ISSN 0023-1584, Kinetics and Catalysis, 2010, Vol. 51, No. 4, pp. 469–474. © Pleiades Publishing, Ltd., 2010.
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Branched-Chain Nature of Hydrogen Combustion in the Detonation Mode

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Received August 11, 2009

Abstract—Minor admixtures of the simplest hydrocarbons can prevent detonation and break down a steady-state detonation wave in hydrogen–air mixtures at atmospheric and higher pressures. Therefore, the determining role in the appearance and propagation of the detonation wave is played by the branched mechanism and, accordingly, by the competing chain branching and termination reactions. Without taking into account these reactions, combustion theory cannot explain the basic regularities of the process, including the concentration limits of detonation.

DOI: 10.1134/S0023158410040026

Interest in gaseous detonation is generated by practical challenges and by problems of combustion theory. This phenomenon has been the subject of numerous works, including specialized monographs (see, e.g., [1–3]), large chapters in books on combustion [4, 5], and thematic collections of works (see, e.g., [6]). This work deals the role of the chain mechanism of reactions in detonation.

The progressively accelerating self-heating of the reaction system and the avalanche-like multiplication of intermediates through their multiply recurring reactions with the initial reactants and with one another are the two different factors causing ignition and combustion [7–9]. Ignition and combustion caused by self-heating are conventionally called thermal. The following two conditions must be satisfied simultaneously for thermal ignition to occur:

$$q_+ > q_-, \quad (1)$$

$$\mathrm{d}q_+/\mathrm{d}T > \mathrm{d}q_-/\mathrm{d}T, \quad (2)$$

where q_+ is the heat evolution rate in the chemical reaction, q_- is the rate of heat dissipation from the system, and T is temperature.

In thermal combustion theory, a chemical process is represented as a single-step reaction in which the product results directly from the initial reactants. The rate of a second-order reaction is conventionally represented as

$$-\mathrm{d}[\mathrm{B}]/\mathrm{d}t = w = k^0[\mathrm{A}][\mathrm{B}]\exp(-E/RT), \quad (3)$$

where [A] and [B] are the concentrations of the initial molecular reactants, t is time, E is the activation energy, and k^0 is the preexponential factor of the rate constant (see, e.g., [10]).

In a branched-chain process, the initial reactants are consumed mainly in their reactions with reactive intermediates—free atoms and radicals. These species are regenerated and multiplied in these reactions, giving rise to branched reaction chains. The rate of the process is given by the equation

$$w = -\mathrm{d}[\mathrm{B}]/\mathrm{d}t = \omega_0 + k_\mathrm{p}[\mathrm{B}]n, \quad (4)$$

where ω_0 is the formation rate of reactive species from molecular reactants alone, n is the concentration of active species, and k_p is the chain propagation rate constant [9].

Along with being involved in regeneration and multiplication reactions, reactive species can disappear through recombination and by turning into radicals incapable of participating in chain combustion. It is, therefore, obvious that the rate of change of the reactive species concentration in chemical reactions is equal to the difference between the formation and disappearance rates of these species:

$$\mathrm{d}n/\mathrm{d}t = \omega_0 + 2k_\mathrm{b}[\mathrm{B}]n - k_\mathrm{t}n = \omega_0 + fn - gn. \quad (5)$$

In this equation, k_b is the rate constant of the reaction between the initial reactant B and a reactive species that multiplies atoms or radicals and, accordingly, leads to chain branching, and k_t is the effective overall rate constant of the disappearance of reactive species (chain termination). For the sake of convenience, the quantities $2k_\mathrm{b}[\mathrm{B}]$ and k_t are conventionally designated f and g [7, 9].

The fundamental difference between the chain and thermal ignition mechanisms implies that there should be a radical difference between the main laws

governing these two types of combustion. For example, the critical condition for chain ignition is that the reactive species multiplication rate exceeds the reactive species disappearance rate. This also follows from Eqs. (4) and (5).

