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LOW-TEMPERATURE FLAMELESS COMBUSTION OF HYDROCARBON DROPLETS IN MICROGRAVITY CONDITIONS

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The physico-mathematical model of droplet combustion coupled with the detailed reaction mechanism of n-dodecane ($C_{12}H_{26}$) oxidation is used to simulate forced ignition and combustion, as well as self-ignition of a n-dodecane droplet in air at normal pressure under microgravity conditions. The choice of n-dodecane is due to the recent American-Russian space experiment CFI (Cool Flame Investigation or “Zarevo”) at the International Space Station using droplets of this hydrocarbon hold in 2017. Calculations show that after the radiative extinction of the hot flame, the droplet can continue evaporating due to exothermic low-temperature oxidation of fuel vapors with multiple flashes of a “blue” flame at a characteristic temperature of about 1000 K. A detailed analysis of the calculation results shows that regular temperature jumps arise from the thermal decomposition of hydrogen peroxide, that is reaction branching with the release of hydroxyl radicals.

The radiative extinction of a hot flame is associated with the formation of a spherical soot shell around the droplet, which contains very small (nanometer range) soot particles. The soot particles absorb a part of the thermal energy of the flame and radiate it into the environment, thereby leading to irreversible energy losses and to a progressive decrease in the droplet burning rate. Such a decrease in the burning rate can lead either to a complete cessation of chemical activity near the droplet (i.e., to a complete flame extinction) or to the establishment of a quasi-stationary regime of flameless droplet combustion (i.e., its low-temperature oxidation with possible temperature jumps). As for the interpretation of the experimental observations of droplet behavior after its radiative extinction, we believe one should speak here of flameless rather than cool-flame combustion.

As an example, Fig. 1 shows the results of calculations of the self-ignition of an n-dodecane droplet of an initial diameter $D_0 = 4$ mm in air at a pressure of 0.1 MPa and at five different initial temperatures $T_0 = 600, 700, 800, 900$ and 1000 K. In Fig. 1, the ordinate is the maximum temperature of the gas around the droplet, T_m . The curve for $T_0 = 600$ K indicates, that droplet self-ignition is multistage. Firstly, after a long induction period (~ 21 s) a “cool” flame appears with a gradual increase in temperature to $T_m \approx 780$ K, followed by a blue flame with a stepped rise in temperature to $T_m \approx 1000$ K, and then a flash of a hot flame arises with

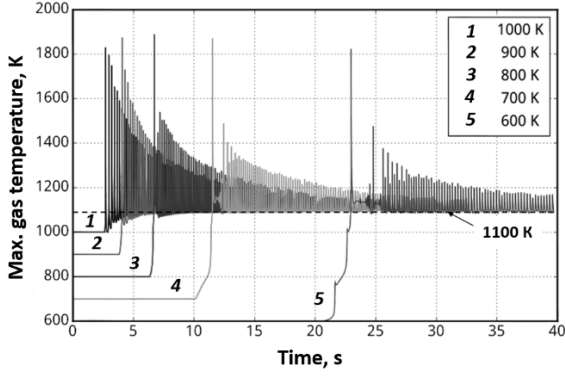


Fig. 1. Time histories of the maximum gas temperature during self-ignition of an n-dodecane droplet

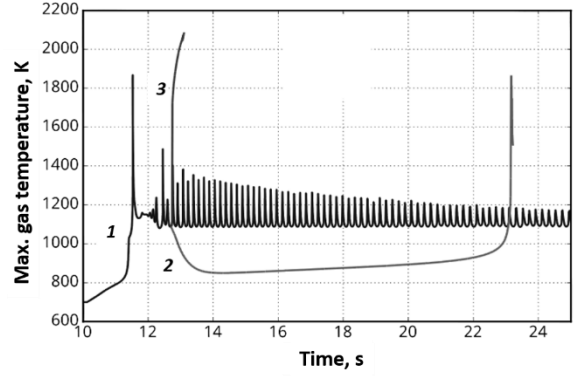


Fig. 2. Results of calculations: complete (1), with deactivated H_2O_2 decomposition (2), and with deactivated soot radiation (3)

an increase in temperature to $T_m \approx 1820$ K. The hot flame extinguishes due to the formation of the soot shell around the droplet and the energy losses associated with soot radiation. When the hot flame extinguishes, the maximum temperature of the gases near the droplet decreases to ~ 1100 K, and after a certain time delay (about 2 s), blue flames appear around the droplet transitioning into flashes of a hot flame, initially irregular and then regular. A similar behavior of the droplet is observed in calculations with different values of the initial air temperature T_0 , with the only difference that as T_0 increases, the multistage self-ignition gradually degenerates: the effects of a stepwise temperature growth at the initial sections of curves $T_m(t)$ become increasingly indistinguishable. It is interesting that the level of the maximum temperature at which regular flashes occur (~ 1100 K) does not depend on T_0 . This fact indicates the existence of some physical and chemical processes determining such a behavior. To identify these processes, we considered in detail what happens in the time intervals between the temperature jumps.

A detailed analysis shows that regular temperature jumps arise from the thermal decomposition of H_2O_2 due to branching reaction $\text{H}_2\text{O}_2 + \text{M} = \text{OH} + \text{OH} + \text{M}$. These jumps appear to be periodic or multiple blue flames, transitioning into hot flames. To finally confirm this, we conducted two mathematical experiments: in the first we equated the rate constant of the H_2O_2 decomposition reaction to zero, and in the second we equated to zero the energy losses caused by soot radiation. The results of both mathematical experiments are shown by curves 2 and 3 in Fig. 2. For convenience, the temperature curve $T_m(t)$ (curve 1) is also shown in the same graph. When the H_2O_2 decomposition reaction is deactivated (curve 2), the regular temperature jumps cease. When the radiative energy losses are switched off (curve 3), a flash of hot flame immediately occurs around the droplet.