

COMBUSTION, EXPLOSION,
AND SHOCK WAVES

Mechanisms of the Oxidation and Combustion of Normal Alkanes:
Passage from C₁–C₄ to C₂H₅

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Abstract—A previously proposed algorithm was applied to constructing an optimal *n*-pentane oxidation mechanism capable of predicting the reaction rate and the formation of the main intermediate and final products. The mechanism can be considered a nonempirical detailed mechanism, since the constituent elementary reactions are kinetically validated. The mechanism is based on two assumptions: it ignores reactions involving double addition of oxygen (first, to a peroxy radical and then to its isomeric form) and isomer compounds and derivatives thereof. For low-temperature autoignition, the mechanism reproduces the stage character of the oxidation of *n*-pentane, more specifically, the emergence of cool and blue flames. The calculation results were compared with the published experimental data.

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INTRODUCTION

At present, based on the kinetic characteristics of numerous intermediate stable molecules and radicals participating in the oxidation and combustion of complex hydrocarbons, detailed mechanisms composed of thousands of reactions involving hundreds of species have been proposed. For example, for *n*-heptane, a mechanism comprised of 2300 reactions and 650 species was developed [1]. Even larger mechanism, consisting of 3872 reactions with 715 species, was compiled in [2]. Despite a number of obvious advantages of such detailed mechanisms, their application to modern multidimensional calculations of reactive flows is unfeasible because of enormous computational cost. Note also that such detailed mechanisms cannot be considered complete: they can be extended signifi-

cantly by including isomers, polyaromatic compounds, soot fullerenes, etc. and the relevant reactions. In addition, there are no reliable, if any, kinetic and thermodynamic data for many species and reactions in such mechanisms, a circumstance that markedly curtails the value of their predictions. It turns out that such mechanisms often provide no adequate description of the multistage oxidation of hydrocarbons accompanied by the emergence of cool and blue flames [3].

In solving actual problems, it is advantageous to use not maximally detailed but optimal mechanisms, including only those processes that determine the reaction rate and the formation of the main intermediate and final products. Such mechanisms, even compact ones, are referred to as nonempirical detailed mechanisms if the constituent reactions have a solid

Table 1. Additional reactants appearing in the mechanism of the oxidation and combustion of *n*-pentane

Species no.	Species	ΔH_f^0 , cal/mol	S_{298}^0 , cal/(mol K)	c_0	c_1	c_2	c_3
55	C ₅ H ₁₂	−34684.0	83.638	−0.358	116.180	−62.219	13.022
56	C ₅ H ₁₁	13536.0	87.328	1.279	106.930	−60.040	15.492
57	C ₅ H ₁₁ O ₂	−14164.0	105.730	2.109	132.620	−81.840	24.192
58	C ₅ H ₁₁ O ₂ H	−49864.0	104.330	1.789	135.320	−81.640	23.592
59	C ₅ H ₁₁ O	−16364.0	96.628	−0.611	131.820	−83.340	26.292
60	C ₄ H ₉ CHO	−55064.0	91.828	10.369	66.826	17.160	−40.308
61	C ₄ H ₉ CO	−19864.0	93.128	10.369	66.826	17.160	−40.308
62	C ₅ H ₁₀	−4984.0	82.928	1.579	99.096	−52.047	10.612
63	C ₅ H ₉	39136.0	82.128	2.189	85.226	−40.840	7.462

