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PHYSICAL CHEMISTRY

Deflagration-to-Detonation Transition in Air Mixtures of Polypropylene Pyrolysis Products

S. M. Frolov[a,b,c,*], V. I. Zvegintsev[d], V. S. Aksenov[a,b], I. V. Bilera[e], V. M. Kazachenko[a,f], I. O. Shamshin[a,c], P. A. Gusev[a,g], and M. S. Belotserkovskaya [c,h]

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Abstract—A new method to determine fuel detonability has been proposed, which is based on measuring the length and time of a deflagration-to-detonation transition (DDT) in a calibration pulsed-detonation wind tunnel (CPDWT). The fuel was polypropylene granules (PG). A test stand was designed and built, which included the CPDWT and a gas generator to obtain PG pyrolysis products (PGPP) at a decomposition temperature to 800°C. Experiments for studying DDT in PGPP–air mixtures were carried out. It was shown that the detonability of PGPP is close to that of a stoichiometric mixture of autogas liquefied petroleum gas with air under normal conditions.

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The problem of increasing the power efficiency of the combustion in the power plants of high-speed aircraft is currently solved by burning fuel in controlled detonation mode, and the corresponding thermodynamic cycle is called the Zel'dovich cycle [2]. We for the first time propose to solve this problem using controlled detonation of solid-fuel pyrolysis products in air. Up to now, such an approach was applied only to deflagration combustion [3–10].

A most important characteristic of the efficiency of using solid fuels in a detonation engine is their detonability. The relative detonability of fuel–air mixtures (FAMs) is usually estimated from the direct detonation initiation energy and the multifront detonation cell size. Measurement of these parameters is difficult and in great error.

Based on the results of our previous studies [11], we propose a new method to determine the fuel detonability: from the length and/or time of a deflagration-to-detonation transition (DDT) in a calibration pulsed-detonation wind tunnel (CPDWT). The CPDWT is a part of a test stand, which also includes an air supply system, a gas generator, a mixer, and also controllers, igniters, and recorders: ionization probes (IPs) and high-response pressure gauges (PGs).

The calibration pulsed-detonation wind tunnel (Fig. 1) comprises a combustor and three sections: a flame acceleration section, a helical section, and a test section. Compressed air is periodically pumped to the mixer, where it is mixed with a combustible gas fed continuously from the gas generator. The air flow rate is found from the pressure change across the air receiver. The combustible gas flow rate is estimated from the time of the complete decomposition of a solid-fuel sample in the gas generator. The mixed FAM is fed from the mixer to the CPDWT combustor, where it is ignited by a car spark plug. The formed flame passes to the flame acceleration section, in which a steel-wire Shchelkin spiral is installed.

Downstream the flame acceleration section is the helical section, which consists of two turns of a helically wound tube. In this section, the compression

[a] *Semenov Institute of Chemical Physics, Russian Academy of Sciences, Moscow, 119991 Russia*
[b] *MIFI National Research Nuclear University, Moscow, 115409 Russia*
[c] *Institute of Systems Research, Russian Academy of Sciences, Moscow, 117218 Russia*
[d] *Khristianovich Institute of Theoretical and Applied Mechanics, Siberian Branch, Russian Academy of Sciences, Novosibirsk, 630090 Russia*
[e] *Topchiev Institute of Petrochemical Synthesis, Russian Academy of Sciences, Moscow, 119991 Russia*
[f] *Bauman Moscow State Technical University (National Research University), Moscow, 105005 Russia*
[g] *Joint Institute for High Temperatures, Russian Academy of Sciences, Moscow, 125412 Russia*
[h] *Institute of Design Automation, Russian Academy of Sciences, Moscow, 117218 Russia*
**e-mail: sergei@frolovs.ru*

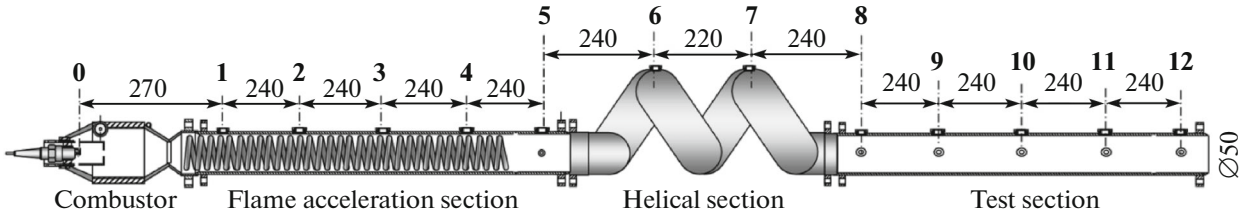

Fig. 1. Scheme of the calibration pulsed-detonation wind tunnel, including base distances (in mm): 0, ignition site; 1–12, measurement sections, in which PIs and/or PGs are installed.

waves are gas-dynamically focused, and self-ignition spots nucleate, which can eventually lead to a DDT by a previously considered mechanism [12] and to further detonation propagation.