The role of the chain avalanche was long recognized only for pressures that are tens of times lower than atmospheric pressure, when there is almost no self-heating (see, e.g., [8, 9, 11]). For near-atmospheric pressures, even when the reactions of atoms and radicals were taken into account, it was believed that combustion is caused by the progressive acceleration of self-heating (see, e.g., [10–14]). When analytically solving the flame propagation equation, the chemical process was represented as a single-step reaction in which the initial reactants directly yield the final product. The temperature dependence of the combustion rate was represented as an Arrhenius function involving empirical parameters derived from experimental data on combustion under the same assumption that the process consists of a single step. In numerical simulations of gas-phase combustion using kinetic networks that include reactions of atoms and radicals, the role of chain branching was not investigated [15] and ignition at atmospheric pressure was interpreted as an explosion caused by self-heating alone (see, e.g., [16, 17]). In addition, the authors that used kinetic networks involving reactions of atoms and radicals often represented the combustion process as a single-step reaction in their subsequent publications.

In our earlier works [18, 19], we drew attention to some contradictions between the facts and the theory that ignores the branched-chain nature of combustion. Below we present some examples.

(1) All combustibility parameters of H_2 are significantly above the same parameters of hydrocarbons, although the molar heat of combustion of H_2 is much lower. The same contradictions are observed when comparing the combustibility properties of other classes of compounds.

(2) The ignition and combustion of H_2 and CH_4 in air, e.g., at 900 K, are inconsistent with the very small rate constants of the reactions of these molecules with O_2 (the activation energy of these reactions is over 220 kJ/mol). The characteristic time of heat evolution in reactors with typical dimensions is three orders of magnitude longer than the heat dissipation time. Therefore, the intermolecular molecular reactions cannot ensure any significant self-heating and, a fortiori, explosion.

(3) Minor admixtures of many compounds exert a strong effect on H_2 combustion at atmospheric pressure, including the concentration limits of detonation [19–21]. Note that the effect of some compounds on the hydrogen ignition limits at atmospheric pressure has long been known. Nevertheless, this effect was ignored by the authors who denied the role of the chain mechanism in combustion.

These contradictions are evidence of the branched-chain character of combustion both at pressures hundreds of times lower than atmospheric and at atmospheric pressure. Self-heating becomes significant only in the course of chain combustion and enhances the chain avalanche [18, 19]. Elucidating the role of reaction chains in different modes of these processes is among the topical problems of chemical kinetics and combustion. In addition, this problem is relevant to chemical control of gas combustion, explosion, and detonation.

This work was aimed at understanding the role of the chain avalanche in the propagating detonation wave. We also studied the dependence of detonation parameters on the type of the elementary step of inhibition. For this purpose, olefins were used as inhibitors along with methane for comparison. We will consider, in brief, the origin of the strong effect of the dopants on detonation, which is observed in spite of the high temperatures typical of this process. By way of example, we will examine hydrogen oxidation as the model process. We will report the influence of the simplest hydrocarbons on the detonation of hydrogen–air mixtures containing 33.5, 45, and 50% hydrogen at initial pressures of 100 and 600 kPa.

EXPERIMENTAL

The experimental setup included a reactor, a vacuum station, gas blenders, and a data acquisition and processing system. The reactor was a stainless steel sectioned tube 15 m in length and 10.1 cm in diameter. The reactor was connected with a narrow initiation section (Fig. 1), in which the initiating detonation of a stoichiometric $H_2 + O_2$ mixture was generated. The hydrogen–air mixtures to be examined, containing different amounts of inhibitors, were prepared in a blender more than 24 h before the experiment. This ensured the perfect mixing of the components. The inhibitors were propene, isobutene, and methane. In the experiments in which detonation was studied at an initial pressure of 100 kPa, the gas to be examined was admitted into the reactor and into the initiation section up to a pressure of 85–90 kPa through the inlet valve located in the middle of the tube. Next, the $2H_2 + O_2$ mixture was admitted through the end of the initiation section up to a total pressure of 100 kPa. This displaced the hydrogen–air mixture from the initiation section and from the initial length of the tubular reactor to a distance of about 0.9–1.0 m from the join of the initiation section and the reactor. This procedure, in which the initiation section-to-reactor volume ratio was taken into account, ensured that boundary between the working and initiating mixture was in the preset place at the beginning of the tube. A similar procedure was used for the initial pressure of 600 kPa. The $2H_2 + O_2$ mixture in the initiation section was ignited with a spark (3 J), and a detonation wave entered the reactor. The distance–time ($x - t$) dia-

grams (Figs. 2–5) and their quantitative reproducibility indicate that the mixtures were prepared accurately.