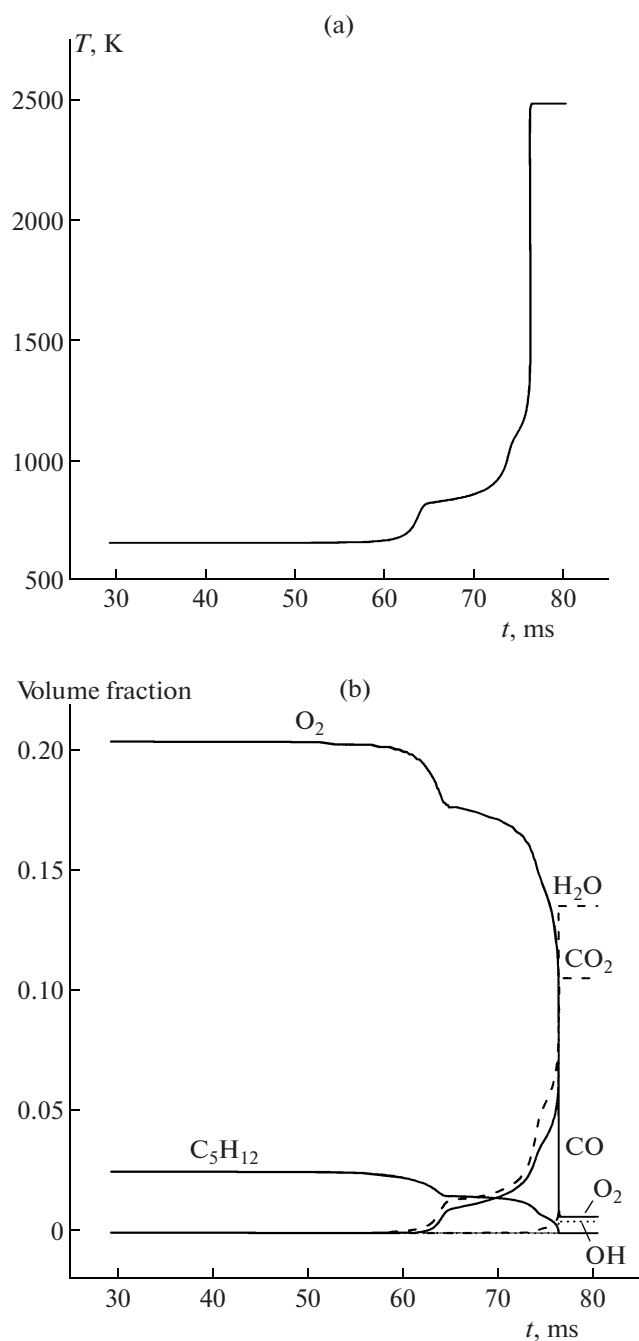


Fig. 1. Calculated time histories of (a) the temperature and (b) concentration of the main reaction products for the autoignition of a 2.54% C_5H_{12} -20.4% O_2 - N_2 -Ar stoichiometric mixture at an initial temperature of $T_0 = 658$ K and an initial pressure of $P_0 = 6.8$ atm.

kinetic substantiation. Thus, there is a nonextensive approach to constructing the mechanisms of the oxidation and combustion of hydrocarbons, which restricts the number of products and reactions but retains the main pathways of the process and principally important types of elementary steps.

The oxidation of alkanes has many common features [3–5]. In the present work, we extended the

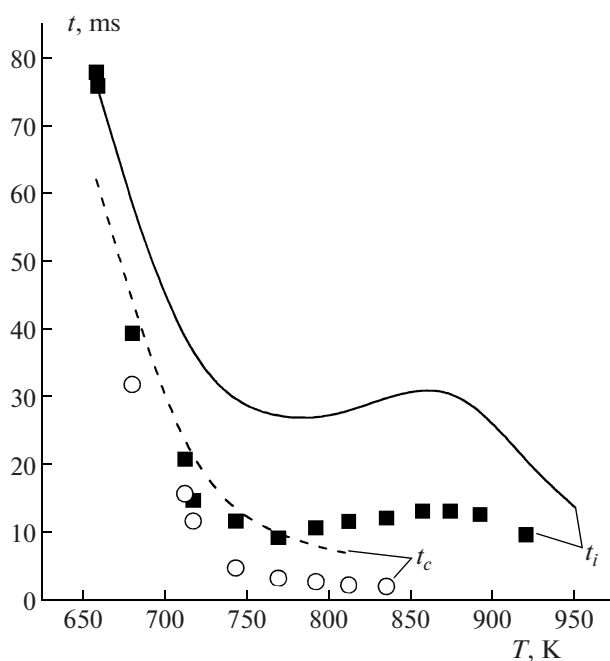


Fig. 2. Comparison of the calculated (curves) and measured (symbols) ignition delay times t_i and t_c at various initial temperatures for a 2.54% C_4H_{10} -20.4% O_2 - N_2 -Ar stoichiometric mixture at initial pressure of $P_0 = 6.8$ -9.2 atm.

algorithm proposed in [5] to developing a mechanism of the oxidation and combustion of n -pentane (C_5H_{12}). This algorithm is based on the principle of nonextensive construction of reaction mechanisms, which is based on two assumptions: (1) low-temperature branching involves a group of reaction with single oxygen addition and (2) oxidation involving isomeric forms can be excluded, since it is slower than that occurring via nonisomerized forms. Although several mechanisms of C_5H_{12} oxidation have been proposed (see, e.g., [6, 7]), the authors of these mechanisms fall short of demonstrating whether these mechanisms describe the available experimental data on multistage oxidation accompanied by the emergence of cool and blue flames before ignition. Constructing the mechanism of C_5H_{12} oxidation based on the algorithm proposed in [5] is important for creating the mechanisms of the oxidation of higher alkanes, n -hexane, n -heptane, etc.