The test section of the CPDWT is a straight smooth tube and is intended for measuring parameters of the produced combustion and detonation waves. To the outlet of the section, an additional tube section 1790 mm in length is connected, through which the combustion products are vented (not shown in Fig. 1).

In the scheme of the CPDWT, the numbers of measurement sections (MSs), in which IPs and PGs are installed, are indicated, and so are the distances between the MSs. There are twelve MSs along the CPDWT. In MSs 1–7 and 10, only IPs are placed, whereas in MSs 8, 9, 11, and 12, both IPs and PGs are located. The operating principle of the IPs and a measurement procedure were described before [13]. The IPs determine the instantaneous position of a flame with an accuracy of ±2 mm. The PGs measure the instantaneous position of a pressure wave with an accuracy of ±6 mm.

The solid fuel was secondary polypropylene granules (PG). The thermal decomposition of PG is performed in the gas generator (a cylindrical stainless-steel reactor). The gas generator is put into a muffle furnace heated to decomposition temperature T_d controlled by a thermocouple with an accuracy of ±5°C. The gas generator operates in the temperature range $650^oC \le T_d \le 800^oC$ at a PG sample weight of 15 g.

A chromatographic analysis of the composition of the gaseous products of the PG pyrolysis showed that they mainly consist of propylene (to 39%), methane (to 21%), ethylene (to 17%), isobutene (to 14%), ethane (to 12%), and propane (to 4%).

Experiments for determining the detonability of FAMs are carried out according to the following procedure. Initially, the cyclogram of the operation of the test stand is specified. The working cycle is adjusted based on the fact that the combustible gas is fed to the CPDWT continuously, and air is supplied portionwise. The air supply duration is chosen based on the air flow rate so that the volume of the gases fed to the CPDWT is larger than the CPDWT volume. After ignition, the air supply is suspended for a short time and then resumed. The pause in the air supply is provided to create a plug of the pyrolysis products between a new portion of the fresh FAM and the products of the combustion at the previous cycle. After that, a cycle of air supply, ignition, and pause is repeated a given number of times ("shots"). The test stand operates autonomously until the complete consumption of the solid fuel in successive shots.

From the flow rates of air and the combustible gas, the air–fuel mass ratio L_o was found. Let us recall that, for stoichiometric FAMs based on hydrocarbons, such as jet fuel, $L_{o,st} \approx 15$. Knowing T_d and L_o, and also the initial air temperature $T_a \approx 20^oC$, one can estimate the FAM temperature at the inlet of the CPDWT at $T_m \approx (T_d + L_oT_a)/(1 + L_o)$.

Figure 2 gives an example of the primary readings of IPs (dashed curves) and PGs (solid lines) in one of the shots in an experiment with a FAM based on PG pyrolysis products (PGPP). Time is counted from the ignition time. The times of abrupt deviations of the IP readings below the baseline are the times of the arrival of a flame front in the corresponding MS (see point and arrow in section 5). Similarly, the times of abrupt deviations of the PG readings above the baseline are the times of the arrival of a pressure wave at the corresponding MS (see point and arrow in section 8). Knowing the distances from all the MSs to the ignition site, based on the data of Fig. 2, one can construct the dependences of the velocities of the flame front and the pressure wave on the travelled distance and find the DDT length L_{DDT} and the DDT time t_{DDT}. As was previously determined [14], detonation emerges when the time delay between the arrivals of a pressure wave and a flame front does not exceed 100 μs; i.e., a FAM self-ignites by shock compression. In sections 8, 9, 11, and 12, there is already almost no time delay between the signals of IPs and PGs; i.e., a detonation wave propagates in the test section. In the considered case, $L_{DDT} \approx 2$ m and $t_{DDT} \approx 15$ ms.

Table 1 presents the results of typical experiments for studying DDT in a FAM based on the products of the PG pyrolysis at $650^oC \le T_d \le 800^oC$, and also experiments with stoichiometric FAMs based on methane and autogas liquefied petroleum gas (LPG). The experiments with methane and LPG were performed for adjusting the procedure and obtaining

