Numerical study of two-dimensional structure of detonation front in two-fuel mixtures

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Abstract. The numerical simulation of a two-dimensional multi-front structure of detonation waves (DWs) in two-fuel mixtures has been carried out. These studies are based on the proposed two-stage generalized model of chemical kinetics of detonation combustion of a two-fuel mixture: hydrogen and carbon monoxide (synthesis gas) with an oxidizer. This kinetics allowed performing for the first time a two-dimensional numerical calculation of the DW parameters and the irregular cellular front structure in this two-fuel mixture at various concentrations of hydrogen. Stoichiometric compositions with oxygen and air as oxidizing agents have been studied. The transverse sizes of detonation cells in the studied mixtures have been obtained. The decrease in the hydrogen concentration leads to a significant increase of the cell size and an increase of the degree of irregularity of DW multi-front structure.

1. Introduction
To date, the numerical simulation of a multi-dimensional multi-front (cellular) structure of a gas detonation wave (DW) is limited, as a rule, to mixtures based only on one fuel with an oxidizer and inert diluents (see, for example, calculations [1, 2]). Apparently, this is due to the lack of appropriate chemical kinetics models suitable for 2D numerical simulation of multi-fuel mixtures and not requiring tremendous numerical calculations. The use of detailed kinetic schemes for the oxidation of hydrocarbon fuels contains, as a rule, hundreds of elementary reactions. On the other hand, these generalized models of detonation kinetics should have sufficient accuracy to describe chemical transformations.

Meanwhile, multi-fuel gas mixtures are widely found in nature and technology. Such mixtures also include a mixture of hydrogen with carbon monoxide (synthesis gas, syngas), used both in the chemical industry and in power engineering. To solve the problems of explosion safety in these sectors of the economy, it is necessary to simulate detonation processes in this mixture. Among other things, it is necessary to numerically calculate the parameters and the two-dimensional multi-front structure of the detonation wave in such a mixture in order to determine such an important parameter in gas detonation as the transverse size of the detonation cell $a_0$. Knowledge of the value of $a_0$ allows us to predict the critical size of the DW propagation channel, the critical energy of direct initiation of the DW, and a number of other important parameters for the origin and propagation of detonation.

In connection with this issue, in present work a two-dimensional numerical simulation of the structure and parameters of the DW in a mixture of synthesis gas with oxygen and air has been carried out. These studies are based on the chemical kinetics model of detonation combustion of a syngas two-fuel mixture proposed by us in [3, 4]. Previously, the parameters of the DW in synthesis gas [5] and the
problems of determining the duration of the induction period for detonation of multi-fuel mixtures [6] were studied by Vasil’ev.

2. Governing equations and chemical model of detonation kinetics

The dynamics of the compressible chemically reactive medium is described by the two-dimensional Euler equations. The chemical reaction in the DW is described according to the two-stage model of the detonation kinetics (a stage of induction period and main heat release stage) first proposed in [7].

A generalized model of detonation kinetics for describing chemical transformations in a two-fuel mixture of carbon monoxide CO and hydrogen H₂ was proposed in [3, 4]. The kinetics is applicable to a mixture of synthesis gas with oxygen, inert diluents and water vapor of the form (1-α)CO+αH₂+α₃O₂+a₄N₂+a₅Ar+a₆H₂O. This generalized kinetic model is a further development of the previously developed models of the chemical kinetics of detonation combustion of hydrogen-oxygen mixtures [8,9] and mixtures based on methane [2]. Currently, the model of detonation kinetics for hydrocarbon two-fuel mixtures of the form (1-α)CO+a₆CₙHₘ+α₃O₂+a₄N₂+a₅Ar+a₆H₂O is at the stage of developing and conducting 2D test simulations.

In this kinetic model, it is assumed that during the induction period chemical transformations do not occur in the mixture, and, accordingly, the molar mass of the gas does not change, and the heat release of the chemical reaction is zero. A semi-empirical Arrhenius-type formula is proposed for calculating the duration of the induction period in mixtures with synthesis gas [4], based on experimental data on the sizes of detonation cells in these mixtures for various values of the hydrogen fraction α. The constants of Arrhenius-type formula for calculating the induction period in pure monofuel mixtures of hydrogen and CO with an oxidizer are assumed to be known from experiment or from detailed chemical modeling.