DEVELOPMENT OF THE KINETIC MECHANISM

According to the algorithm proposed in [5], to construct a kinetic mechanism of the oxidation of a C_nH_{2n+2} hydrocarbon, it is advantageous to rely on the mechanism developed for the preceding analogue in the homologous series $C_{(n-1)}H_{2(n-1)+2}$; this refers to the reactions and reactants. Therefore, the mechanism of oxidation and combustion of C_4H_{10} was based on that of n -butane, which was composed of 288

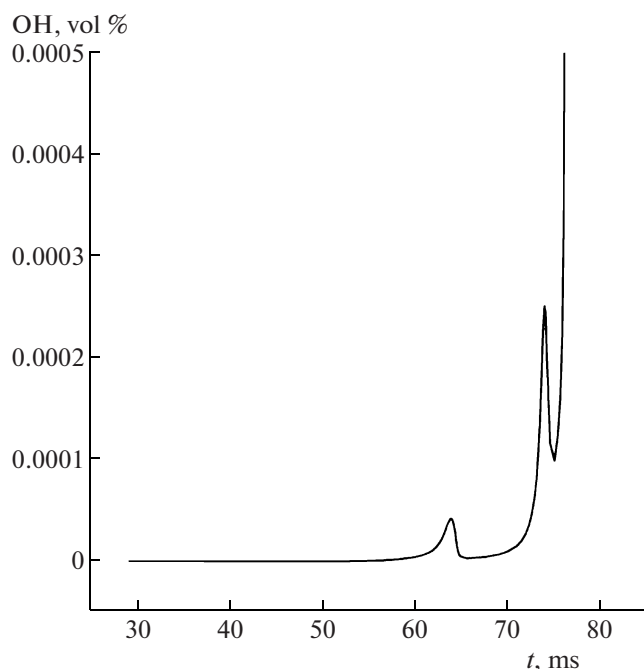


Fig. 3. Calculated time history of the hydroxyl concentration for the multistage autoignition of a 2.54% C_5H_{12} –20.4% O_2 – N_2 –Ar stoichiometric mixture at an initial temperature of $T_0 = 658$ K and an initial pressure of $P_0 = 6.8$ atm.

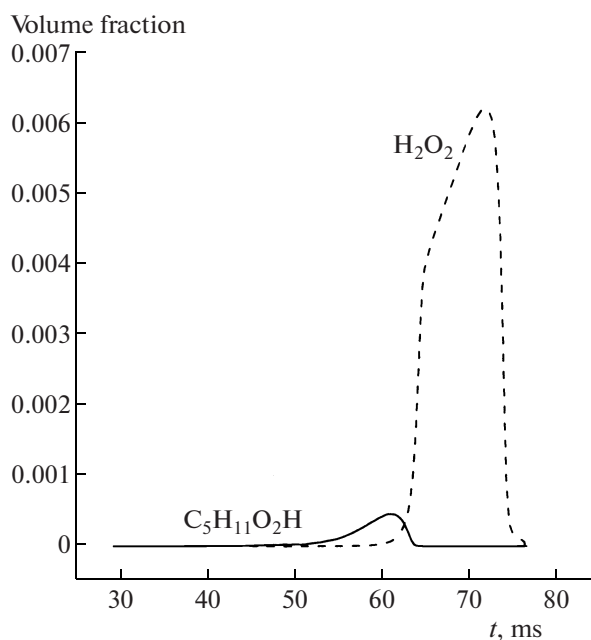


Fig. 4. Calculated time histories of the $C_5H_{11}O_2H$ and H_2O_2 concentrations for the multistage autoignition of a 2.54% C_5H_{12} –20.4% O_2 – N_2 –Ar stoichiometric mixture at an initial temperature of $T_0 = 658$ K and an initial pressure of $P_0 = 6.8$ atm.

reversible reactions with 54 species [5]. To extend the scheme to C_5H_{12} , we introduced 9 new species and 97 elementary steps, so that the new mechanism consisted of 385 reactions involving 63 species.