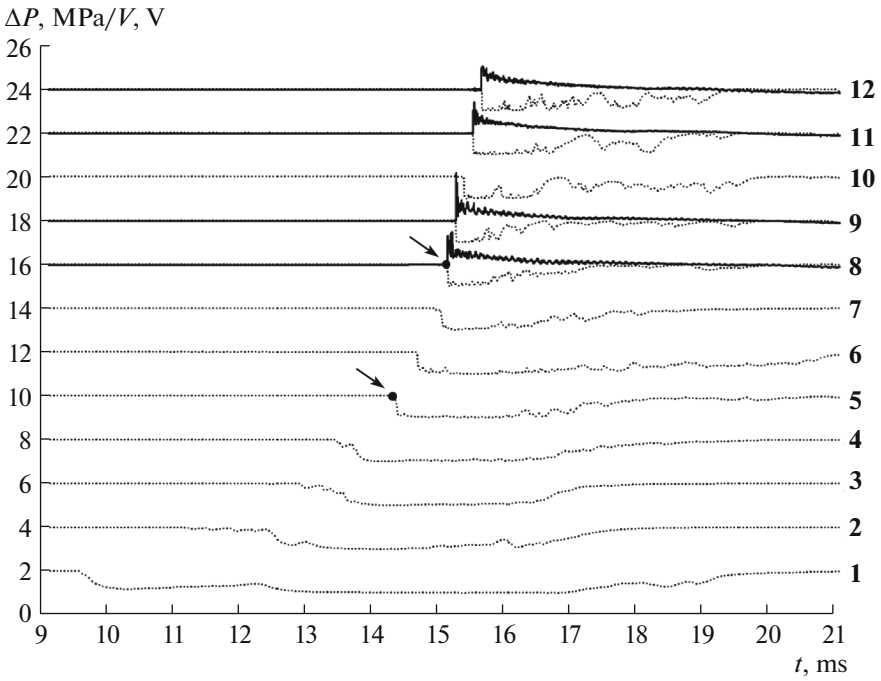

Fig. 2. Primary readings of IPs (voltage V, V) in MSs 1–12 (dashed lines) and PGs (gauge pressure ΔP, MPa) in MSs 8, 9, 11, and 12 (solid lines) in a single shot in an experiment with an FAM based on the products of the PG pyrolysis at a decomposition temperature of 700°C.

comparative data. Unlike PGPP, which were fed to the CPDWT in the heated state, the FAMs based on methane and LPG were delivered to the CPDWT at room temperature. Table 1 presents all the most important parameters of the experiments and the results of measuring L_{DDT} and t_{DDT}, and also the average detonation velocities.

Experiments 38, 39, and 40 were conducted at $T_d \approx 700$°C. Table 1 shows that L_o from experiment 38 to experiments 39 and 40 decreases from 13.5 to 11.2. Because $L_{o,st} \approx 15$, one can conclude that, in all these experiments, there is an excess of fuel in the FAM: the excess air coefficient $\alpha = L_o/L_{o,st} < 1$. The FAM tem-

Table 1. Results of several experiments for studying DDT in FAMs based on methane, LPG, and PGPP

No. of experiment/fuel	89 LPG	59 PGPP	38 PGPP	39 PGPP	40 PGPP	61 PGPP	82 methane
Decomposition temperature T_d, °C	–	653	705	703	710	804	–
Initial pressure in receiver, MPa	–	0.37	0.40	0.37	0.33	0.40	–
Final pressure in receiver*, MPa	–	0.31	0.37	0.33	0.30	0.33	–
Air flow rate (average), g/s	–	2.5	2.7	2.4	2.2	2.9	–
Fuel flow rate (average), g/s	–	0.2	0.2	0.2	0.2	0.26	–
Air-to-fuel mass ratio L_0	15.3	12.1	13.5	11.8	11.2	11.0	17.3
Excess air coefficient α	1.00	0.81	0.90	0.79	0.74	0.74	1.00
Relative mass of solid residue, %	–	4.9	7.3	7.3	7.3	18.0	–
Number of shots	6	8	8	10	6	6	6
Estimated FAM temperature at CPDWT inlet, T_m, °C	20	68	74	73	77	85	20
L_{DDT}, m	~2	~2	~2	~2	~2	~2	~2
t_{DDT}, ms	12.9	12.9	10.6	11.2	11.7	8.6	15.1
Average detonation velocity, m/s	1800	1730	1800	1800	1800	1770	1715

*Equilibrium pressure after keeping for 5 min.

