MACROKINETIC MODEL FOR CALCULATION OF SOOT EMISSIONS IN DIESEL ENGINE

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Abstract: The macrokinetic model of soot formation is proposed, which may be included in the detailed and reduced kinetic mechanisms of hydrocarbon fuel oxidation and combustion. The model includes three overall irreversible reactions, namely, the acetylene pyrolysis reaction and two soot oxidation reactions — by carbon dioxide and water vapor. Arrhenius parameters entering the rate constants of overall reactions were obtained from the best fit of the results of calculations of soot yields obtained based on the macrokinetic model and on the thoroughly validated detailed kinetic mechanism (DKM). For a number of hydrocarbons (CH_4, C_3H_8, i-C_8H_{18}, n-$C_{10}H_{22}$, n-$C_{14}H_{30}$, C_6H_6, C_7H_8, and C_2H_5OH), the values of soot propensity coefficient with respect to the reference fuel (n-heptane) are obtained. The macrokinetic model is applied to multidimensional calculations of 14 different operating modes of diesel engine using the DKM of oxidation and combustion of high hydrocarbons supplemented with the DKM of NOx formation. A satisfactory agreement between the calculated and measured results for soot and NOx emissions is obtained.

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