After the end of induction period and the beginning of the heat generation stage, one differential kinetic equation is used to calculate the average molar mass of the gaseous reacting mixture [1, 2, 4, 9]. Based on this value and using algebraic formulas, the amount of heat release is calculated, as well as the temperature and pressure in this zone.

In our previous numerical simulation [1] of the two-dimensional regular cellular DW structure in hydrogen–oxygen mixtures with the proposed kinetics of heat-release stage, good agreement was obtained between the numerical results and experimental data on the detonation cell size over a wide range of initial pressures below 1 atm and degrees of dilution with argon.

The system of governing equations was closed by the well-known thermal equation of state for an ideal gas.

Numerical simulation has been performed for a stoichiometric syngas–air and syngas–oxygen mixtures at normal initial conditions p₀=1 atm and T₀=298.15 K.

DW propagation in a two-dimensional straight-line channel has been studied. The slip conditions (impermeable solid wall) [10] were imposed on the upper, lower, and left boundaries of the channel, and the right boundary was subjected to the condition of an undisturbed initial state of the gas. The detonation wave was initiated near the left closed end of the channel and propagated from left to right along the x axis. The size and energy of the initiation source [1, 2] were chosen sufficiently large to ensure a supercritical regime of DW direct initiation in investigated mixtures.

3. Numerical method

The resultant systems of equations were solved numerically using the code based on the finite-volume scheme [10] with the fourth-order MUSCL TVD reconstruction [11] and the advanced HLLC algorithm [12] for an approximate solution of the Riemann problem. In implementation of this algorithm for the case of a chemically reacting mixture, the “energy relaxation method” [13] was used. This method eliminates the problem of numerical solution of the Riemann problem for a medium with a complicated nonlinear equation of state (including that with a variable ratio of specific heats). Integration in time was performed with second-order accuracy by using recently developed additive semi-implicit Runge-Kutta methods [14].
The use of adaptive moving grids with the total number of cells \( N_x \) in the \( x \) direction with local refinement (uniform grid with the cell size \( h_x \) and the cell number \( N_{x1} \) in the vicinity of a leading shock front and a nonuniform grid with cell number \( N_{x2}=N_x-N_{x1} \) that occupied the region between the closed left end of the channel and the beginning of the uniform grid) allowed us to have a fine resolution where necessary, using a significantly smaller number of cells, as compared with a uniform splitting of the computational domain. A uniform motionless grid with the total number of cells \( N_x \) and cell size \( h_y=H/N_y \) was used in the \( y \) direction, where \( H \) is the height of channel. Almost in all calculations \( h_x = h_y \). The special preliminary computations have been performed for studied mixtures to determine required numerical grid resolution that is needed to get grid-independent results.

The time step was determined at each time layer of the solution from the stability condition [10]. In the present simulations, the values of the Courant number were CFL=0.3–0.4. The codes are parallelized with MPI library using the "domain decomposition" technique. In this study, the base calculations were carried out on 256 processor cores and \( N_x=2000 \), \( N_{x1}=1750 \), \( N_y=2000 \).

4. Results of simulation

The detonation cell size for the syngas-based mixture has been determined in a procedure similar to that used in the numerical study of hydrogen mixtures [1]. The initial height of the channel \( H \) has been chosen rather arbitrarily; usually, it was assumed to be slightly higher than the presumed transverse size of the cell \( a_0 \). Further variation of \( H \) in the calculations affected the number of primary (main) transverse waves (TWs) remaining at the DW front after its initiation and the establishment of a self-sustained Chapman–Jouguet detonation regime. The value of \( H \) has been found at which two equal and antisymmetrically moving TWs remained on the front of the DW, thus, the cell size was determined as \( a_0=H \).

