Numerical modeling of soot formation at diesel-like conditions

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The objective of this work was to use our unified kinetic model [1] for simulation of soot-forming combustion at diesel-like conditions. Resulting data were obtained at a base diesel-like operating condition, corresponding to a near top dead center compression temperature (850 K) and pressure (3.5 MPa). Data were taken for n-heptane as a “surrogate” diesel fuel in one of the fuel-rich patterns of burning jet in immediate flame proximity, where equivalence ratio $\phi$ was equal 3.0. Our original unified kinetic model comprises of 372 species and 4782 reactions and consists of two principal components: gas-phase chemistry of high-temperature n-heptanes’ oxidation, and modified soot particle dynamics, which describes the start and evolution of the particles. The predictive power of our model was tested with injection of small amounts of H\textsubscript{2}O\textsubscript{2} and H\textsubscript{2} additives into a rich n-heptane—air mixture patterns. These additives, as it is known, influence both the processes of ignition and soot formation. In particular, very small amounts of injected H\textsubscript{2}O\textsubscript{2} enable to reduce ignition delay as well as to suppress soot formation during diesel-like combustion. The numerical simulations were validated against experimental results available in the literature. A good quantitative fit between the data calculated via the unified kinetic model and experimental data has been attained. The completed analysis might give new insights into the initial roots of soot formation process and create a magic cure for their depletion.