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Flame Front Model with the Clusters Condensation

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Abstract. The processes model in a flame during the n-alkanes air mixture combustion initiation is proposed, taking into account the supramolecular structures formation possibility in the peroxide clusters form. This approach is justified by the n-alkanes melting temperatures correlation with their autoignition temperatures and anti-knock indexes. The condensation possibility is provided for such high molecular structures. Boiling temperatures values at flame front pressures characteristic were evaluated. To predict the peroxide clusters melting temperatures, a formula developed earlier for the hydrocarbons condensed state was used, which takes into account the length and molecular weight of modeled clusters. Expected peroxide clusters melting temperatures were predicted for conditions of dimeric and tetrameric structures. A linear dependence was used to recalculation the obtained values in boiling temperatures. It is shown that the calculated clusters phase transitions characteristic temperatures can be realized in the flame front preparatory zone. Based on the condensation theory, the flame front thickness and the minimum non-extinguishing sphere radius during ignition were estimated: the obtained data closely coincide with these parameters known values.

Introduction

Flame combustion developmental processes are explained by several theories within their paradigms [1]. The thermal theory treats the combustion process as a "black box", the input and output parameters for which are the material and energy balances components in a generalized form; it does not take into account the chemical transformations mechanisms, but considers the certain processes heat accumulation possibility. The peroxide theory takes into account the oxidation intermediate stages presence in the peroxide compounds formation form, which is observed in the flame; but the proposed phasing contradicts the combustion reaction high speed. The chain theory additionally predicts the free radicals formation in hydrocarbon oxidation processes, which have sufficient energy to activate the next molecule with the formation of more than one flame active center, which causes the reaction paths branching and its acceleration. But radicals are already products of some reaction, that is, the theory does not describe the flame initiation mechanism except in the case of ignition by an electric discharge, when ions become primary active centers. That is, there is a need to formulate a generalized explanation regarding the first elementary act, which leads to the next chemical equilibrium shift in the system.

Some researchers predict the quasi-liquid formation in the flame, which at the molecular level forms nanopores, in walls of which significant pressures are formed with the molecules emission possibility, shock ionization, which initiates the detonation combustion [2]. Nanopores are separated by the molecules double layer: this is similar to the foam structure, where the walls have some properties of a solid. According to a similar mechanism, seam detonation in coal nanopores with the methane release in quantities greater than the pores volume is also predicted [3, 4]. But the

provides the melting condition instead of "-170 ºC" for the dimer – "-15 ºC ". The n-alkanes peroxide tetramers model has expected melting points of "-49–180 ºC ", boiling points of "130–1200 ºC ", dew points up to 900 ºC. Such temperatures can be realized in the flame front preparatory zone, and compression effects further facilitate the condensation processes. Based on such a minimum volume of the combustible air mixture, which is sufficient for the formation of a condensate continuous film from peroxide clusters on the sphere surface, the minimum non-extinguishing flame sphere radius, which is spreading capable, is determined, 3 δ_{ff} (3 flame front thicknesses), which is slightly less than the known spark ignition rating of 3.7δ_{ff}. The difference is determined by the fact that in the electric discharge event, the middle zone of this sphere no longer contains the combustible substance molecules, which capable to the clustering by the peroxide mechanism, but contains the plasma. Thus, the substance peroxide clustering theory with the condensation allows us to describe the processes in the flame.

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