Active oxygen species in combustion

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Active oxygen species (AOS – ozone O_3, molecular singlet oxygen $O_2(a)$ (0.98 eV) and $O_2(b)$ (1.63 eV), atomic oxygen $O(^3P)$ and $O(^1D)$ (1.97 eV)) play an important role in the combustion, especially when it is initiated by plasma [1, 2]. In recent years, a wide interest to them is because the processes involving AOS can be used to expand the limits of combustion and ignition. In order to reduce harmful emissions, primarily nitrogen oxides NO_x, requires reduction of the maximum gas temperature in the combustion chamber. For this purpose, the use of lean air-fuel mixture is preferable, as this also leads to a reduction in fuel consumption. Expanding the limits of combustion and ignition with the increase in the ratio "air/fuel" is one of the most pressing problems in the theory of combustion. These limits can be extended by external impact: plasma, chemical or the light (laser).

Creation of non-equilibrium plasma with high levels of reduced electric field, E/N, and a significant level of energy load may provide a high yield of oxygen atoms at O_2 plasma dissociation. The oxygen atoms enter into rapid chemical reactions with hydrocarbons and cause initiation of the combustion process. The possibility of using an electric discharge has been experimentally demonstrated in terms of thermal engines, such as in [1, 3]. Selective excitation of internal degrees of freedom of ozone and oxygen molecules by laser radiation can also increase the limits of the ratio "air/fuel".

With an excess of O_2 (the atmosphere, the air-fuel mixture, oxygen-containing plasma), oxygen atoms are effectively removed in the three-body recombination process

$$O + O_2 + M \rightarrow O_3(v) + M.$$

This forms a highly reactive $O_3(v)$ molecule which, together with the atomic oxygen may play an important role in the initiation of combustion, recovery of ozone in the atmosphere, etc. These processes were not previously included in the kinetic scheme of planetary atmospheres, combustion and oxygen-containing plasma. The vibrational excitation of ozone greatly accelerates the rate of reactions with O and $O_2(a)$ [4]. To determine the role of the reaction pathways to the dynamics of ozone in the atmosphere, in the combustion and in oxygen-containing plasma, new kinetic data are required that are not currently available in the literature and databases.

Plasma–chemical processes in air–fuel mixtures result in the formation of $O_2(b)$ molecules that may activate chain reactions in the combustion zone. Analysis of the reaction kinetics involving $O_2(b)$ is difficult due to the fact that there is little published data concerning the deactivation kinetics at temperatures above 350 K. In this report a new kinetic data related to $O_3(v)$ and $O_2(b)$ are presented.

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