A specially developed computational code and the algorithm from [5] were used to select additional species (their thermodynamic functions, enthalpy $\Delta H_{f,298}^\circ$, entropy S_{298}° , and heat capacity at constant pressure $c_p = c_0 + c_1 T/10^3 + c_2 T^2/10^6 + c_3 T^3/10^9$ are summarized in Table 1) and reaction (Table 2).

The critical phenomena in chemical kinetics, including the emergence of a cool and/or blue flame during multistage autoignition are versatile, being observed only at certain ratios between the rates of different elementary steps. Describing such critical phenomena normally requires a correction of rate constants within a theoretically admissible range or within the experimental error limits. As to the new *n*-pentane oxidation mechanism, such corrections were applied to a limited number of reactions (the reactions of *n*-pentane with hydroperoxide radicals and the reactions of pentyl with molecular oxygen).

TESTS OF THE MECHANISM

The proposed kinetic mechanism was tested against the published data experimental results on the oxidation and autoignition of C_5H_{12} . The kinetic

simulations were performed using a standard kinetic code [5].

Experimental Data from [8]

The experiments described in [8] were conducted at moderate pressures and temperatures. Figure 1 shows the calculated time dependences of the temperature (Fig. 1a) and concentrations of the main reaction products (Fig. 1b) for the autoignition of *n*-pentane–oxygen mixtures diluted with nitrogen or argon at low and medium temperatures. The first stepwise rise in temperature, at ~ 63 ms (Fig. 1a), is associated with the emergence of a cool flame. At ~ 72 ms, a blue flame appears and gives rise to the second step in the temperature time history. At ~ 76 ms, a hot flame (explosion) arises, and the temperature rapidly increases to ~ 2500 K. This behavior is indicative of a multistage character of the autoignition of *n*-pentane, a sequence of cool, blue, and hot flames.

That the reaction accelerates in the cool-flame regime can be explained by the decomposition of pentylhydroperoxide ($C_5H_{11}O_2H$) with the formation of a hydroxyl and pentoxyl. This acceleration gives rise to a negative temperature coefficient of the reaction rate: when the overall ignition delay time t_i at a higher temperature is longer than that at a lower one (Fig. 2). Figure 2 also shows the temperature dependence of the delay time of cool flame emergence t_f . Note the tem-