As a first stage, the multi-front structure of the DW in a stoichiometric mixture of 0.9CO+0.1H\(_2\)+0.5O\(_2\) synthesis gas with oxygen \((\alpha=0.1)\) has been investigated. To begin with, the 2D cellular structure of the DW in a wide channel with a height of \( H=3.25 \) cm was studied after detonation reached a self-sustaining Chapman–Jouguet regime with a constant (on average) propagation velocity. Simulation has shown that for a given value of \( H \), there are about 10–11 detonation cells on the front of the DW. In addition to the main transverse waves, there is a significant amount of secondary (smaller, but sometimes not less intensive) TWs on the front. A similar structure of the DW was obtained in simulation of the detonation in methane based mixtures [2]. In general, the cellular structure of the DW in a mixture of synthesis gas \((\alpha=0.1)\) with oxygen is rather irregular, and the movement of the main TWs is rather unharmonic (chaotic).

To reveal the prevailing transverse size of the detonation cell \( a_0 \), a series of numerical experiments with decreasing channel height \( H \) has been carried out; as a result, \( H=0.3 \) cm \( \geq a_0 \) and \( H=0.25 \) cm \( \leq a_0 \) has been obtained. These calculations have a higher spatial resolution than in the case of \( H = 3.25 \) cm. Analysis of 2D flow fields shows that at the front of the DW in this mixture at \( H= a_0 \) there are several secondary TWs and a significant numbers of tertiary and even smaller TWs. At some points in time, unburned gas packets are observed behind the DW front. So, the features of the DW multifront structure in the mixture under consideration are investigated, and the size of the detonation cell is defined as \( 0.25 \leq a_0 \leq 0.3 \) cm. Note that this \( a_0 \) well corresponds to the \( a_0 \) size for this mixture calculated using the Vasil’ev Nikolaev analytical formula [15].

Similarly, a two-dimensional multifront (cellular) DW structure has been numerically investigated in a stoichiometric mixture of synthesis gas with air \((1-\alpha)CO+\alpha H_2+0.5 Air\), using a variation of the channel width \( H \). Figure 1 shows the simulation of the DW structure for \( \alpha=0.3 \) after the detonation reaches a self-sustaining regime with a constant (on average) propagation velocity. Two-dimensional flowfields of numerical Schlieren-visualization (figure 1a) and normalized density (figure 1b) in a channel with height \( H=0.35 \) cm are shown. The symbols AA and BB show a pair of main transverse waves.

With a given value of \( H \), these TWs are almost symmetrical about the channel axis and move in the opposite direction, as it should be in a classical detonation cell. At the time shown, the BB main
bottom TW a little earlier come to the channel wall and already completes the process of reflection. The AA upper TW is in the process of reflection: its head has not yet reached the wall of the channel. The symbols aa and bb show some of the numerous secondary TWs, both smaller in size and in amplitude, also existing on the leading shock front of the DW.

Further, a series of calculations with the variation of $H$ has been carried out for $\alpha=0.1$. The multi-front structures of DW in channel with $H=1.2$ cm is shown in figure 2. In this case, we have also two almost identical main TWs. Comparing the structure of the DW in figure 1 and figure 2, it may be concluded that with a decrease of the hydrogen concentration in the mixture, the degree of irregularity of the multi-front structure of the DW front increases, the number of secondary TWs on the wave front increases, and the formation of unburned gas packets behind the wave front begins. Such a gas package is designated as P1 on figure 2.

So, in the series of 2D numerical simulation of detonation in a syngas-air mixture, it was found that the transverse size of the detonation cell at $\alpha=0.3$ is $a_0=0.35$ cm, and at $\alpha=0.1$ it is $a_0=1.2$ cm. Calculations for different values of $H$ show that 2D multi-front structure of the DW qualitatively coincides with the DW structure in the syngas-oxygen mixture, that is, it is moderately irregular.

5. Discussion and Concluding Remarks

The two-step reduced model of the chemical kinetics of detonation combustion of a mixture of two combustibles: hydrogen and carbon monoxide (synthesis gas) with an oxidizing agent has been proposed. This allowed performing a two-dimensional numerical calculation of the parameters and the cellular structure of the detonation wave in this two-fuel mixture with oxygen and air at various concentrations of hydrogen.

