Features of flame propagation caused by heterogeneous reactions of intermediate particles

Azatyan Vilen V.,[1*] Alymov Mikhail I.,[2] Prokopenko Vyacheslav M.[2]
Abramov Sergey K.,[2] Kazansky Vladimir B.[3]

[1] *Scientific Research Institute for System Analysis RAS, Nakhimovsky prospect, 36, building 1, 117218, Moscow, Russia*

[2] *Merzhanov Institute of Structural Macrokinetics and Materials Science, Ac. Osipyan Str. 8, 142432, Chernogolovka, Russia*

[3] *N. D. Zelinsky Instituteof Organic Chemistry RAS, Leninsky Prospect, 47, 119991, Moscow, Russia*

** E-mail: vylenazatyan@yandex.ru*

Flame propagation is one of the main modes of gas-phase combustion, passing under certain conditions into an explosion and detonation. Despite the strategic role in technology and importance for the theory of combustion, the implementation of this combustion mode, as well as its main regularities, until recently, could not be explained. Combustion accompanied by self-heating was considered as a single stage reaction of the initial molecules, caused only by an increase in temperature. The role of reaction chains was ignored. The dependence of the flame velocity on the dimensions of the reactor was explained only by a change in heat removal. To describe the rate of the process, the calculated parameters were hypothetically selected according to the observed combustion rate and according to a conventionally accepted equation. In a series of our works, however, it was shown that due to very high activation energies exceeding 200 kJ/mol, the rates of intermolecular reactions are thousands of times lower than the rates of real combustion reactions. It was found that the combustion of gases during any self-heating proceeds only through chain mechanisms. One of the important stages of chain processes is the chemisorption of atoms and radicals, because of which active particles are removed from the reaction medium, and thus the only combustion path is blocked.

To reveal and study the role of heterogeneous recombination of active particles in flame propagation, the process was carried out with varying the efficiency of heterogeneous recombination all other parameters of the system being kept unchanged. For this purpose, the reactor was preliminarily rinsed with solutions providing the specified efficiency of heterogeneous recombination. It was found that over the surfaces created in this way, the flame velocities differ up to ten times. This means that the walls affect combustion not only by removing heat, but even more so by breaking the reaction chains. An important feature of combustion was also a change in the characteristics of the flame because of its impact on the surface. The pulsating mode of combustion also depends on the properties of the surface. The obtained results indicate the need to consider heterogeneous reactions both in the theory of flame propagation and in practice, for example, when selecting materials for combustion chambers. It also follows from the obtained data that the results of numerical simulation of gas combustion can be reliable only if heterogeneous reactions of atoms and radicals and

their role in the formation of concentration and temperature gradients are to be taken into account.