Table 2. Mechanism of the oxidation and combustion of *n*-pentane

Reaction no.	Reaction	<i>A</i> , l, mol, s	<i>E/R</i> , K
1	$C_5H_{12} + O_2 = C_5H_{11} + HO_2$	0.400E+10	0.239E+05
2	$C_5H_{12} + OH = C_5H_{11} + H_2O$	0.630E+10	0.600E+03
3	$C_5H_{12} + H = C_5H_{11} + H_2$	0.930E+11	0.403E+04
4	$C_5H_{12} + O = C_5H_{11} + OH$	0.505E+12	0.483E+04
5	$C_5H_{12} + HO_2 = C_5H_{11} + H_2O_2$	0.600E+09	0.856E+04
6	$C_5H_{10} + H = C_5H_{11}$	0.189E+10	0.315E+03
7	$C_5H_{11} + O_2 = C_5H_{10} + HO_2$	0.220E+10	0.800E+04
8	$C_5H_{11} + OH = C_5H_{10} + H_2O$	0.600E+10	0.000E+00
9	$C_5H_{12} = H + C_5H_{11}$	0.359E+14	0.376E+05
10	$C_5H_{12} = CH_3 + C_4H_9$	0.404E+16	0.421E+05
11	$C_5H_{12} = C_2H_5 + C_3H_7$	0.195E+17	0.428E+05
12	$C_5H_{11} + H = C_5H_{10} + H_2$	0.600E+10	0.000E+00
13	$C_5H_{11} + CH_3 = C_5H_{10} + CH_4$	0.351E+09	-0.106E+03
14	$C_5H_{11} + C_2H_5 = C_5H_{10} + C_2H_6$	0.158E+11	0.466E+03
15	$C_5H_{11} + C_3H_7 = C_5H_{10} + C_3H_8$	0.138E+09	0.488E+03
16	$C_5H_{11} + C_4H_9 = C_5H_{10} + C_4H_{10}$	0.138E+09	0.488E+03
17	$C_5H_{11} + O = C_5H_{10} + OH$	0.200E+12	0.000E+00
18	$C_5H_{11} + O_2 = C_5H_{11}O_2$	0.400E+08	-0.500E+03
19	$C_5H_{12} + CH_3O_2 = C_5H_{11} + CH_3O_2H$	0.100E+11	0.650E+04
20	$C_5H_{12} + C_2H_5O_2 = C_5H_{11} + C_2H_5O_2H$	0.100E+11	0.650E+04
21	$C_5H_{12} + C_3H_7O_2 = C_5H_{11} + C_3H_7O_2H$	0.100E+11	0.650E+04
22	$C_5H_{12} + C_4H_9O_2 = C_5H_{11} + C_4H_9O_2H$	0.100E+11	0.650E+04
23	$C_5H_{12} + C_5H_{11}O_2 = C_5H_{11} + C_5H_{12}O_2$	0.100E+11	0.650E+04
24	$C_5H_{12}O_2 = C_5H_{11}O + OH$	0.500E+16	0.200E+05
25	$C_5H_{11}O = CH_2O + C_4H_9$	0.158E+15	0.797E+04
26	$C_5H_{11}O = CH_3CHO + C_3H_7$	0.312E+15	0.113E+05
27	$C_5H_{11}O = C_2H_5CHO + C_2H_5$	0.374E+15	0.103E+05
28	$C_5H_{11}O = C_4H_8O + CH_3$	0.775E+14	0.108E+05
29	$C_5H_{11}O = C_5H_{10}O + H$	0.688E+12	0.626E+04
30	$C_5H_{11}O_2 + H = C_5H_{11}O + OH$	0.236E+11	-0.161E+04
31	$C_5H_{11}O_2 + CH_3 = C_5H_{11}O + CH_3O$	0.364E+09	-0.166E+03
32	$C_5H_{11}O_2 + C_2H_5 = C_5H_{11}O + C_2H_5O$	0.827E+09	-0.649E+03
33	$C_5H_{11}O_2 + C_3H_7 = C_5H_{11}O + C_3H_7O$	0.630E+09	0.000E+00
34	$C_5H_{11}O_2 + C_4H_9 = C_5H_{11}O + C_4H_9O$	0.630E+09	0.000E+00
35	$C_5H_{11}O_2 + C_5H_{11} = C_5H_{11}O + C_5H_{11}O$	0.630E+09	0.000E+00
36	$C_5H_{11}O_2 + CH_2O = C_5H_{12}O_2 + HCO$	0.320E+09	0.564E+04
37	$C_5H_{11}O_2 + CH_3CHO = C_5H_{12}O_2 + CH_3CO$	0.315E+09	0.560E+04
38	$C_5H_{11}O_2 + C_2H_5CHO = C_5H_{12}O_2 + C_2H_5CO$	0.315E+09	0.554E+04
39	$C_5H_{11}O_2 + C_4H_8O = C_5H_{12}O_2 + C_4H_7O$	0.315E+09	0.554E+04
40	$C_5H_{11}O_2 + C_5H_{10}O = C_5H_{12}O_2 + C_5H_9O$	0.315E+09	0.554E+04
41	$C_5H_{11} + HO_2 = C_5H_{11}O + OH$	0.300E+11	0.000E+00
42	$C_5H_{11} + O_2 = C_5H_{10}O + OH$	0.400E+10	0.900E+04
43	$C_5H_{11} + C_2H_5 = C_5H_{12} + C_2H_4$	0.625E+09	0.335E+03
44	$C_5H_{11} + C_3H_7 = C_5H_{12} + C_3H_6$	0.190E+10	0.000E+00
45	$C_5H_{11} + C_4H_9 = C_5H_{12} + C_4H_8$	0.190E+10	0.000E+00
46	$C_5H_{11} + C_5H_{11} = C_5H_{12} + C_5H_{10}$	0.190E+10	0.000E+00
47	$C_5H_{11} + O_2 = CH_2O + C_4H_9O$	0.400E+09	0.700E+04
48	$C_5H_{11} + O_2 = CH_3CHO + C_3H_7O$	0.400E+09	0.700E+04
49	$C_5H_{11} + O_2 = C_2H_5CHO + C_2H_5O$	0.400E+09	0.700E+04

Table 2. (Contd.)

