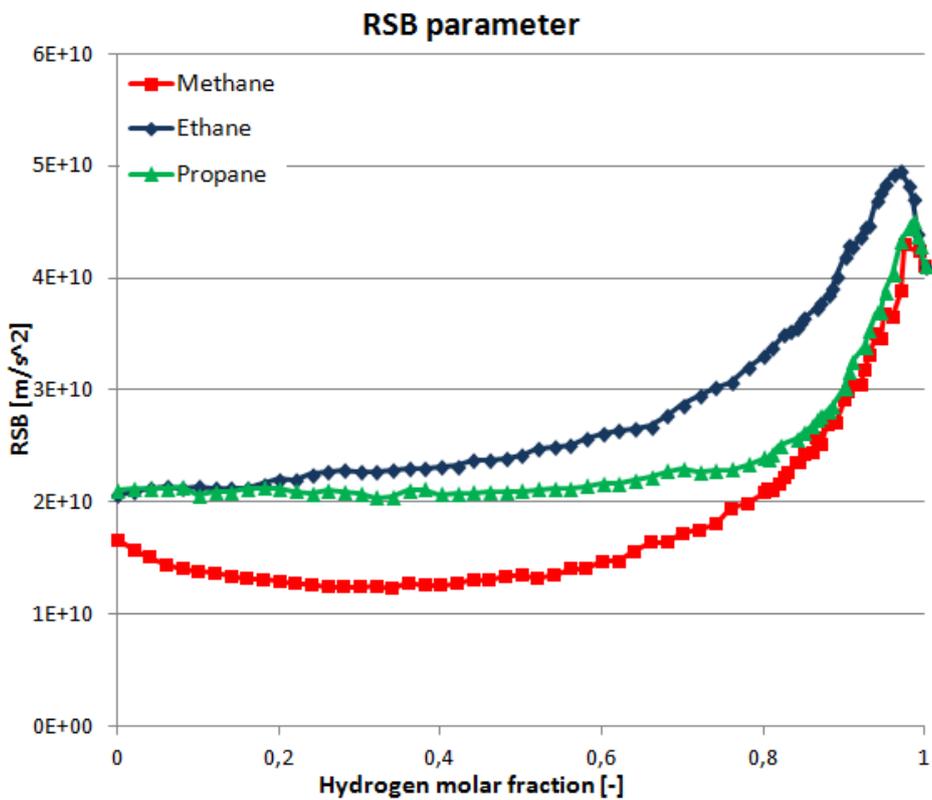


Figure 5. RSB parameter [m/s^2] as a function of hydrogen molar fraction in fuel [-]

The RSB parameter [3–5] was proposed for qualitative description of the propensity to develop instabilities, strong internal pressure waves and turbulence in the reaction zone. Unlike the parameter χ , the diagram of the RSB parameter is similar for all of mixtures of interest. The maximum values of the RSB for all mixtures are reached with mixtures of $X_{H_2} = 97\%–98\%$. Propane and ethane mixtures are characterized by an increasing monotonic function of the RSB with H_2 molar fraction. This increase is stronger for higher H_2 concentrations. Minimum values of the RSB for those two mixtures are obtained for pure ethane or propane, which in fact are almost the same, $RSB \approx 2.1E+10 \text{ m/s}^2$. On the contrary, methane mixtures reaches minimum value of RSB for $X_{H_2} \approx 35\%$ ($RSB \approx 1.2E+10 \text{ m/s}^2$). The highest propensity to develop turbulence, hotspots and instabilities in reaction zone is for mixtures of ethane or propane. Methane remains the most resistant to instabilities. This propensity is smaller for lower concentration of H_2 .

4.0 DETONATION CELL

4.1 Detonation cell width

Due to lack of experimental data for hydrogen-air mixtures with a dope of methane, propane or ethane it was decided to interpolate data for pure species into mixtures with a variable composition. An experimental detonation cell sizes were given for mixtures where the fuel is pure hydrogen ($X_{H_2} = 1$), methane ($X_{CH_4} = 1$), ethane ($X_{C_2H_6} = 1$) or propane ($X_{C_3H_8} = 1$).

Following experimental detonation cell width were used for stoichiometric mixtures:

- methane + air: $\lambda = 350 \text{ mm}$, [27]

- ethane + air: $\lambda = 54 \text{ mm}$, [28]

- propane + air: $\lambda = 46 \text{ mm}$, [29]

- hydrogen + air: $\lambda = 8 \text{ mm}$, [28]

initial conditions were 293 K and 101325 Pa.

