Numerical Simulation of Localized Preflame Autoignition in Enclosures

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ABSTRACT

The phenomenology of the process under investigation includes flame ignition and propagation in an enclosure, 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. For modeling such phenomena a novel computational approach based on the coupled 3D Flame-Tracking – Particle (FTP) method is used. The Flame Tracking technique implies continuous tracing of the mean flame surface and application of the laminar/turbulent flame velocity concepts. The Particle method 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 hydrocarbon fuel oxidation in wide ranges of initial temperature, pressure, and equivalence ratio.

As an example of FTP method implementation, we considered a vertical cylindrical vessel 172 mm in diameter and 360 mm high initially filled with the homogeneous stoichiometric *n*-heptane – air mixture at initial pressure 1 atm and elevated initial temperature 500 K. The mixture was ignited by a spark plug near the bottom wall. At the end of flame propagation (at about 93 ms after ignition, Fig. 1), preflame autoignition occurred in the upper part of the cylinder leading to a sharp pressure rise. Figure 2 shows the results of calculation in terms of the temperature iso-surface $T = 735$ K at $t \approx 93$ ms. One can see volumetric hot spots ahead of the flame. In a short time interval, these hot spots transformed to localized exothermic centers giving birth to spontaneous ignition waves traversing the preflame zone at a very high apparent velocity on the level of 4–5 km/s. By other words, a nearly homogeneous preflame explosion occurred. The abrupt pressure rise resulted in the formation of a shock wave propagating towards the cylinder bottom and producing high overpressure peaks after reflections.

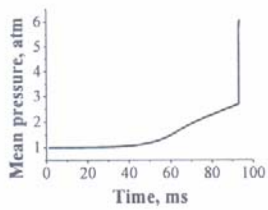

Fig. 1: Predicted pressure history in the cylindrical enclosure

Fig. 2: Temperature iso-surface prior to preflame autoignition