NUMERICAL EVALUATION OF SOOT FORMATION CONTROL AT DIESEL-LIKE CONDITIONS BY USING SURROGATE FUELS

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Abstract: A detailed kinetic modeling is carried out to examine the influence of the molecular structure of different surrogate hydrocarbon fuels on the characteristic features of the initial phase of the formation of soot particles and on the ignition delay time under diesel-like conditions. Mixtures of n-heptane (n-C_7H_{16}) and hexadecane (cetane, $C_{16}H_{34}$) are used as the base fuels. The lighter hydrocarbons in the model were represented by n-heptane (n-C_7H_{16}) and the heavier hydrocarbons — by hexadecane ($C_{16}H_{34}$). The class of naphthenes (cycloalkanes) was represented by decalin ($C_{10}H_{18}$) and tetralin (bi-cyclin) ($C_{10}H_{12}$). At the first stage, the effect of the above hydrocarbons introduced separately into the base fuel was investigated. For the base fuel, the soot yield, the ignition delay time, the temperature, and the pressure in the virtual combustion chamber were preliminarily calculated in a position close to the top dead center of the piston. Then, in turn, all tested hydrocarbons of different chemical classes and subclasses were "injected" into the initial reactive mixture to determine the individual activity with respect to the stages of nucleation and formation of solid soot particles. When aromatic hydrocarbons (benzene, naphthalene, and anthracene) were added, the dependence of the ignition delay time on the additive ratio demonstrated a complex nonlinear character. As the concentration of the additive increases, the ignition delay of the mixture of the base fuel with addition of naphthalene decreases in comparison with other added aromatic hydrocarbons, while the amount of soot generally increases. A heavier aromatic hydrocarbon causes a greater increase in the soot yield. At the second stage, several surrogate fuels were tested to determine the synergistic effect of the influence of hydrocarbons introduced into the base fuel (naphthenes, aromatic hydrocarbons, and olefins). The results of numerical experiments at this stage showed that when these hydrocarbons were separately introduced into the base fuel, an increase in the concentration of naphthenes introduced markedly increases the content of soot particles but, at the same time, reduces the ignition delay time of the mixture. Such numerical modeling allows one to outline possible ways to create low-toxic surrogate diesel fuels (in terms of the content of soot particles).

Keywords: ignition kinetics; kinetics of soot formation; numerical simulation; surrogate diesel fuels; naphthenes, aromatic and olefin additives; soot reduction

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