After traveling 0.9–1.0 m, the distance at which the space occupied by the stoichiometric mixture ends, the detonation wave in the absence of an inhibitor propagates with a constant velocity, as is shown in Fig. 2. Therefore, if no detonation occurs in the presence of an inhibitor with this initiation procedure, this is only due to chain termination under the action of the inhibitor.

The flame front, shock wave, and detonation were monitored using eight piezoelectric sensors (clock frequency of 300 MHz) arranged along the tube and eight photosensors in opposite positions (Fig. 1). The photosensors were adjusted so that they could detect only luminescence from detonation and from the flame front. The light emission from the shock wave in the absence of a flame was below their sensitivity limit. The arrangement of each pressure sensor–photosensor pair in the same cross section of the tube allowed detonation, the flame front, and the shock wave to be distinguished and studied separately. Indeed, as the detonation wave was running, we simultaneously recorded the signals from each pressure sensor–photosensor pair. In the case of a shock wave traveling without combustion (when the inhibitor prevented detonation), only signals from the pressures could be recorded. The resulting oscillograms were used to determine the detonation, shock wave, and burning velocities and the distance between the shock wave and the flame front. The detonation wave pressure was determined from the height of the pressure peak.

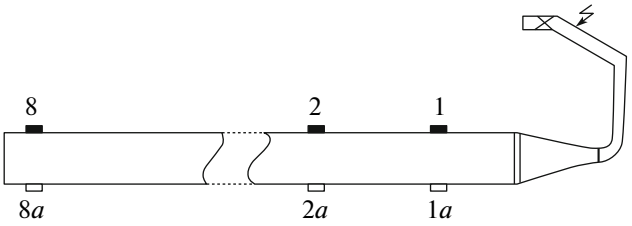

Fig. 1. Schematic of the reactor for investigation of the detonation of hydrogen–air mixtures: (*1*, *2*, ..., *8*) pressure sensors; (*1a*, *2a*, ..., *8a*) photosensors.

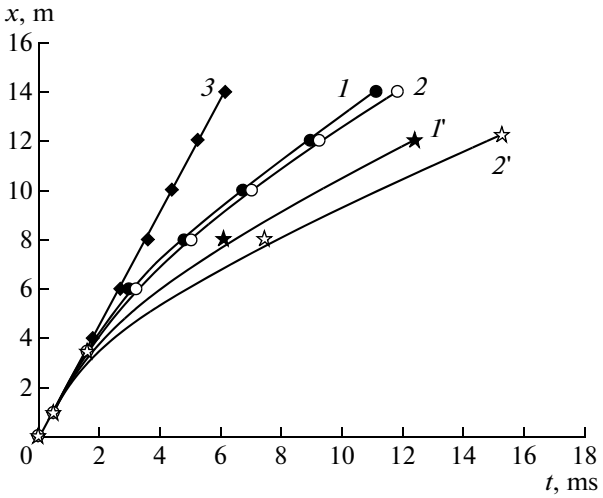

Fig. 2. *x*–*t* diagrams of (*1*, *2*) shock waves, (*1'*, *2'*) combustion fronts, and (*3*) detonation for the 45% H_2 + air mixture containing (*1*, *1'*) 2.5% propene, (*2*, *2'*) 2.5% isobutene, and (*3*) no dopant.

RESULTS AND DISCUSSION

Straight line *3* in Fig. 2 refers to the 45% H_2 + air mixture containing no inhibitor. Clearly, the pressure and light emission signals in each cross section throughout the tube length were detected synchronously, indicating that this is a detonation wave. The oscillogram of the synchronous pressure and light emission signals in one of the runs is presented in Fig. 3. Figure 2 also demonstrates that, after entering the reactor, the detonation wave somewhat slows down over a distance of 1 m and then travels with a constant velocity. The *x*–*t* diagrams recorded for the same mixture in different runs almost coincide. Therefore, the boundary between the stoichiometric and working mixtures was crossed in the same way in all runs. Similar results were obtained for the 50% H_2 + air and 33.8% H_2 + air mixtures.

