

Analysis of the Kinetic Data Described Oxygen-Hydrogen Mixtures Combustion

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Abstract

The main bases contained kinetic data on rate constants of gas-phase chemical reactions in H₂-O₂ system published up to 2008 were analyzed. The generalized database with rate constants of reactions between components in ground electronic states is presented. Several combustion mechanisms were tested by comparison of experimental results and simulation of ignition delay-times of oxygen-hydrogen mixtures behind a front of incident shock wave. The problems of available combustion mechanisms for H₂-O₂ gas mixtures are marked.

Introduction

An interest to combustion modeling has a long history, and at present it does not failed. At last years some new works were appeared, and detailed kinetic mechanisms of oxygen-hydrogen mixtures combustion were analyzed by authors. First of all, it is Konnov's work [1] supported substantially on review of Baulch and coauthors [2]. The database chemical reactions with corresponding kinetic coefficients was tested in [1] using experimental data obtained in reflected shock waves, burners, flowing reactors.

The base of kinetic data in the present work is founded on the analysis of earlier published combustion mechanisms and is substantially similar to data [1]. The essential difference of present work is that the testing of proposed reaction mechanism and several others was fulfilled by comparison with the results of own measurements of hydrogen ignition delay-time behind the front of incident shock waves. Gas pressure range was from parts of atmosphere up to several atmospheres. The reduced mechanism [3] was also tested.

The mechanism of hydrogen combustion

In the present work the data of earlier published databases on combustion modeling [1, 4-21] are compared, and under their discussion the conclusions concerning recommended values of rate constants are made. In details the selection of recommended rate constants is discussed in [22]. The results are given in Table 1.

Together with reactions important for combustion, the reactions involving ozone, some reactions of dissociation and others reactions inessential for combustion were also included to Table 1. In other bases of combustion data these reactions are absent. In Table 1 the reactions of dissociation-recombination with argon as collisional partner were also included. The rate constants of dissociation and recombination were represented only in low pressure limits.

If there was enough data concerning rate constants for direct and reverse reactions, both values of rate constants were included in Table 1 (reaction number is the same one for both directions, reverse reaction

number has sign "minus"). If a rate constant for one direction was known, then in Table 1 this value was only included. When the data on measured rate constants of dissociation or recombination for collisional partner M were absent, one of the essential sources of rate constant uncertainties in different works was the significant scatter of partner efficiencies, often exceeding one order. In the present work it is recommended to use the following efficiencies of partners M (their values were obtained as a result of data average given in works [4, 7-9, 14]): Ar : O : H : N₂ : O₂ : H₂ : OH : O₃ : HO₂ : H₂O : H₂O₂ = 1 : 11.7 : 5.5 : 1.7 : 3.3 : 2.8 : 2.9 : 17 : 17 : 17 : 17.

In works [2, 5-8, 15] the reaction H₂+O₂=OH+OH (27) was not taken into account in combustion mechanisms. Authors of theoretical and experimental study [28] considered the rate constant of this reaction equal to zero. Author of works [1, 9, 11] kept this reaction in the model of hydrogen combustion from theoretical work [34] ($k=2.04 \cdot 10^{12} \cdot T^{0.44} \cdot \exp(-39000/T)$, cm³/mol.c, T=298-1000K) "only for the base completeness". Indeed, this rate constant is 2-3 orders smaller than parallel hydrogen-oxygen product channel H₂+O₂=H+HO₂. (It is necessary to note, however, that on the site [10] (renewed in 2007) for hydrocarbon combustion mechanism the same author presented significant greater rate constant from [35]: $k=2.5 \cdot 10^{12} \cdot \exp(-19628/T)$, cm³/mol.c, T=1400-2500K).

The authors of many publications consider necessary to take into account the reaction (27) to make fitting of their calculations and available experimental data on ignition delay-times, the velocity of flame expansion and so on. In [3] the rate constant (27) from [33] was recommended: $k=1.7 \cdot 10^{13} \cdot \exp(-24044/T)$ cm³/mol.c. Still greater rate constants were used in [36-38]. In particular, in [36] the rate constant was given equal to $k=6 \cdot 10^{14} \cdot \exp(-24180/T)$ cm³/mol.c for agreement of experimental data and results of modeling.

