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Peroxide Conditions Modeling for the Combustion Occurrence

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Abstract. The oscillations presence of the substance condensed state parameters and the n-alkanes combustion process was analyzed. It is shown that the smallest substance structural unit that describes such features is a dimer, a hexamer for methane, and a trimer for ethane. The cluster "equivalent length" based on the framework number atoms in the continuous chain and without taking into account cluster side parts was used as a modulating parameter. Attention was drawn to the dependences similarity for water solubility and the autoignition temperature of n-alkanes. It is proposed to take into account clustering involving water molecules for the water solubility, and oxygen molecules in the peroxide groups form that form similar clusters for combustion processes. It is accepted that the solubility limit is determined by the condition of all water molecules aggregation by the substance, and in combustible mixtures the substance aggregates all available oxygen in the air. Corresponding peroxide proportions allow the burning limits, detonation limits, stoichiometric concentration and cold flame limit to be described. An approximation formula has been developed that describes the general dependence of the n-alkanes and 2-methylalkanes autoignition temperature based on values of the cluster length and the monomer molecular weight.

1 Introduction

In knowledge several areas, there is important information about combustion processes: conditions for substances technical use, forecasting the fires development and their extinguishing, the combustion products formation [1]. These processes description involves conducting a studies number about the initiation, general occurrence conditions, combustion spread, as well as on the substances combustion [2]. These stages are characterized by certain parameters [3], but they do not always have a simple logical sequence in hydrocarbons homologous series, which requires explanation [4, 5].

Thermal theory analyzes the balance between heat release and heat loss from the combustion area, but combustion heats have a simple logical sequence, proportional to the atoms number in the combustible substance, and do not reflect the fire hazard parameters values periodicity [6, 7]. The oxidation peroxide theory considers the oxidation intermediate stage presence with the peroxide compounds formation in the combustion [8]. But on its own, this theory does not describe the combustion process well. The chain theory assumes the presence of the chemical reactions sequential branched chain involving free radicals and peroxide compounds. Free radicals play the active flame centers role and carriers of combustion reaction activation energy [9]. But this theory does not completely describe the first elementary act at the combustion initiation stage. That is, radicals are reaction products, for example, thermal molecules destruction, which begins after providing the system with the activation energy. Such an assumption does not explain cold flame initiation well.

Some studies predict the nanoporous quasi-liquid presence in the flame; the conditions in the nanopore are sufficient for the pressures occurrence that can cause the molecules emission from its wall and impact ionization [10]. This model assumes the bimolecular condensed film formation of the combustible substance in the nanopore walls form. This mechanism is also used to describe the

5 Conclusion

Oscillation of changes in melting temperatures, water solubility and combustion parameters of n-alkanes was revealed. The supramolecular structure has a significant influence on the substance solid state properties. It was also observed that the change in tai in the n-alkanes homologous series has common features with the water solubility γ. Based on this, the possible clustering scheme modeling during the combustion initiation was carried out. We explained the limited solubility as the all water molecules aggregation by the solute molecules certain number. By analogy, during the combustion initiation at any combustible concentrations, combustible substance molecules aggregate all oxygen molecules in the form of peroxide complexes. In the work, certain proportions between peroxide groups and a combustible substance cluster are established, which correspond to LFL and UFL, LEL and UEL, the stoichiometric concentration of complete combustion and the cold flame limit with R=0.99: for LFL – $\beta = 3n_c+1$; for UFL – $\beta = 0{,}25n_c+1$; for the complete combustion stoichiometric concentration – $\beta = 1{,}5n_c+0{,}5$; for LEL – $\beta = 2n_c$; for UEL – $\beta = 1n_c$; 6) for the cold flame limit, a states mixture with $\beta = 0.5$ and with $\beta = 0.5n_c$ in the ratio 95/5 %. Based on the length and molecular weight of the smallest cluster, the introduced indicator "melting ease", formula (3) was developed for predicting the tai of n-alkanes, which works with R = 0.996.

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