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Turbulent Combustion with Localized Preflame Autoignition of Hydrogen-Air Mixture in an Enclosure

S.M. Frolov, V.S. Ivanov
Semenov Institute of Chemical Physics RAS, 119991, Moscow, Russia

Numerical simulation of flame propagation with preflame autoignition in enclosures is a complex problem. The phenomenology of the process includes flame ignition and propagation, unburned mixture compression and heating, as well as formation of hot spots and fast-spreading localized explosions in the preflame region. The localized explosions evolve from the sites with the minimum induction time and traverse the preflame zone as spontaneous ignition waves with the propagation velocity depending on the local instantaneous distributions of temperature and mixture composition.

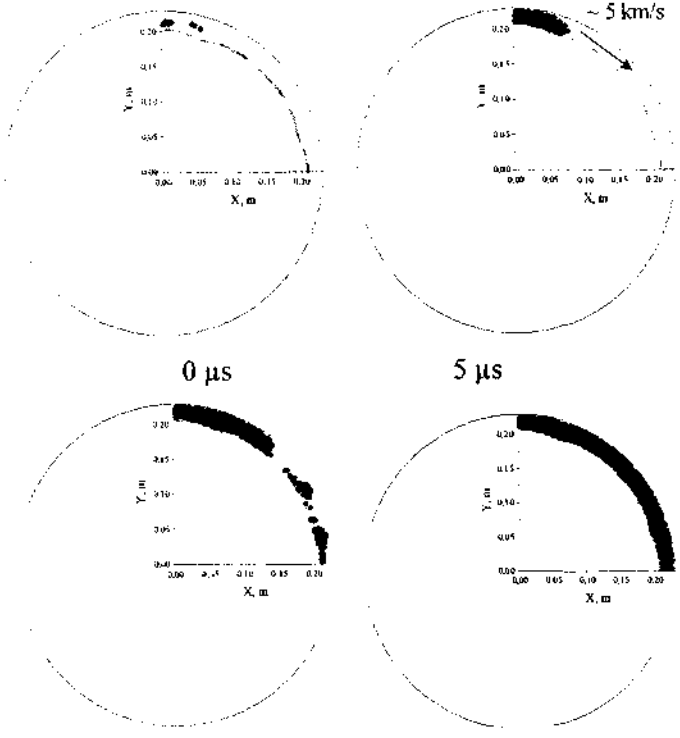
In this study, for modeling such phenomena we used a novel computational approach based on the coupled Flame-Tracking – Particle (FTP) method. The Flame Tracking technique [1] implies continuous tracing of the mean flame surface and application of the laminar/turbulent flame velocity concepts. The Particle method [2] is based on the joint velocity – scalar probability density function approach for simulating reactive mixture autoignition in the preflame zone. The coupled algorithm was supplemented with the database of tabulated laminar flame velocities as well as reaction rates of fuel oxidation in wide ranges of initial temperature, pressure, and equivalence ratio for premixed hydrogen – air compositions. The look-up tables contained information on flammability limits to identify the conditions of flame quenching. The main advantage of the FTP method is that it covers both possible modes of premixed combustion, namely, frontal and volumetric, and is based on clear phenomenology.

As numerical examples, autoignition of reactive mixtures in closed vessels of different geometries were considered, namely, in a cylindrical enclosure 0.452 m in diameter and in cubic enclosure with the side wall 0.2 m long. The wall temperature was kept constant (293 K). The vessels were filled with the stoichiometric hydrogen – air mixture at initial pressure 10 atm and temperature 900 K for the cylinder and 850 K for the cube. These initial temperatures were chosen to ensure preflame autoignition.

Figure 1 shows the predicted flame shape and the positions of autoignition sites (black points) at different time instants for the cylindrical vessel just after the first autoignition events. Autoignition of precompressed and preheated hydrogen – air mixture ahead of the flame starts in several locations and spreads at a very high apparent velocity (up to 5 km/s) along the gap between the flame and a cold wall. In 20 μs after the first autoignition events, nearly all mixture in the gap is burned except for a thin near-wall layer where the temperature is lower than in the central regions of the gap. As could be expected, the autoignition pattern depended on the number of notional particles adopted in the calculations. However when the mean number of particles per computational cell was sufficiently large (on the level of 10–15 and more) this dependence was weak. The effect of the computational grid on the autoignition pattern was also studied in detail.

The phenomenology of processes in the cubic enclosure was the same as in the cylinder. However preflame autoignition occurred in cube corners and traversed the unburned mixture with a considerably higher apparent velocity as compared to the cylinder (about 20 km/s).

Thus, the possibility of localized preflame autoignitions of fuel – air mixture in multiple hot spots has been successfully demonstrated in calculations. It was shown that the method is capable of quantitatively describing the phenomenology of combustion in enclosures with local appearance and anisotropic propagation of autoignition waves ahead of the propagating flame.



0 µs 5 µs

10 µs 15 µs

Fig.1 Snapshots of hydrogen – air preflame autoignition in the cylindrical enclosure filled with the stoichiometric hydrogen – air mixture

Very similar features are observed experimentally at abnormal ("knocking") operation of spark-ignition piston engines. Autoignition always occurs in several spots ahead of the propagating flame and then traverses the preflame zone exhibiting anisotropy and propagation nonuniformity.

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Experimental Studies of Methane-Air Flame Acceleration in Tubes with Obstacles

V.S. Aksenov, S.M. Frolov, V.S. Ivanov, A.E. Mailkov,
A.A. Skripnik, V.A. Smetanyuk
Semenov Institute of Chemical Physics RAS, 119991, Moscow, Russia

Investigation of methane – air flame acceleration in semi-closed volumes is of practical importance, in particular for safety reasons in coal mines, natural gas transportation systems, process plants, etc. According to numerous experimental observations in laboratory-scale tubes and channels with regular obstacles, flames in the stoichiometric methane – air mixture can spontaneously accelerate to the visible propagation velocity on the order of 900-1000 m/s. Depending on the experimental conditions, further flame propagation can be either quasistationary or decelerating. However,