

## 59. MODELING OF ISO-OCTANE AND N-HEPTANE AUTO-IGNITION UNDER CONDITIONS RELEVANT TO SPARK IGNITION ENGINES

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According to qualitative analysis [1] the abnormal combustion in engines ('knock') can be caused by multi-stage auto-ignition of unburned mixture pockets.

A new detailed reaction mechanism is suggested for studying auto-ignition of iso-octane, n-heptane and their mixtures in air under conditions relevant to those in an end-gas of spark ignition engines. The mechanism consists of a non-empirical block of elementary reactions for the oxidation of  $C_1$ - $C_2$ -hydrocarbons and an auto-ignition block including, apart from elementary reactions, a few overall reactions. In total, it accounts for 284 reactions with 43 species.

At low temperature, reaction branching is assumed to proceed due to alkyl peroxide decomposition, while at larger temperature due to decomposition of hydrogen peroxide and through the reactions of formaldehyde. With further temperature increase a branching process starts to go mainly through the reaction of H atom with oxygen. Transition between the branching mechanisms occurs as a result of temperature increase in the course of alkyl peroxide radical decomposition.

The mechanism has been validated by comparing the predicted results on reaction dynamics with available experimental data for the variety of n-heptane - iso-octane - air mixtures within the wide range of governing parameters, namely, temperature 650 - 1200 K, pressure 15 - 40 bar, equivalence ratio 0.5 - 2.0. The comparison has been made for the auto-ignition delay dependencies on temperature, pressure and mixture composition, for the dependencies of the induction time of cool flame and hot explosion on temperature, for the concentration of intermediate products (formaldehyde and octane peroxide radical) depending on the temperature, and for the pressure histories in the course of auto-ignition. The mechanism provides the negative temperature dependence of ignition delay within the transition region and gives satisfactory quantitative predictions.

For the sake of implementing the reaction mechanism in a multi-dimensional fluid dynamic code, the mechanism has been systematically reduced. The reduction procedure is based on the selection of governing reactions at either current state of the reacting mixture. The combination of the reactions selected during the calculations is treated as a reduced kinetic mechanism. The shortest mechanism thus obtained consists of 21 reactions with 21 species. This mechanism shows a satisfactory agreement with available experimental data and with the results given by the complete reaction mechanism.

/1/ Sokolik, A.S., "Self-Ignition, Flame and Detonation in Gases", Israel Program for Scientific Translation, Jerusalem, 1963.