In the present work the rate constant for reaction (27) was selected from work [33]. Indeed in a number of cases, the generation of active agents in this reaction allowed to reach the better agreement of experiments and simulation. However, it is necessary to remember the use of this reaction contradicts the mentioned theoretical and experimental data.

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Table 1. Reaction mechanism for H₂–O₂ system.
 $k = AT^n \exp(-E/T)$, (cm³/mol)^{m-1}/s (m is reaction order); the value Δlg k is uncertainty factor.

	Reaction	M	T, 10 ³ K	A	n	E, K	Δlg k	Source
1	H ₂ +M→H+H+M	H ₂	2.5 - 8	9.03·10 ¹⁴	0	48350	0.5	[2]
		H ₂ O	0.6 - 2	8.43·10 ¹⁹	-1.1	52530	0.7	[2]
		Ar	2.5 - 8	2.23·10 ¹⁴	0	48350	0.3	[2,12]
-1	H+H+M→H ₂ +M	H ₂	0.2 - 5	1.0·10 ¹⁷	-0.6	0	0.5	[23]
		H ₂ O	0.3 - 2	1.0·10 ¹⁹	-1	0	0.7	[23]
		H	0.3 - 5	3.2·10 ¹⁵	0	0	0.5	[23]
		Ar	0.2 - 2.5	6.53·10 ¹⁷	-1	0	0.5	[2,16]
2	O ₂ +M→O+O+M	O ₂	2 - 8	9.8·10 ²⁴	-2.5	59380	0.3	[17]
		O	2 - 8	3.5·10 ²⁵	-2.5	59380	0.4	[17]
		O ₃ , H ₂ O	2 - 5	1.2·10 ¹⁹	-1	59380	1.0	[24]
		Ar	3 - 18	1.8·10 ¹⁸	-1	59380	0.3	[17]
-2	O+O+M→O ₂ +M	O ₂	0.3 - 5	8.0·10 ¹⁷	-1	0	0.5	[1,25]
		O	0.3 - 5	2.88·10 ¹⁸	-1	0	0.3	[1]
		O ₃	0.3 - 4	1.3·10 ¹⁴	0	-900	0.8	[24]
		H ₂ O	0.2 - 4	3.51·10 ¹⁴	0	-900	0.3	[8]
		Ar	0.3 - 5	1.0·10 ¹⁷	-1	0	0.3	[1]
3	O ₃ +M→O ₂ +O+M	O ₂	0.2 - 1	1.54·10 ¹⁴	0	11600	-	[24]
		O	0.2 - 1	2.48·10 ¹⁵	0	11430	-	[24]
		O ₃	0.2 - 1	4.4·10 ¹⁴	0	11600	0.2	[24]
		Ar	0.2 - 1	2.48·10 ¹⁴	0	11430	0.1	[17]
-3	O ₂ +O+M→O ₃ +M	O ₂	0.1 - 0.3	6·10 ²⁰	-2.6	0	0.1	[6]
		O	0.2 - 0.4	7.2·10 ¹⁹	-1.9	0	-	[24]
		O ₃	0.2 - 1	4.97·10 ¹⁹	-1.9	0	-	[24]
		Ar	0.2 - 0.37	7.2·10 ¹⁸	-1.9	0	0.1	[19]
4	H+O+M→OH+M	H ₂	0.3 - 3	2.0·10 ¹⁹	-1	0	-	[1,9]
		O ₂	0.3 - 3	1.35·10 ¹⁹	-1	0	-	[1,9]
		H ₂ O	2.95 - 3.7	1.1·10 ²⁰	-1	0	0.5	*
		Ar	2.95 - 3.7	6.75·10 ¹⁸	-1	0	0.5	[1,9]
5	H ₂ O+M=H+OH+M	O ₂	2 - 6	3.5·10 ¹⁵	0	52920	-	[22]
		H ₂ O	2 - 4	2.26·10 ¹⁶	0	52920	0.2	[16]
		Ar	2 - 4	1.35·10 ¹⁵	0	52920	0.3	[2]
-5	H+OH+M→H ₂ O+M	H ₂	0.3 - 1.25	1.61·10 ²²	-2	0	0.5	[7]
		O ₂	0.3 - 3	2.2·10 ²²	-2	0	-	[22]
		OH	1.74 - 1.9	8.34·10 ¹⁵	0	0	-	[26]
		H ₂ O	0.3 - 3	1.4·10 ²³	-2	0	0.5	[16]
		Ar	0.3 - 3	8.34·10 ²¹	-2	0	0.3	[16]
6	O ₂ +H+M→HO ₂ +M	H ₂	0.3 - 2	8.55·10 ¹⁹	-1.4	0	0.5	[1]
		O ₂	0.3 - 0.7	5.69·10 ¹⁸	1.094	0	0.11	[1,27]
		H ₂ O	0.3 - 2	3.63·10 ¹⁹	-1.0	0	0.1-0.3	[2]
		Ar	0.3 - 2.	6.9·10 ¹⁸	-1.2	0	0.1-0.2	[2]
7	H ₂ O ₂ +M→OH+OH+M	Ar	1 - 1.5	2.29·10 ¹⁶	0	21960	0.2	[2]
		N ₂	0.7 - 1.5	1.21·10 ¹⁷	0	22900	0.2	[16]
-7	OH+OH+M=H ₂ O ₂ +M	N ₂	0.25 - 1,4	2.38·10 ¹⁹	-0.8	0	0.4	[2]
8	H ₂ +O ₂ →H+HO ₂		0.4 - 2.3	7.4·10 ⁵	2.43	26926	0.3-0.5	[28]
-8	H+HO ₂ →H ₂ +O ₂		0.25 - 1	1.05·10 ¹⁴	0	1030	0.3	[1,2]
9	H+HO ₂ →H ₂ O+O		0.3 - 1	3.0·10 ¹³	0	866	0.5	[18]
10	H ₂ +OH→H+H ₂ O		0.25 - 2.4	2.17·10 ⁸	1.52	1740	0.1-0.3	[1,2]
-10	H ₂ O+H→H ₂ +OH		0.8 - 2.5	4.52·10 ⁸	1.6	9030	0.2	[2]
11	OH+OH→H ₂ O+O		0.25 - 2.4	3.35·10 ⁴	2.42	-970	0.15	[1,2,29]
12	O ₂ +H→OH+O		0.8 - 3.5	2.06·10 ¹⁴	-0.097	7560	0.1-0.2	[1,2]
-12	OH+O→H+O ₂		0.25 - 3	1.21·10 ¹⁴	-0.352	-113	0.2	[2]
13	H ₂ +O→OH+H		0.3 - 3	5.1·10 ⁴	2.67	3165	0.2	[12,30]