The reaction zone width δ is related to the detonation cell size λ by a factor A :

$$\lambda = A \cdot \delta \quad (10)$$

It was assumed that factor A depends linearly from hydrogen molar fraction X_{H_2} in mixture:

$$A_{X,CH_4} = X_{CH_4} \cdot A_{CH_4} + X_{H_2} \cdot A_{H_2} \quad (11)$$

$$A_{X,C_2H_6} = X_{C_2H_6} \cdot A_{C_2H_6} + X_{H_2} \cdot A_{H_2} \quad (12)$$

$$A_{X,C_3H_8} = X_{C_3H_8} \cdot A_{C_3H_8} + X_{H_2} \cdot A_{H_2} \quad (13)$$

where A_{CH_4} , $A_{C_2H_6}$, $A_{C_3H_8}$ and A_{H_2} were leaded from Equation 7 and appropriate δ was used from calculations.

Two methods were used for δ assessment. The first one was based on ZND theory. The initial conditions were 300 K and 101325 Pa. Calculations were provided for stoichiometric mixtures using mechanism validated in previous section. The second method of calculation of the reaction zone width was based on Gavrikov's formula [2], Eq. 1. Figure 6 presents detonation cell sizes for both methods.

Detonation cell width λ computed using ZND model provides similar pattern of ethane or propane mixtures. In a wide range of hydrogen molar fraction 0–75% the detonation cell size equals to $\sim 50 \text{ mm}$, then it decreases to 8 mm. Methane mixtures have the widest cells in range of $X_{H_2} = 0–65\%$, beginning from 350 mm for pure methane. For $X_{H_2} = 65\%–100\%$ these cells are narrower than cells of hydrogen mixtures with addition of propane or ethane. Summarizing, hydrogen-air mixtures with addition of ethane or propane have similar propensity for detonation and it is higher than for mixtures with addition of methane. Detonability of methane mixtures increases with H_2 concentration in fuel faster than detonability of ethane and propane mixtures. Gavrikov's formula provides noticeably

different results. For $X_{H_2} = 28\%$ propane cell width reaches the maximum value of 148 mm, what indicates the difference in mixtures' detonability. Additionally, diagram of cell width for methane decreases slower for ZND model. Based on Gavrikov's formula, in range of $X_{H_2} = 12\%–100\%$ methane or propane mixtures have similar detonability, which is lower than detonability of mixture of propane. In the rest of range the most detonable are methane mixtures.

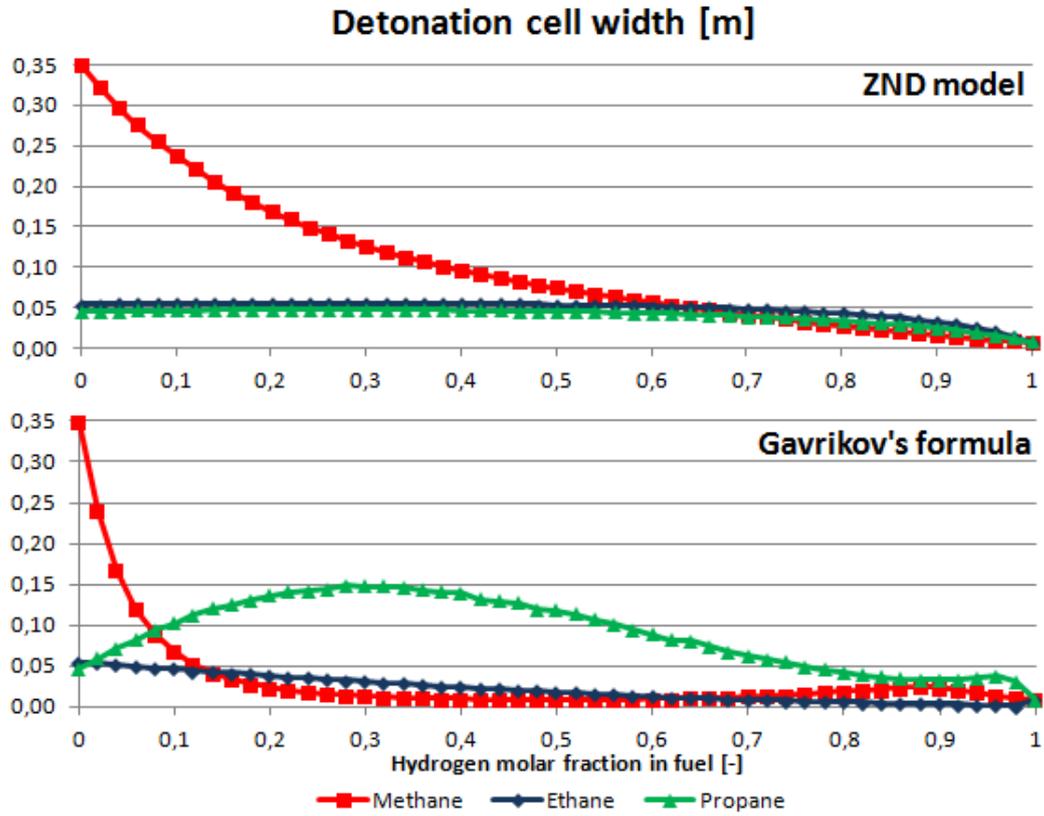


Figure 6. Detonation cell width [m] computed using Gavrikov's formula and ZND model