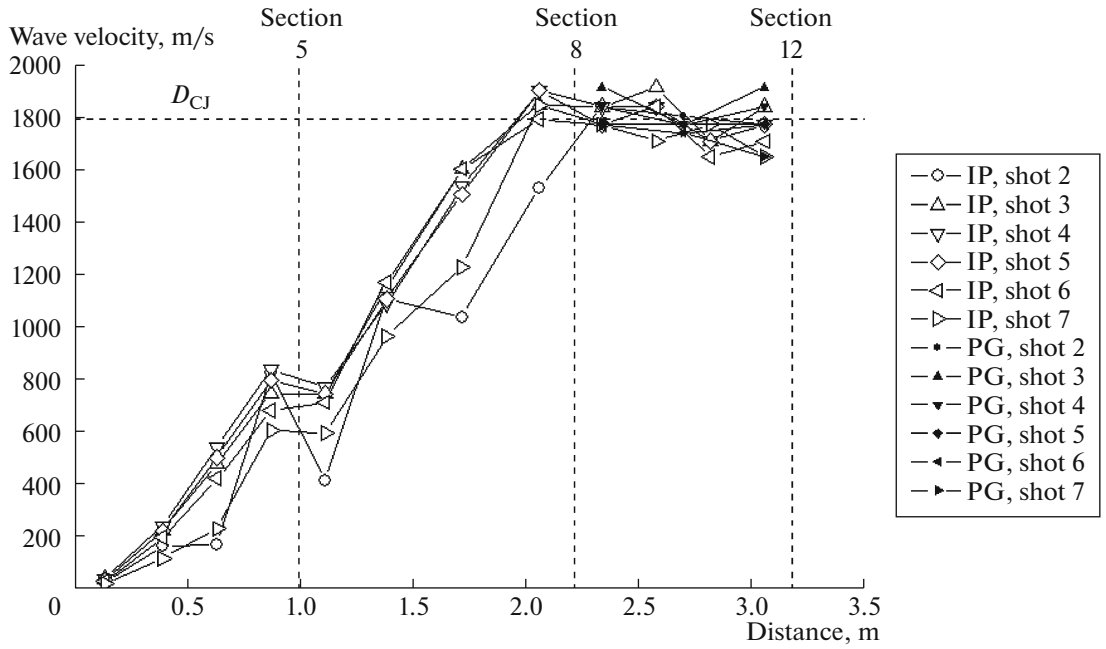

Fig. 3. Dependences of the velocities of the flame front and the pressure wave on the travelled distance in six successive shots 2–7 in experiment 40 with an FAM based on PGPP.

perature at the CPDWT inlet in these experiments is $T_m \approx 75$°C.

Let us demonstrate, by the example of Fig. 3 for experiment 40, how the flame accelerates from shot to shot. Figure 3 shows the dependences of the velocities of the flame front and the pressure wave on the travelled distance in six successive shots 2–7. In all the six shots, there was a DDT with subsequent propagation of a detonation wave at a constant velocity on the order of 1700–1870 m/s in the test section of the CPDWT. In all the shots, the DDT occurred between MSs 7 and 8 at the outlet of the helical section; i.e., $L_{DDT} \approx 2$ m. The DDT length L_{DDT} varied insignificantly, regardless of the change in the FAM composition from shot to shot. In experiments 38 and 39, L_{DDT} was the same. The DDT time was minimal in experiment 38 ($t_{DDT} \approx 10.6$ ms) and maximal in experiment 40 ($t_{DDT} \approx 11.7$ ms); i.e., as it was expected, enriching a FAM with fuel decreased its detonability.

In experiments 59 and 61, which were carried out at $T_d \approx 650$°C and 800°C, there were also a DDT and propagation of detonation waves in the test section of the CPDWT at quasi-stationary velocities of 1650–1800 and 1650–1900 m/s, respectively. In these experiments, the DDT also occurred between MSs 7 and 8 at the outlet of the helical section of the CPDWT; i.e., $L_{DDT} \approx 2$ m. A comparison of the DDT times in experiments 59, 40, and 61 showed that this time was minimal in experiment 61 ($t_{DDT} \approx 8.6$ ms) and maximal in experiment 59 ($t_{DDT} \approx 12.9$ ms); i.e., increasing decomposition temperature T_d from 650 to 800°C increases the FAMs detonability.

In the experiments with the stoichiometric FAMs based on methane and LPG, a DDT with $L_{DDT} \approx 2$ m was also observed, but the DDT times t_{DDT} were 13 and 15 ms, respectively. Moreover, in the methane–air mixture, the limiting (spin) detonation mode was detected. This means that the detonability of the FAM based on PGPP at decomposition temperatures T_d from 650 to 800°C is comparable with or even exceeds the detonability of the stoichiometric FAM based on LPG under normal conditions.

Thus, we proposed a new method to determine fuel detonability, which is based on measuring the length and time of DDT in a CPDWT. A most important distinguishing feature of the CPDWT is that it operates in pulsed–periodic mode; therefore, a single experiment gives sufficient information for determining the DDT length and time. Experiments for studying DDT in PGPP–air mixtures were conducted. It was demonstrated that, in air mixtures enriched with fuel ($0.73 \le \alpha \le 0.90$) at normal pressure and elevated initial temperature (70–90°C), the detonability of PGPP is close to that of a stoichiometric mixture of LPG with air under normal conditions.

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