14	$\text{HO}_2 + \text{O} \rightarrow \text{OH} + \text{O}_2$		0.22 - 1	$1.63 \cdot 10^{13}$	0	-224	0.1-0.5	[2]
15	$\text{HO}_2 + \text{H} \rightarrow \text{OH} + \text{OH}$		0.25 - 1	$4.46 \cdot 10^{14}$	0	700	0.15	[2]
16	$\text{OH} + \text{HO}_2 \rightarrow \text{H}_2\text{O} + \text{O}_2$		0.25 - 2	$2.9 \cdot 10^{13}$	0	-250	0,2	[1]
			+	$9.3 \cdot 10^{15}$	0	8810	0.5	**
17	$\text{OH} + \text{O}_3 \rightarrow \text{O}_2 + \text{HO}_2$		0.2 - 0.45	$1.03 \cdot 10^{12}$	0	940		[5]
18	$\text{O}_3 + \text{O} \rightarrow \text{O}_2 + \text{O}_2$		0.2 - 0.4	$4.82 \cdot 10^{12}$	0	2060	0.3	[5,6]
19	$\text{O}_3 + \text{H} \rightarrow \text{OH} + \text{O}_2$		0.2 - 0.4	$8.44 \cdot 10^{13}$	0	470	0.7	[5]
20	$\text{HO}_2 + \text{O}_3 \rightarrow \text{OH} + \text{O}_2 + \text{O}_2$		0.25 - 0.34	$5.85 \cdot 10^{-4}$	4.57	-693		[6]
21	$\text{H} + \text{H}_2\text{O}_2 \rightarrow \text{HO}_2 + \text{H}_2$		0.3 - 1	$1.69 \cdot 10^{12}$	0	1890	0.5	[14,16]
22	$\text{HO}_2 + \text{HO}_2 \rightarrow \text{H}_2\text{O}_2 + \text{O}_2$		0.3 - 1.25	$1.03 \cdot 10^{14}$	0	5556	0.4	[1,31]
			+	$1.94 \cdot 10^{11}$	0	-709		**
23	$\text{H} + \text{H}_2\text{O}_2 \rightarrow \text{H}_2\text{O} + \text{OH}$		0.3 - 1	$1.02 \cdot 10^{13}$	0	1800	0,3	[14]
24	$\text{OH} + \text{H}_2\text{O}_2 \rightarrow \text{H}_2\text{O} + \text{HO}_2$		0.24 - 1.7	$1.93 \cdot 10^{12}$	0	215	0.2	[1,2,32]
			+	$1.70 \cdot 10^{18}$	0	14800	0.5	**
25	$\text{O} + \text{H}_2\text{O}_2 \rightarrow \text{H}_2\text{O} + \text{O}_2$		0.3 - 2.5	$9.6 \cdot 10^6$	2	2000	0.5	[15]
26	$\text{O} + \text{H}_2\text{O}_2 \rightarrow \text{OH} + \text{HO}_2$							[15] ***
27	$\text{H}_2 + \text{O}_2 \rightarrow \text{OH} + \text{OH}$		0.5 - 2.2	$1.7 \cdot 10^{13}$	0	24044		[33]