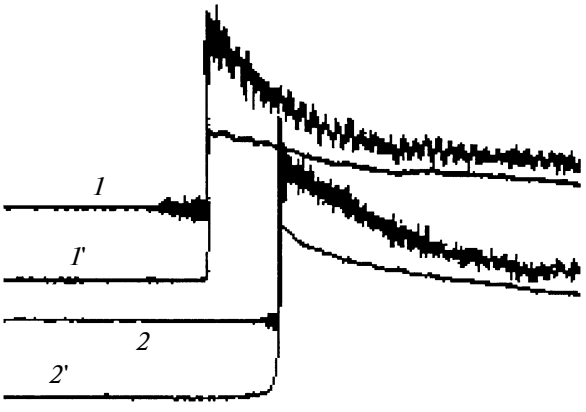

Fig. 3. Oscillograms of the (*1*, *2*) shock wave and (*1'*, *2'*) flame front under detonation conditions in two different cross sections of the tubular reactor.

The detonation velocity corresponding to straight line *1* in Fig. 2 is 2030 m/s, which is in good agreement with the experiments and calculations reported by Lewis and Elbe [11]. Note that Lewis and Elbe did not take into account the chain character of the reaction in their calculations [11]. It might, therefore, seem that the agreement between these calculations and experimental data confirms the popular view ignoring the chain nature of the chemical process in detonation. However, the data obtained for the same hydrogen–air mixture, but with dopants, indicate radical changes in detonation parameters. In the presence of

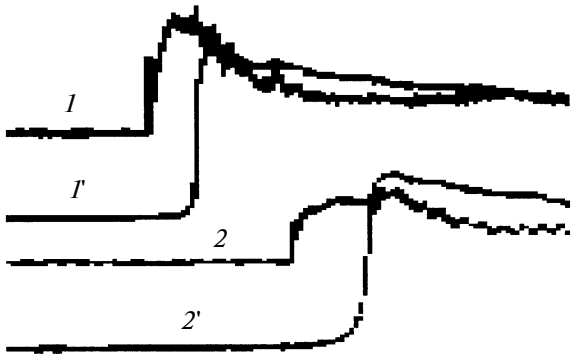

Fig. 4. Oscillograms of the (*1*, *2*) shock wave and (*1'*, *2'*) flame front in two successive measurement cross sections of the tubular reactor after the breakdown of detonation in the mixture containing 3% propene.

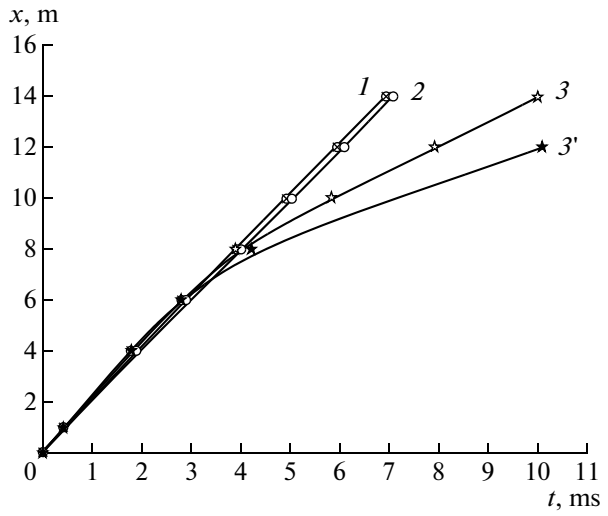

Fig. 5. Effect of isobutene on detonation in the 33.8% H_2 + air mixture [25]. Isobutene concentration (%): (*1*) 0, (*2*) 2.0, and (*3*, *3'*) 2.3 (*3*, shock wave; *3'*, combustion front).

3% isobutene in the 45% H_2 + air mixture, the detonation wave breaks down almost immediately after the entry of the initiating detonation wave into the reactor. Indeed, *x*–*t* diagrams *2* and *2'* in Fig. 2 demonstrate that the flame front lags behind the shock wave, which, as a consequence, also begins to slow down. A double unsteady-state discontinuity travels along the tube, consisting of a decelerating shock wave and a flame front moving behind it with an increasing lag. This situation is also illustrated in Fig. 4. Two pairs of shock wave and light emission oscillograms referring to two successive measurement cross sections are shown here. The upper oscillograms (*1*, *2*), which refer to the shock wave, are ahead of the lower oscillograms (*1'*, *2'*), which characterize luminescence. In going along the tube, the distance between the wave and light emission fronts increases and the signal intensities decrease, indicating that the process is damped.