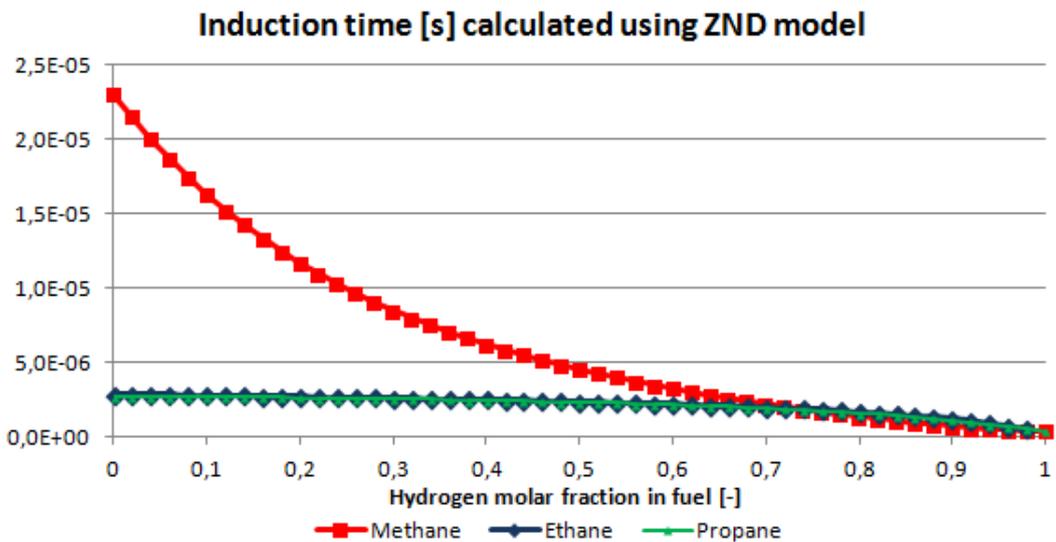


Figure 7. Induction time [s] computed using ZND model

5.0 INDUCTION TIME

Figure 7 presents the induction time τ_i for mixtures of interest calculated using ZND model. The pattern of the diagram is very similar to detonation cell width calculated with ZND model. The difference between ethane and propane mixtures is less than 5% (smaller than for cell width, where maximum difference is 24%). In range of $X_{H_2} = 0\%–74\%$ methane mixtures have longer induction times, than mixtures of propane or ethane. The induction time decreases with increase of hydrogen molar fraction in fuel. The longest induction delay time is obtained for pure methane ($\tau_i = 2,3E-05$ s). For pure propane or ethane induction time equals to $\tau_i = 2,8E-05$ s. Pure hydrogen has the shortest ignition delay time (two orders of magnitude, $\tau_i = 3,85E-07$ s).

6.0 CONCLUSIONS

In this study, the detonation propensity of stoichiometric hydrogen-air mixtures with addition of methane, ethane or propane has been analyzed in range of 0%–100% hydrogen molar fraction in the fuel. The χ parameter, its dimensional form a_c [3–5], the detonation cell width λ [2] and the induction delay time τ_i were assessed. The detailed chemical kinetic reaction mechanism – GRI-mech 3.0 was used as a result of validation of calculated ignition delay times against experimental data. All parameters indicate significantly different behavior of methane mixtures, particularly for lower concentration of H_2 in fuel. Although these hydrogen-poor mixtures develop irregular cellular structure (χ), induced detonations have low propensity for hotspots and instabilities formation in the reaction zone (a_c), what is consistent with relatively low detonability of mixture (τ_i, λ). Comparing ethane and propane mixtures, ethane has slightly more irregular cellular structure (χ) and it is more prone to generate turbulence in the reaction zone (a_c). The most detonable mixtures are those with high hydrogen molar fraction (τ_i, λ). The effect of hydrogen addition on mixture properties depends on the hydrocarbon fuel. Noticeably different cell sizes obtained with ZND model and Gavrikov's formula for mixtures of hydrogen and light hydrocarbons require further experimental investigation.

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