*) The efficiencies of collisional partners proposed in the present work were used.

***) The rate constant is represented as a sum: $k = A_1 T^{n_1} \exp(-E_1/T) + A_2 T^{n_2} \exp(-E_2/T)$

****) The rate constant is usually given for reaction (25). The ratio k_{25}/k_{26} is unknown.

The testing of combustion mechanisms

In the present investigation the delay-times of oxygen-hydrogen mixtures ignition behind the front of the shock wave measured in shock-tube experiments were compared with calculated ones. The combustion mechanisms of present work and mechanisms published in [1, 3, 39] were tested.

In experiments, the time between arrival of shock wave front to test section of shock tube and appearance at this section of OH radical emission, recorded at wavelength 306.4 nm was measured [40]. The gas mixtures diluted by argon up to 79-97% were studied for different $\text{O}_2\text{-H}_2$ concentration ratios (from 5:1 up to 1:20). The pressure in shock wave was changed from 0.7 up to 2 atmospheres. At high temperatures ($T > 2000\text{K}$) the main limitation of delay-times measurements was the time resolution (about 1 microsecond). In this case the uncertainty of measured delay time is $\pm 15\text{-}20\%$. At low temperatures ($T < 900\text{K}$) the delay time is long (milliseconds), and the ignition takes place near the contact between a shock wave and driver gas in the shock tube. The error of delay time measurements may exceed 20%. At the intermediate temperatures 1100-2000K the uncertainty does not exceed 10%. In detail the experiment is presented in [40].

In calculations the chemical transformations behind incident shock wave were described by ordinary differential equations for quantity Y_i which represents a component mole number per mass unit of the gas mixture:

$$\rho \frac{dY_i}{dt} = \sum_r (\bar{v}_{ir} - v_{ir}) \left(k_{fr} \prod_i (c_i)^{v_{ir}} - k_{br} \prod_i (c_i)^{\bar{v}_{ir}} \right) \quad (1)$$

Here c_i is a component mole number per volume unit,

k_{fr}, k_{br} are the rate constants of direct and reverse chemical reactions, respectively.

