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Cluster Mechanism of the Explosive Processes Initiation in the Matter

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Abstract. The relationship between substance characteristic temperatures: autoignition, melting, flash, boiling is demonstrated and analyzed. Based on the oscillatory and step changes presence, a conclusion was made about the supramolecular structures presence and periodicity in the n-alkanes homologous series. A method for modeling equivalent lengths of peroxide supramolecular structures for predicting the explosion and fire hazard parameters of n-alkanes is proposed. An approximation dependence was developed for predicting autoignition temperatures t_{ai} of n-alkanes. It is shown that stoichiometric concentrations of the various supramolecular peroxide structures formation accord to different flammability and explosion limits. A correlation between t_{ai} and Anti-Knock Index (AKI) was established. An approximation dependence was developed for predicting n-alkanes AKI. The detonation propensity index K_D was introduced based on cluster supramolecular structures modeling and melting temperatures. It is shown that K_D indicator correlates with the n-alkanes AKI and the explosives detonation velocity. The possibility of taking into account during calculations the supramolecular structures presence at the combustion stage confirms their existence.

1 Introduction

Explosive processes are often used in the industry, for military purposes, and they also become the consequences of safety rules violating for handling certain substances. However, corresponding mechanisms for the transformations initiation in substances or combustible mixtures have not been definitively established. Therefore, improving theoretical models that explain these processes and developing appropriate mathematical models for predicting the explosive processes development remains an urgent issue. Spontaneous decomposition of explosive substances with the energy release can be modeled as autoignition according to a chain mechanism, since this process is characterized by the reactions jump-like self-acceleration. For this combustion occurrence type, the thermal explosion model is also used, when at a critical temperature in each mixture part, heat release begins and the temperature rises without heat loss to neighboring zones. For such a process, it is possible to propose the instantaneous emergence model of a substance supramolecular structure. Then, at the next stage, these unstable supramolecular structures will be destroy and transform by free radical mechanisms.

Establishing the substance's ability reasons to undergo explosive transformations can provide a new perspective on explosive substances properties and creates new opportunities for ensuring the explosive processes safety. These questions are related to solving the establishing problem the first elementary act of substance state changing before the explosion. Therefore, establishing the substance structure peculiarities at explosive transformations initial stages is an urgent scientific task.

2 Literature Review

The occurrence of explosive and fire hazards can be considered in three directions: the detonation danger, the autoignition danger, and the presence of explosion hazard concentration

5 Conclusion

It was established the supramolecular structures presence during the combustible air mixture autoignition initiation, which is evidenced by the change fluctuation in t_{ai} in the n-alkanes homologous series, which is typical for t_{mp} as opposed to t_{bp}. On the basis of equivalent lengths modeling of peroxide supramolecular compounds, methods for predicting such parameters of the n-alkanes explosion and fire hazard as t_{ai}, AKI, LEL, UEL, LDL, UDL, combustion reaction stoichiometric concentration is created. The substances propensity indicator to detonation K_D was developed based on t_{mp} values and supramolecular structures modeling, this indicator correlates with n-alkanes AKI and the explosives velosity detonation. Formula (2) describes t_{ai} based on the cluster equivalent length n_{Ceq} and the combustion reaction stoichiometric coefficient with R=0.999 and the average absolute deviation of 4.1 °C. The close nature of t_{ai} to AKI with R=0.95 is shown. Formula (3) describes the dependence of AKI(n_{Ceq}) with R=0.998 and an average absolute deviation of 3 scale units. The K_D indicator correlates with the AKI of n-alkanes with R = 0.92, and also correlates with the detonation velosity with $R^2 = 0.95$. The possibility of taking into account the supramolecular structures presence at the combustion stage in the calculations confirms their existence.

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