Reaction no.	Reaction	A , l, mol, s	E/R , K
50	$C_5H_{11} + O_2 = C_4H_8O + CH_3O$	0.400E+09	0.700E+04
51	$C_5H_{11} + OH = CH_3 + C_4H_9O$	0.185E+11	-0.194E+04
52	$C_5H_{11} + OH = C_2H_5 + C_3H_7O$	0.891E+11	0.417E+03
53	$C_5H_{11} + OH = C_3H_7 + C_2H_5O$	0.117E+12	-0.232E+03
54	$C_5H_{11} + OH = C_4H_9 + CH_3O$	0.107E+11	0.480E+03
55	$C_5H_{11} + H = CH_3 + C_4H_9$	0.388E+11	0.546E+03
56	$C_5H_{11} + H = C_2H_5 + C_3H_7$	0.187E+12	0.318E+03
57	$C_5H_{11} + H = CH_2 + C_4H_{10}$	0.423E+08	0.302E+04
58	$C_5H_{11} + H = C_2H_4 + C_3H_8$	0.722E+07	-0.641E+04
59	$C_5H_{11} + H = C_3H_6 + C_2H_6$	0.251E+10	-0.677E+04
60	$C_5H_{11} + H = C_4H_8 + CH_4$	0.116E+08	-0.711E+04
61	$C_5H_{11} + O = H + C_5H_{10}O$	0.702E+09	0.565E+03
62	$C_5H_{11} + O = CH_3 + C_4H_8O$	0.791E+11	-0.952E+03
63	$C_5H_{11} + O = C_2H_5 + C_2H_5CHO$	0.381E+12	-0.118E+04
64	$C_5H_{11} + O = C_3H_7 + CH_3CHO$	0.318E+12	-0.111E+04
65	$C_5H_{11} + O = C_4H_9 + CH_2O$	0.162E+12	-0.352E+01
66	$C_5H_9O + HO_2 = C_5H_{10}O + O_2$	0.530E+08	0.000E+00
67	$C_5H_{10}O + OH = C_5H_9O + H_2O$	0.100E+11	0.000E+00
68	$C_5H_{10}O + H = C_5H_9O + H_2$	0.140E+11	0.165E+04
69	$C_5H_{10}O + O = C_5H_9O + OH$	0.568E+10	0.780E+03
70	$C_5H_{10}O + HO_2 = C_5H_9O + H_2O_2$	0.600E+09	0.500E+04
71	$C_4H_9 + HCO = C_5H_{10}O$	0.223E+11	0.352E+01
72	$C_4H_9 + CO = C_5H_9O$	0.187E+09	0.242E+04
73	$C_5H_9O + H = C_4H_9 + HCO$	0.485E+10	0.240E+04
74	$C_5H_9O + O = C_4H_9O + CO$	0.369E+10	0.646E+03
75	$C_5H_{10} + OH = C_5H_9 + H_2O$	0.900E+11	0.325E+04
76	$C_5H_9 + H_2 = C_5H_{10} + H$	0.853E+11	0.533E+04
77	$C_5H_9 + O_2 = C_3H_7O_2 + C_2H_2$	0.242E+11	0.396E+04
78	$C_5H_{10} + HCO = C_5H_9 + CH_2O$	0.600E+11	0.900E+04
79	$C_5H_{10} + CH_3 = C_5H_9 + CH_4$	0.107E+09	0.268E+04
80	$C_5H_{10} + C_2H_5 = C_5H_9 + C_2H_6$	0.481E+10	0.325E+04
81	$C_5H_{10} + C_3H_7 = C_5H_9 + C_3H_8$	0.420E+08	0.328E+04
82	$C_5H_{10} + C_4H_9 = C_5H_9 + C_4H_{10}$	0.420E+08	0.328E+04
83	$C_3H_7 + C_2H_2 = C_5H_9$	0.141E+10	0.143E+04
84	$C_5H_{10} = C_2H_3 + C_3H_7$	0.390E+14	0.379E+05
85	$C_5H_{10} = C_3H_5 + C_2H_5$	0.140E+14	0.446E+05
86	$C_5H_{10} = C_4H_7 + CH_3$	0.289E+13	0.439E+05
87	$C_5H_{10} + O_2 = C_5H_9 + HO_2$	0.600E+11	0.236E+05
88	$C_5H_{10} + O = C_4H_9 + HCO$	0.404E+10	0.226E+03
89	$C_5H_9 + OH = C_4H_9 + HCO$	0.485E+10	-0.352E+01
90	$C_5H_9 + H = C_3H_8 + C_2H_2$	0.917E+10	0.362E+03
91	$C_5H_9 + O = C_4H_9 + CO$	0.485E+10	-0.352E+01
92	$C_5H_9 + O = C_3H_7O + C_2H_2$	0.405E+11	-0.662E+02
93	$CH_3 + C_4H_9 = C_5H_{10} + H_2$	0.248E+14	0.191E+05
94	$C_2H_5 + C_3H_7 = C_5H_{10} + H_2$	0.513E+13	0.193E+05
95	$C_5H_{10} + H + H = CH_3 + C_4H_9$	0.356E+10	-0.415E+04
96	$C_5H_{10} + H + H = C_2H_5 + C_3H_7$	0.172E+11	-0.438E+04