According to one-dimension model these equations must be solved using algebraic relations of mass, impulse and energy conservation. At accurate definition it is the same that equations (1) must be integrated under conditions of adiabatic process connecting gas pressure and density by Relay-Michelson relation.

In present experiments the gas mixtures contained high argon concentration. This allows consider chemical transformations at constant-volume process because of low heat generation and weak influence of combustion on gas dynamic parameters in such mixtures. Below in calculations an enthalpy of each component $H_i(T)$ is calculated using Gibbs function $\Phi_i(T)$ from [41]:

$$H_i(T) = T^2 \partial \Phi_i(T) / \partial T + H_i(0).$$

The delay-time was calculated as a maximum of gas temperature gradient during ignition. This value was compared with the measured distance (in microseconds) between the front of the shock wave and the beginning of OH radical emission appearance (except testing of mechanism [39]). Basically in this case the calculated time may be slightly longer than measured one. However, this difference does not exceed uncertainties of delay-time measurements.

Testing of combustion mechanism [39] was carried out by comparison of calculated and measured delay-times as the time between the front of the shock wave and the maximum emission of OH radical achievement.

The calculations were performed using the code described ibidem.

In [1] the comparison of ignition delay-times calculations with results of shock tube experiments was made for the data obtained in reflected shock waves.

Testing kinetic mechanism of present work was carried out for two values of rate constant of reaction $H_2+O_2=OH+OH$ taken from [34] (mechanism 1) and [33] (mechanism 2).

There are some differences between kinetic mechanism of present work and investigation [1]. In mechanism [1] the rate constants of several dissociation-recombination reactions were presented both in low and high pressure limits. Also the reaction $HO_2+HO_2+M=H_2O_2+O_2+M$ was included in mechanism [1], and it was shown that it is essential at high gas pressure. These reactions are not presented in our mechanism. Some others particularities of our mechanism were discussed in [22].

Reduced mechanism [3] contains seven reactions (-1), (-5), (10)-(13), (27) (numeration is given in agreement of Table 1). The rate constants of reactions (-5), (10)-(13) in [3] are close or coincide with the rate constant values proposed in the present work. Data of reaction (27) were taken from [33]. The rate constants of recombination reaction (-1) coincide for $M=H_2$.

In our previous work [39] both reactions between components in ground electronic states and processes involving electronically excited molecules O_2^* , OH^* and atoms O^* were taken into account. For reaction (27) the rate constant was taken from work [34]. The difference in rate constants for reactions of components in ground electronic states is slight between data [39] and present mechanism.

Reduced mechanism [3] contains seven reactions (-1), (-5), (10)-(13), (27) (numeration is given according to Table 1). The rate constants of reactions (-5), (10)-(13) in [3] are close or coincide with the rate constants proposed in the present work. The rate constant of reaction (27) were taken from [33]. The rate constants of recombination reaction (-1) coincide for $M=H_2$.

In our previous work [39] the reactions between components in ground electronic states and processes involving electronically excited molecules O_2^* , OH^* and atoms O^* were taken into account. The difference in rate constants between data [39] and present mechanism is inessential for components in ground electronic states.

Discussion of testing results

In Fig.1-5 the results of comparison of measured ignition delay times with calculated ones are presented for all the combustion mechanisms tested. The comparison was carried out for different initial compositions of mixture H_2-O_2-Ar , initial pressures and temperatures behind a front of shock wave in temperature range 850-2500K.

In Fig.1, 2 it is shown that the whole array of experimental data is satisfactorily described with the help of most of mechanisms under study for mixtures with reach content of hydrogen ($O_2 : H_2 =1:20, 1:10$). The mechanism 1 was exclusive because in it for chain

initiation reaction $H_2+O_2\rightarrow OH+OH$ the rate constant was taken from [34] where its value is negligible quantity. In Fig.1-4 the arrows show sharply increase of delay times calculated using mechanism 1 (arrow 1) and using mechanism [1] (arrow 2). In figures experimental values are shown by black squares.