Since the inhibitor slows down the reaction and the flame moves with a decreasing velocity, combustion does not generate a compression wave that can produce a sufficiently strong shock wave and, accordingly, detonation before itself. Thus, the addition of 3% isobutene to the 45% H_2 + air mixture prevents detonation even after strong initiation. In the presence of 3% propene, the detonation wave breaks down somewhat later, after traveling a distance of 2.5–3.0 m.

The effects of isobutene and propene on the detonation wave cannot be due to dilution: measurements demonstrate that inert gas concentrations far exceeding the above olefin concentrations are required for the breakdown of detonation. In addition, it is clear from Fig. 2 that the effectiveness of a dopant depends on its chemical composition.

Since detonation is inhibited, the chemical process is a chain process and is, therefore, due to reactions of atoms and radicals. In the process considered, these species are obviously $OH^{\cdot}$ radicals and H atoms. The presence of hydrogen atoms and O_2 molecules inevitably brings about the fast reaction

$$H + O_2 = OH^{\cdot} + O \qquad (I)$$

which multiplies active free valences and reactive intermediate species causing chain branching. A comparison between the known rate constants of the O_2 + H_2 reaction and the chain branching reaction (I) [22, 23] suggests that, under combustion conditions, O_2 reacts mainly with hydrogen atoms; that is, the reaction proceeds via the chain branching route. The slowdown of combustion and the breakdown of detonation under the action of isobutene are caused by the reaction

$$H + i\text{-}C_4H_8 = C_4H_9^{\cdot}, \qquad (II)$$

in which the active chain carrier—atomic hydrogen—is replaced by the $C_4H_9^{\cdot}$ radical, which is incapable of regenerating chain carriers for hydrogen combustion. Reactions of this radical lead eventually to the disappearance of free valences and, therefore, to chain termination. This slowdown of the process is inhibition. The inhibition reaction (II) is in competition with reaction (I). Note that combustion is slowed down despite the fact that reaction (II) is exothermic.

As the inhibitor concentration is decreased or the O_2 concentration is raised, the distance traveled by the detonation wave before its breakdown lengthens. For example, in the 33.8% H_2 + air mixture containing 2.3% isobutene, the detonation wave breaks down only 6.5 m from the reactor entrance (Fig. 5). Up to the breakdown point, the detonation wave velocity is almost invariable and is equal to the velocity observed in the absence of an inhibitor: up to this point in time, curves *3* and *3'* in the *x*–*t* diagram (Fig. 5), coincide with straight line *1*. After the detonation wave travels 6.5 m, the reaction zone begins to lag behind the shock

wave increasingly and the latter also begins to decelerate. Thus, detonation, which is steady-state up to this point, breaks down under the action of the dopant, indicating that the process is not a single-step reaction, but a branched-chain one. Therefore, the competition between chain branching and chain termination plays the determining role. Obviously, the significance of this competition is not due to the presence of the inhibitor. The inhibitor only accentuates the role of this competition and, accordingly, branched-chains in detonation. Since the inhibitor is uniformly distributed in the hydrogen–air mixture, the observed behavior of the detonation wave suggests that this wave is affected by the inhibitor from the instant it enters the reactor and weakens monotonically as the combustion reaction slows down while traveling along the tube. Once the decreasing reaction rate reaches a certain value, the flame zone begins to lag behind the shock wave and the energy of the reaction can no longer sustain detonation. In the run represented by curve *3* in Fig. 5, this takes place at a distance of 6.5 m.

The detonation velocity in the 33.8% H_2 + air mixtures containing 2% isobutene or less is equal to the detonation velocity in the undoped mixture. Therefore, the reaction rate does not decrease below its critical value at least up the end of the tube. However, it is not impossible that a somewhat lower rate of the chain process is established at these inhibitor concentrations and that this slower process is no less capable of sustaining detonation.

The above data demonstrate that the detonation parameters depend even on the molecular structure of the inhibitor. Owing to the increased reactivity of the π bond at the tertiary carbon atom in its molecule, isobutene inhibits detonation more strongly than propene, in which the π bond is at the secondary carbon atom. The effect of methane, whose molecule has no π bond, is substantially weaker than the effect of propene or isobutene. This is indicated by the fact that, unlike propene and butene, 4% methane does not prevent detonation in the 50% H_2 + air mixture, but only breaks it down in the sixth meter along the tube (Fig. 6).