the mechanism of the oxidation and combustion of C_4H_{10} follows

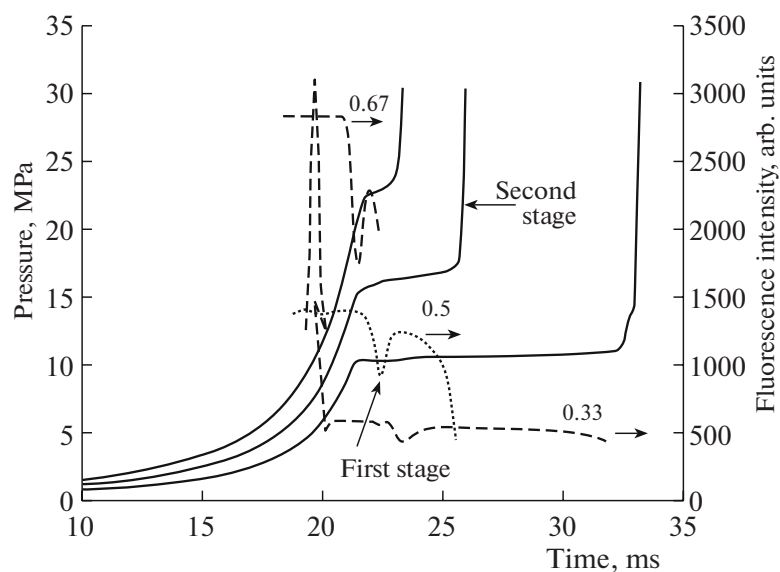


Fig. 5. Experimental results on the autoignition of a 2.04% C_5H_{12} -16.32% O_2 -Ar mixture in a rapid-compression machine at initial pressures of 0.67, 0.5, and 0.33 atm [9].

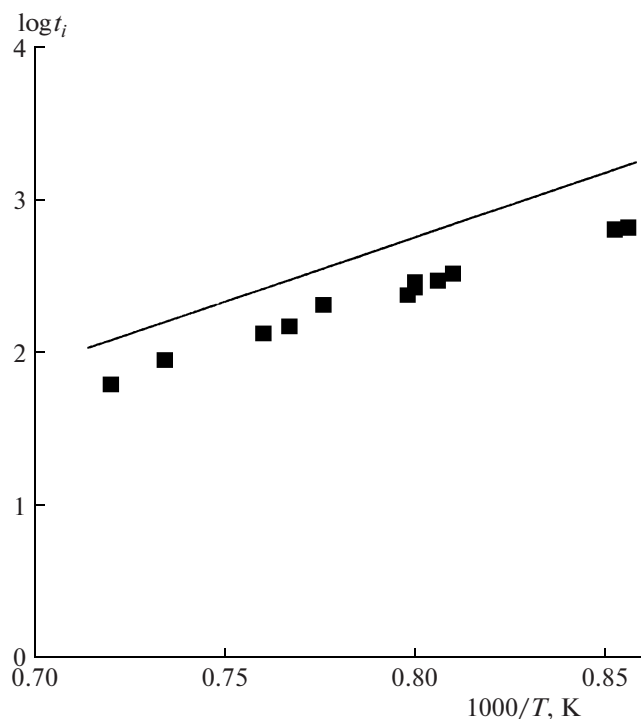


Fig. 6. Comparison of the calculated (line) with the experimental ([10], symbols) temperature dependence of the ignition delay time t_i (in μs) for a 2.04% C_5H_{12} -16.32% O_2 -Ar mixture at pressures of $P_0 = 8.27$ -9.46 atm.