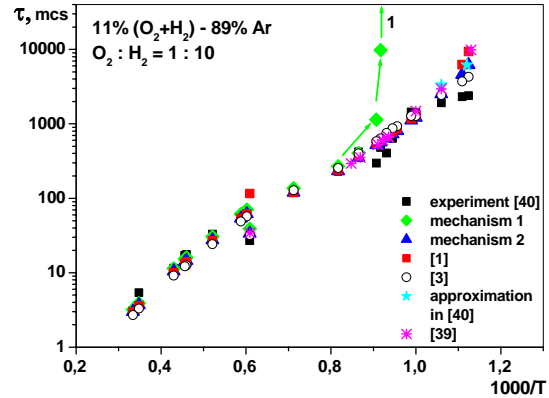


Fig. 1. Ignition delay times versus temperature. Mixture is 1% O_2 -10% H_2 -89% Ar.

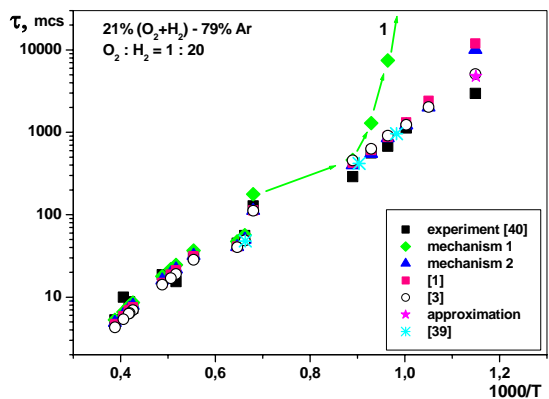


Fig.2. Ignition delay times versus temperature. Mixture is 1% O_2 -20% H_2 -79% Ar.

Ignition delay times calculated in according of mechanism 1 considerably exceed the measured ones at temperatures lower 1100K. At that, the same value of rate constant is used in Konnov's mechanism [1], however the calculations agree well with the experimental data obtained for indicated gas mixtures. As it was noted in [1], the role of chain termination reaction $H+O_2+M\rightarrow HO_2+M$ sharply increases with temperature decrease lower 1100K. Because of the efficiencies of different collisional partners M are greater in the present work than in [1], the contribution of this reaction into chain termination process is greater, and the delay times calculated on mechanism 1 begin to differ from experimental values at temperatures about 1000K and lower.

With decrease of hydrogen concentration in initial mixture ($O_2 : H_2 =1:4, 1:2$), the calculations using the database [1] and mechanism 1 of present work show the sharp increase of delay time at $T<1100K$ (Fig. 3.4). Note that in both cases the small value of rate constant for reaction (27) is taken from [34]. When the greater

value of rate constant of reaction (27) is selected from [33], the experimental ignition delay times are well described up to 850K using mechanism 2 of the present work and other databases [3, 39] in which the rate constant of reaction (27) from [33] or close values are used. The similar picture is observed for gas mixture $O_2 : H_2 = 1:1$ diluted by argon up to 92% .

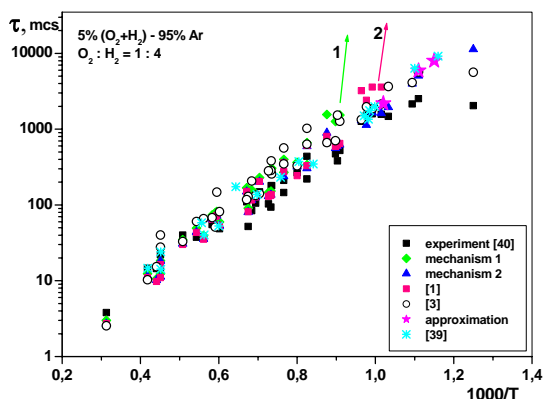


Fig.3. Ignition delay times versus temperature. Mixture is 1% O_2 -4% H_2 -95% Ar.

