RANKING OF FUEL–AIR MIXTURES IN TERMS OF THEIR PROPENSITY TO DEFLAGRATION-TO-DETONATION TRANSITION

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The term "detonability" with respect to fuel–air mixtures (FAMs) implies the ability of a reactive mixture of a given composition to sup-

port the propagation of a stationary detonation wave in various thermodynamic and gasdynamic conditions. The detonability of FAMs, on the one hand, determines their explosion hazards during storage, transportation, and use in various sectors of the economy and, on the other hand, the possibility of their practical application in advanced energy-converting devices operating on detonative pressure gain combustion.

The detonability of reactive mixtures is a relative concept. As a method for its evaluation, one can take a comparison of the mean cell size of multifront detonation propagating in a premixed FAM of a particular fuel under normal conditions with the cell size of any selected (reference) FAM. In this case, the mean size of the detonation cell in the reference FAM is taken as a measure of detonability and the detonability of all other FAMs is estimated with respect to this measure: the larger the cell size, the lower the detonability. As a method for estimating FAM detonability, one can also compare the critical energy of direct initiation of spherical detonation in a quiescent premixed FAM under normal conditions with the critical energy of direct initiation of spherical detonation of any reference FAM. Other methods and measures for assessing the relative detonability of a given FAM include the comparison of FAMs by the critical diameter of detonation transmission from a tube to an unconfined volume and/or by the limiting diameter of detonation propagation in a straight tube with smooth walls. In addition, the methods and measures for assessing the relative detonability can include the comparison of FAMs by the run-up distance of the deflagration-to-detonation transition (DDT), first proposed by Sokolik and Shchelkin in 1933. To complete the picture, one should also mention methods for evaluating the detonability of motor fuels for internal combustion engines in terms of the Octane number, described in detail in national and international standards.

It is worth noting that all of the above methods and measures for evaluating the detonability of FAMs are based solely on the experiment: the current level of development of the detonation theory does not yet allow reliable assessment of the detonability of FAMs in different conditions based on unambiguous scientifically grounded criteria. The experimental determination of the detonation cell size, the energy of direct initiation of spherical detonation, the critical diameter of the transmission of detonation from the tube into an unconfined volume,
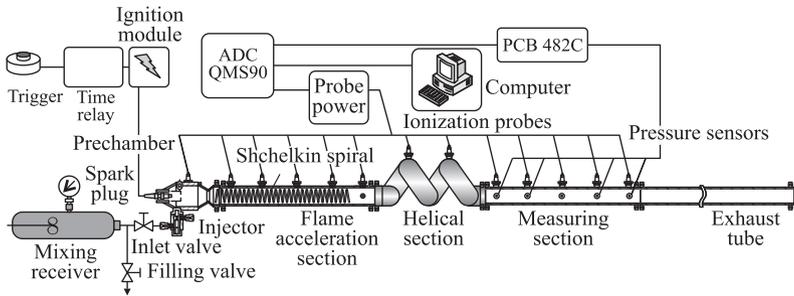
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Figure 1 Schematic of the test bench with the SDT

and/or the limiting diameter of detonation propagation in a straight tube with smooth walls, even for gaseous FAMs, is accompanied with great difficulties and with large measurement errors.

We propose herein an alternative method for estimating the detonability of FAMs based on measuring the DDT run-up time in a standard detonation tube (SDT) under substantially identical thermodynamic and gasdynamic conditions. This method is applicable to gaseous premixed and nonpremixed compositions and to two-phase FAMs based on liquid and solid fuels. The objective of this work is to develop the experimental technique for simple and reliable estimation of the comparative detonability of FAMs.