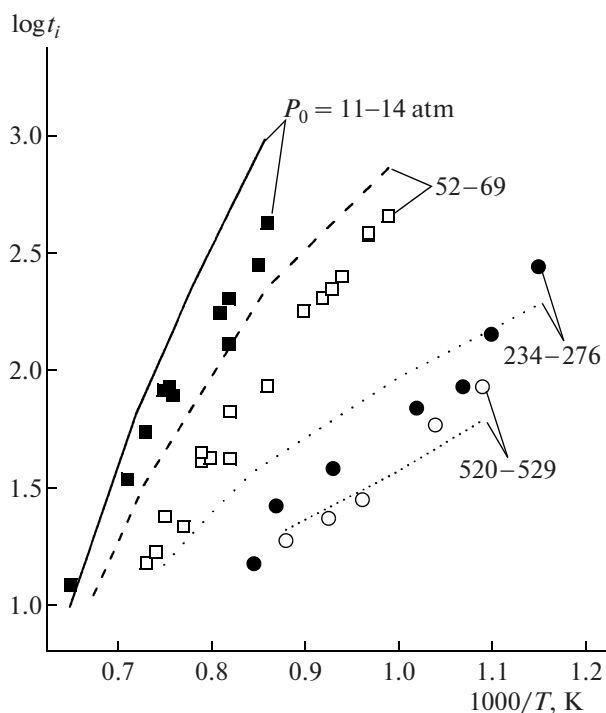


Fig. 7. Comparison of the calculated (curves) with the experimental ([11], symbols) temperature dependences of the ignition delay time t_i (in μs) for a 1.27% C_5H_{12} -20.64% O_2 - N_2 mixture at pressures of $P_0 = 11$ -529 atm.

perature dependences of t_i and t_c were calculated as described in [5].

The emergence of a blue flame is associated with the decomposition of hydrogen peroxide (H_2O_2). The cool and blue flames featured spikes in the hydroxyl concentration (Fig. 3) because of the consecutive

decomposition of pentylhydroperoxide and hydrogen peroxide (Fig. 4).

Cool and blue flames were observed at high pressures in experiments on a rapid-compression machine. Figure 5 (borrowed from [9]) shows that, at an initial compression pressure of 0.33 atm, a cool and

blue flame appeared at ~ 0.23 ms and ~ 0.32 ms, respectively; then, at ~ 0.33 ms, the stage of thermal explosion begins [9, Fig. 5, p. 375], although the authors paid no attention to this phenomenon.

Experimental Data from [10]

Figure 6 compares the calculated (straight line) and measured (in [10], symbols) ignition delay times for a 2.04% n -C₅H₁₂–16.32% O₂–Ar mixture at high initial temperatures and pressure of $P_0 = 8.27$ – 9.46 atm. As can be seen, the calculated and measured values are in satisfactory agreement.

Experimental Data from [11]

Figure 7 compares the calculated (curves) and measured (in [11], symbols) ignition delay times for a 1.27% n -C₅H₁₂–20.64% O₂–Ar mixture at high initial temperatures and pressures ($P_0 = 11$ – 529 atm). Note that the calculated and measured values are in satisfactory agreement.

Experimental Data on Flame Propagation from [12, 13]

To test the kinetic mechanism still further, we calculated the laminar flame speed u_n for a stoichiometric n -pentane–air mixture under normally conditions ($P_0 = 1$ atm, $T_0 = 293$ K). The calculation method was described in detail in [14]. We obtained $u_n = 29.3$ m/s; the measured values were reported to be $u_n = 36$ cm/s [12] and 43 cm/s [13].

CONCLUSIONS

A kinetic mechanism of the oxidation and combustion of n -pentane was proposed. This mechanism can be considered a nonempirical detailed mechanism, since the constituent reactions are kinetically substantiated. This mechanism is based on two assumptions: it ignores reactions involving double addition of oxygen (first, to a peroxy radical and then to its isomeric form) and isomer compounds and derivatives thereof. For low-temperature autoignition, the mechanism reproduces the stage character of the oxidation of n -pentane in the form of cool and blue flames. The calculation results were found to be in satisfactory agreement with

the available experimental data over wide range of pressure, temperatures, and initial mixture compositions. The proposed mechanism is intended for use in constructing a detailed mechanism of the oxidation and combustion of n -hexane.

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