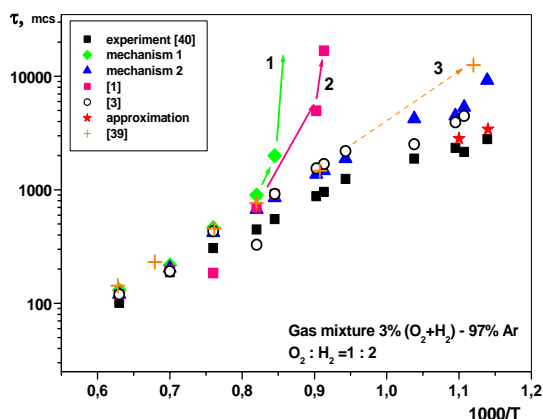


Fig.4. Ignition delay times versus temperature. Mixture is 1% O_2 -2% H_2 -97% Ar.

So, the comparison of experimentally measured ignition delay times with the calculated ones shows that neglect of reaction (27) (or the use of negligibly small values of the rate constant) does not allow to calculate satisfactorily the ignition delay times for oxygen-hydrogen mixtures specified behind the front of incident shock waves at temperatures lower 1100K. At the same time, as it was noted above, there are no serious bases to use the great values of this rate constant and to take account of reaction (27) in combustion models.

Experiments with small hydrogen content in gas mixture ($O_2 : H_2 = 5:1$, 95% Ar) were fulfilled for more narrow temperature range 1225-2316 K and pressures 1-1.5 atm (Fig. 5). In the picture it is seen that for all the mechanisms in study the calculated delay times exceed the experimental ones, and the use of reduced base in [3] shows the most calculated values. In this case the excess of calculated value amounts to factor 2.75 at $T=1225K$.

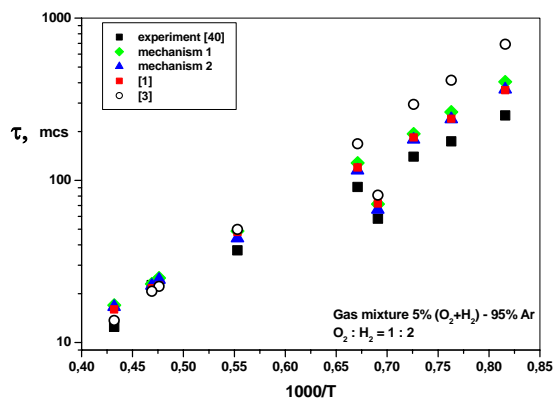


Fig.5. Ignition delay times versus temperature. Mixture is 4.17% O_2 - 0.83% H_2 - 95% Ar.

Conclusion

In summary, it is well to note that the use of available mechanisms of oxygen-hydrogen combustion not always allows describing the process of hydrogen combustion behind the front of shock wave. In particular, for gas mixtures with oxygen excess (4.17% O_2 -0.83% H_2 -95% Ar), calculated delay times are greater than in experiments at $T < 2000K$. For gas mixtures with advanced hydrogen concentration, at $T < 1000K$ the auto-ignition process has been possible to describe only using the reaction (27) with the great values of its rate constant in combustion mechanism.

Considering the “fitting” character of reaction (27), we can conclude that in combustion models under consideration there are no important real processes connected with the chain branching and production of active agents in shock wave conditions, especially at $T \sim 1000K$.

Apparently, it is appropriate to revise the mechanism of chemical transformations of oxygen-hydrogen combustion and to attract alternative mechanisms including processes for vibrationally and electronically excited components. By our opinion, the alternative mechanism proposed in [42-44] has perspectives. The reaction (27) was not concluded in this mechanism. The main difference of this kinetic model from traditional ones is the consideration of reaction $H+O_2=O+OH$ as a complex process with production of nonequilibrium vibrationally excited intermediate $HO_2(v)$ which provides the chain combustion processes and production of electronically excited components (in particular OH^*) even at temperatures about 1000K.

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