Simulation of detonation in a stoichiometric mixture of 0.9CO+0.1H$_2$+0.5O$_2$ syngas with oxygen ($\alpha=0.1$) has shown that the cellular structure of the detonation wave in the mixture under consideration is irregular. It is characterized by a moderately chaotic uncoordinated movement of the main TWs, the existence of numerous secondary (sometimes tertiary) TWs at the leading shock front, forming a hierarchy of the decreasing in size DW front perturbations, and a spontaneous formation of unreacted gas packets behind the DW front.
The detonation cell size in this mixture is $0.25 \leq a_0 \leq 0.3$ cm. Note that the experimental cell size in a pure stoichiometric hydrogen-oxygen mixture ($\alpha = 1.0$) under standard initial conditions is $a_0 = 0.14 \div 0.16$ cm [16]. The DW structure in a pure hydrogen mixture is regular. Thus, as follows from the calculations performed a strong dilution of the hydrogen-oxygen mixture with carbon monoxide leads to a significant increase in the cell size. And the original regular multifront DW structure is replaced by an irregular structure.

An increase in the cell size with a decrease in the fraction of hydrogen was also obtained for the detonation in the mixture of synthesis gas with air. There are $a_0 = 0.35$ cm for $\alpha = 0.3$ and $a_0 = 1.2$ cm for $\alpha = 0.1$. This result corresponds qualitatively to the experimental data [17], which show the growth of $a_0$ in syngas-air mixture. However, the cell size $a_0$ obtained in the 2D calculations is approximately $2 \div 2.5$ times smaller than the experimental cell size [17].

The quantitative difference between the calculated cell size and the experimental data for this two-fuel mixture can be apparently explained by incompletely accurate kinetics of the induction period [18,19] found in our 2D calculations. These so-called global kinetics models are obtained from the processing of experimental data on ignition delays at low initial pressures in the hydrogen mixture. Empirical dependences in the form of analytical formulas [18,19] describe the duration of the induction period for a pure monofuel hydrogen mixture as a function of the initial concentration of the reacting components (initial pressure) and the current temperature of the mixture. And they, apparently, are not entirely accurate when extrapolating to pressures close to atmospheric.

Additional calculations of the detonation in a pure ($\alpha = 1.0$) stoichiometric mixture of hydrogen with oxygen and air under standard initial conditions have given the following results. For an oxygen mixture, 2D calculation using induction kinetics [18] has given $a_0 = 0.075 \div 0.08$ cm, and with [19] kinetics cell size is $a_0 = 0.08$ cm. These values are about 1.9 times smaller than the experimental size $a_0 = 0.14 \div 0.16$ cm [16]. Calculation results in our work [1] and the data of additional calculations with increased spatial resolution, presented here, show that up to the initial mixture pressure $p_0 = 0.4$ atm there is a perfect match (within the measurement error) of the calculated values of $a_0$ with experimental values of $a_0$ for hydrogen-oxygen mixture. When the initial pressure increases, the discrepancy described above appears.
Figure 3. Detonation wave structure in a stoichiometric pure hydrogen-air mixture ($\alpha=1$) in channel with $H=0.3$ cm, flowfields of: (a) numerical Schlieren-visualization; (b) normalized density.

Figure 3 presents the calculation of the detonation of a hydrogen-air mixture in a channel with $H=0.30$ cm. The kinetics of the induction period by [19] has been used. Based on the analysis of the flow fields for different $H$, it can be concluded that the calculated cell size $a_0$ is close to 0.3 cm. Indeed, at $H=0.30$ cm, we have two almost perfectly symmetrical TW labeled as AA and BB, see figure 3. This $a_0$ value is much smaller than the experimental data $a_0=1.0\div1.5$ cm. Apparently, an additional error in determining the duration of the induction period according to [18, 19] for detonation of a hydrogen–air mixture is introduced by a change in the initial concentration of the reacting components of the mixture due to dilution of the initial pure mixture with inert nitrogen. It may be assumed that the concentration dependence of the duration of the induction period is more complex than that presented in the formulas [18, 19].

Thus, it becomes necessary to construct the corrected global kinetics of the induction period for hydrogen mixtures, which gives more realistic results at initial pressures close to 1 atm. We plan to address this issue in our future research.

Acknowledgments
The authors gratefully acknowledge the financial contribution from the Russian Foundation for Basic Research (Grant No. 17-03-01351). The research was carried out using supercomputers at Joint Supercomputer Center of the Russian Academy of Sciences (JSCC RAS).

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