Thus, because of the determining role of the competition between chain branching and chain termination, the correlation between chemical structure and reactivity also shows itself as the dependence of the macrokinetic and gas-dynamic characteristics of the process on the molecular structure of the dopant. As is clear from Fig. 2, detonation in the presence of isobutene breaks down sooner and more abruptly than in the presence of the same amount of propene. The data presented in Figs. 5 and 6 demonstrate that, by varying the concentration and chemical properties of the dopant, it is possible to break down the detonation wave at a preset distance from its origination point.

Now we will consider why the dopants affect detonation in spite of the high temperature. It follows from Eq. (5), which establishes a linear relationship between dn/dt and n, that n depends exponentially on the difference $2k_b[B] - k_t$ [9, 18, 19]. From this fact and expression (4), it follows that the process rate w also depends exponentially on $2k_b[B] - k_t$. The effective overall rate constant k_t contains the product $k_{In}[In]$ as a summand, where k_{In} is the rate constant of the inhibition event and [In] is the inhibitor concentration. This exponential dependence on the rate constant of the inhibition event itself ensures the strong effect of the dopant on the process rate. This effect is further strengthened by the fact that $2k_b$ and $k_{In}[In]$ appear in the exponent as their difference. In addition, the rate constants appear in the exponent as their Boltzmann factors, making the temperature dependence of the process rate extremely strong. As a consequence, even a slight decrease in the mixture temperature caused by inhibition exerts a very strong effect on the process rate.

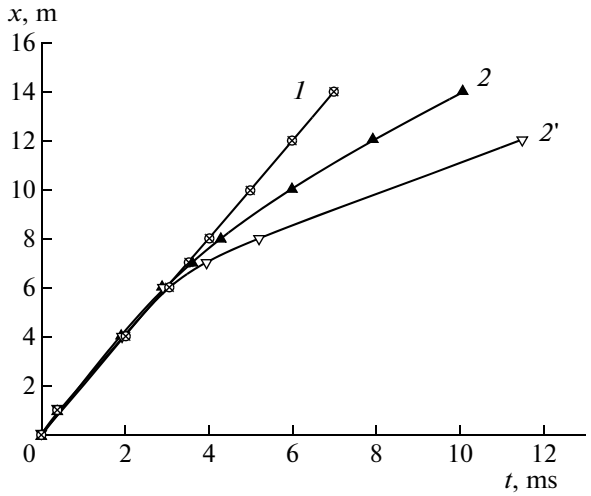

Fig. 6. Breakdown of detonation under the action of methane. Mixture composition: (*1*) 50% H_2 and (*2*, *2'*) 50% H_2 + 4%CH_4; (*2*) shock wave; (*2'*) combustion front.

The above data and the results of our previous studies [19–21, 24] demonstrate that revealing and taking into consideration the branched-chain character of the chemical process in the detonation of hydrogen–air mixtures has made it possible to plausibly account for the observed facts and to predict and discover the breakdown of the developed detonation wave by inhibitors and the different efficiencies of different dopants. This has made possible chemical control of detonation parameters through the introduction of appropriate dopants. It should be expected that the chain branching and termination reactions largely determine the structure of the detonation front.

Note that the dependence of deflagration on the chemical properties of the dopant has also been predicted and discovered [19, 26, 27]. Therefore, without taking into account the chain branching and termination reactions, it is also impossible to explain the observed features of flame propagation.

CONCLUSIONS

The influence of effective inhibitors on the detonation of hydrogen–air mixtures is evidence that the chemical process involved in detonation occurs via a branched-chain mechanism. It is this mechanism that ensures the high reaction rates necessary for the intensive shock compression of the gas. Accordingly, the basic characteristics of detonation are determined by the competition between the chain branching and chain termination reactions. Inside the concentration range of detonation (i.e., far from the critical conditions), if the chain branching rate exceeds greatly the termination rate, combustion will proceed very intensively as explosion, which can generate and sustain detonation. Use of the above effective dopants enabled us to reveal the determining role of the competition between chain branching and chain termination in detonation under any detonation wave propagation conditions. These dopants provide means to prevent detonation and to break it down at a preset distance from its initiation point. By contrast, the conventional view of the chemical process that ignores the chain branching and termination reactions can only formally account for some detonation parameters in a limited range of initial conditions.

ACKNOWLEDGMENTS

This study was supported by a grant from the Presidium of the Russian Academy of Sciences (program nos. 15P and 12P) and by the Russian Foundation for Basic Research (project no. 03-08-010301a).

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