

NUMERICAL SIMULATION OF SOOT EMISSION REDUCTION AT A DI DIESEL ENGINE

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Abstract: A detailed kinetic modeling of the formation of soot particles during ignition and combustion of a rich *n*-heptane–air mixture ($\varphi = 3.0$) is carried out under conditions of a diesel combustion chamber. The possibility of a detailed kinetic modeling of the ignition and soot formation processes within the framework of a unified kinetic model is demonstrated. The predictive power of this model is tested for the injection of H₂O₂ and H₂ additives into a rich *n*-heptane–air mixture. These additives influence both the processes of ignition and soot formation. The kinetic parameters were kept constant in all calculations. A good qualitative agreement between the simulation results and the available experimental data is observed.

Keywords: ignition kinetics; kinetics of soot formation; numerical simulation; spray of burning diesel fuel; hydrogen peroxide additives; soot reduction

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References

1. Agafonov, G. L., I. V. Bilera, P. A. Vlasov, I. V. Zhil'tsova, Yu. A. Kolbanovskii, V. N. Smirnov, and A. M. Tereza. 2016. Unified kinetic model of soot formation in the pyrolysis and oxidation of aliphatic and aromatic hydrocarbons in shock waves. *Kinet. Catal.* 57(5):557–572.
2. Basevich, V. Ya., A. A. Belyaev, V. S. Posvyanskii, and S. M. Frolov. 2010. Mechanism of the oxidation and combustion of normal paraffin hydrocarbons: Transition from C₁–C₆ to C₇H₁₆. *Russ. J. Phys. Chem. B* 4:985–993.
3. Agafonov, G. L., I. V. Bilera, P. A. Vlasov, Yu. A. Kolbanovskii, V. N. Smirnov, and A. M. Tereza. 2015. Soot formation during the pyrolysis and oxidation of acetylene and ethylene in shock waves. *Kinet. Catal.* 56(1):12–30.
4. Basevich, V. Ya., P. A. Vlasov, A. A. Skripnik, and S. M. Frolov. 2008. Modelirovanie sazheobrazovaniya v dvigatelyakh vnutrennego sgoraniya [Soot formation modeling in internal combustion engines]. *Goren. Vzryv (Mosk.) — Combustion and Explosion* 1:40–43.
5. Baturin, S. A. 1982. *Fizicheskie osnovy i matematicheskoe modelirovanie protsessov rezul'tiruyushchego sazhevydeleniya i teplovogo izlucheniya v dizelyakh* [Physical fundamentals and mathematical modeling of the processes of total soot formation and thermal radiation in diesel engines]. Leningrad: Leningrad Polytechnic Institute. D.Sc. Diss. 441 p.
6. Dec, J. E. 1997. A conceptual model of DI Diesel combustion based on laser-sheet imaging. SAE Paper No. 970873.
7. Born, C., and N. Peters. 1998. Reduction of soot emission at a DI Diesel engine by additional injection of hydrogen peroxide during combustion. SAE Paper No. 982676.
8. Trapel, E., P. Ifeacho, and P. Roth. 2004. Injection of hydrogen peroxide into the combustion chamber of diesel engine: Effects on the exhaust gas behavior. SAE Paper No. 2004-01-2925.
9. Svistula, A. E. 2007. Snizheniye sazhevydeleniya i raskhoda topliva v dizele prisadkoy gaza i vody k toplivu [Reduction of soot formation and fuel consumption in a diesel by water and gas additives to the fuel]. *Polzunovskiy Vestnik [Polzunov Herald]* 4:95–103.
10. Fomin, V. M., Kh. Yu. Ranzi, R. R. Khakimov, and D. V. Shevchenko. 2011. Rol' vodoroda kak khimicheskogo reagenta v kineticheskom mekhanizme uglerodoobrazovaniya v dizele [Role of hydrogen as a chemical reagent in the kinetic mechanism of soot formation in a diesel engine]. *Vestnik Rossiiskogo universiteta druzhby narodov: Seriya: Inzhenernye issledovaniya* [Bull. of the Peoples' Friendship University of Russia. Ser. engineering research] 3:91–99.

11. Borisov, A. A., A. B. Borunova, K. Ya. Troshin, Yu. A. Kolbanovskii, and I. V. Bitera. 2014. O roli dobavok vodoroda v formirovanii sazhi pri okislitel'noy konversii metana

[About the role of hydrogen additives in soot formation during oxidative conversion of methane]. *Goren. Vzryv (Mosk.) — Combustion and Explosion* 7:100–106.

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