Figure 1 shows the schematic of a test bench with the SDT. The main element of the bench is an open-type pulse-detonation tube which includes a prechamber and three sections: (*i*) a flame acceleration section with a Shchelkin spiral; (*ii*) a helical section of the tube for gasdynamic focusing of a shock wave; and (*iii*) a measuring section, a straight and smooth section for measuring pressure in the propagating detonation wave and the velocity of detonation. The bench includes control units, ignition and registration systems, and measuring probes. The most important feature of the SDT is its operation in a pulse-periodic mode: fuel and air are fed into the tube and periodically ignited with a predetermined frequency, so that enough statistics are gathered in one experiment to determine the DDT run-up time. The helical section of the SDT ensures that the DDT in FAMs of different compositions always occurs ahead of the measuring
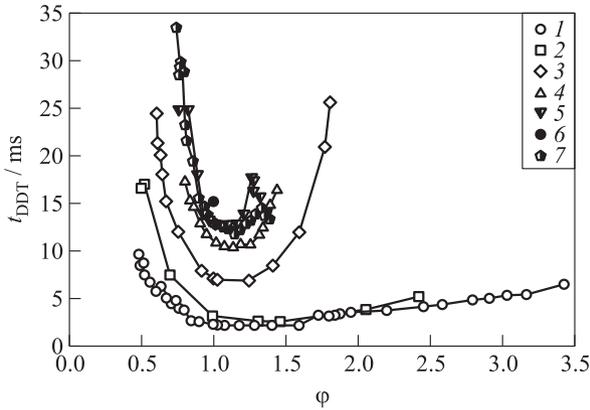
Figure 2 Dependences of the measured DDT run-up time t_{DDT} on the fuel-to-air equivalence ratio φ in FAMs of various combustible gases; each point corresponds to the mean of 10–20 experiments: 1 — H_2; 2 — C_2H_2; 3 — C_2H_4; 4 — C_3H_6; 5 — $C_3H_8 + C_4H_{10}$; 6 — CH_4; and 7 — C_5H_{12}

section, i. e., the DDT run-up distance is limited by the exit from the helical section.

The most interesting results of multiple experiments are presented in Fig. 2 which shows the dependences of the measured DDT run-up time t_{DDT} on the fuel-to-air equivalence ratio φ in premixed FAMs of different combustible gases. The absolute value of the DDT run-up time varies from ~ 2 to ~ 34 ms, i. e., by a factor of 17. All $t_{DDT}(\varphi)$ curves are U-shaped with the pronounced minima for compositions slightly enriched in fuel ($\varphi = 1.1$–1.4). The tails of the U-shaped curves sharply go upward at the concentration limits of DDT, especially at the lower limit. In this case, the curves located above are embedded in the curves located below, i. e., for the upper curves, the boundaries of the existence of detonation are narrower than for the lower ones. For any given φ, hydrogen FAMs possess the shortest measured DDT run-up time and methane FAMs possess the longest measured DDT run-up time. The data in Fig. 2 can be used directly for a comparative assessment of the detonability of different premixed FAMs using the DDT run-up time t_{DDT} as a detonability measure.

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According to Fig. 2, one can rank premixed FAMs in descending order of their detonability under the same conditions as follows:

$$H_2 > C_2H_2 > C_2H_4 > C_3H_6 > C_5H_{12} > C_3H_8 + C_4H_{10} > CH_4 .$$

It is interesting that FAMs based on n-pentane turn out to possess somewhat higher detonability than FAMs based on the propane–butane blend, which is inconsistent with the ranking of FAM detonability in terms of the average cell size of multifront detonation. Apparently, the difference in obtaining a detonation via DDT and via direct initiation manifests itself: in DDT, the main role is played by low-temperature self-ignition of FAM behind a relatively weak shock wave, whereas in the direct initiation of detonation, the high-temperature self-ignition of FAM behind a strong shock wave is of primary importance. With an increase in the number of carbon atoms in the alkane molecule, the low-temperature self-ignition delay in the region of the negative temperature coefficient of the reaction rate is known to decrease. This means that the heavier alkane hydrocarbons should exhibit higher detonability in terms of the DDT run-up time than the lighter ones, and the ranking shown above confirms this implication.

Another interesting outcome from Fig. 2 is that the detonability of acetylene appears to be lower than that of hydrogen. This is also not consistent with the ranking of FAM detonability in terms of the average cell size of multifront detonation. Apparently, here, the difference in obtaining a detonation via DDT and via direct initiation also manifests itself: the flame velocity in hydrogen-based FAMs is considerably larger (50% to more than 100%) than that in the acetylene-based FAMs at normal conditions, thus influencing the DDT time, whereas in the direct initiation of detonation, the difference in flame velocities plays no important role.

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