MODELING OF THE DIESEL-ENGINE OPERATION PROCESS WITH EXHAUST GAS RECIRCULATION ON THE BASIS OF A DETAILED KINETIC MECHANISM OF FUEL COMBUSTION

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Abstract: The work is devoted to the combustion process modeling in engines equipped with the exhaust recirculation system. An approach for calculating the fresh mixture composition, when the atmospheric air is diluted with the combustion products, is suggested. The object of investigations is a passenger car diesel engine in an operation mode with 37% air dilution with combustion products. To verify the suggested approach, numerical experiments are performed on the basis of three-dimensional model of the operation process in combination with the detailed reaction mechanism of n-heptane oxidation and combustion. The verification confirmed the correctness of the suggested approach and highlighted that the accurate estimation of initial air composition is necessary for the adequate modeling of the operation process of the engines with exhaust gas recirculation.

Keywords: diesel; CFD; detailed reaction mechanism; multistage self-ignition

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References

1. Reif, K. 2012. Dieselmotor-Managament. Systeme, Komponenten, Steuerung und Regelung. Springer Vieweg. 545 p.
2. Merker, G., C. Schwarz, and R. Teichmann. 2012. *Grundlagen Verbrennungsmotoren. Funktionsweise, Simulation, Messtechnik*. Wiesbaden: Vieweg+Teubner Verlag. 823 p.
3. Diwakar, R., and S. Singh. 2008. NOx and soot reduction in diesel engine premixed charge compression ignition combustion: A computational investigation. *Int. J. Engine Res.* 9. doi: 10.1243/14680874JER00308.
4. Shuai, S., N. Abani, T. Yoshikawa, R. D. Reitz, and S. W. Park. 2009. Simulating low temperature diesel combustion with improved spray models. *Int. J. Therm. Sci.* 48:1786–1799. doi: 10.1016/j.ijthermalsci.2009.01.011.
5. Zehni, A., R. K. Saray, and K. Poorghasemi. 2017. Numerical comparison of PCCI combustion and emission of diesel and biodiesel fuels at low load conditions using 3D-CFD models coupled with chemical kinetics. *Appl. Therm. Eng.* 110:1483–1499. doi: 10.1016/j.applthermaleng.2016.09.056.
6. Sergeev, S. S., S. M. Frolov, and B. Basara. 2017. Chislennoe modelirovanie sgoraniya i obrazovaniya vrednykh veschestv v tsilindre dizelya s primeneniem detal'nogo kineticheskogo mekhanizma okisleniya n-geptana [Numerical modeling of combustion and pollutants formation in cylinder of diesel using a detailed kinetic mechanism of n-heptane oxidation]. *Goren. Vzryv (Mosk.) — Combustion and Explosion* 10(2):26–34.
7. Sergeev, S. S., S. M. Frolov, and B. Basara. 2017. Raschet sgoraniya v dizele s primeneniem detal'nogo kineticheskogo mekhanizma okisleniya topliva [Calculation of

combustion in a diesel engine using a detailed kinetic mechanism of fuel oxidation]. *5th Minsk Colloquium (International) on Physics of Shock Waves, Combustion and Detonation Proceedings*. Minsk: A. V. Luikov Institute of Heat and Mass Transfer of the National Academy of Sciences of Republic of Belarus. 157–158.

8. Hanjalic, K., M. Popovac, and M. Hadziabdic. 2004. A robust near wall elliptic relaxation eddy-viscosity turbulence model for CFD. *Int. J. Heat Fluid Fl.* 25:897–901.
9. Frolov, S. M., F. S. Frolov, and B. Basara. 2006. Simple model of transient drop vaporization. *J. Russ. Laser Res.* 27(6):562–574.
10. Smetanyuk, V. A., and S. M. Frolov. 2004. Isparenie i gorenie kapli uglevodorodnogo topliva. III. Progrev kapli v gazovom potoke s uchetom vnutrennikh dvizheniy zhidkosti [Evaporation and combustion of hydrocarbon fuel droplet. Part III. Droplet heating in gas flow with regard for internal liquid circulation]. *Khim. Fiz.* 23(7):40–48.
11. Avdeev, K. A., F. S. Frolov, and S. M. Frolov. 2006. Nestatsionarnyy teploobmen metallicheskikh chastits s gazom [Nonstationary heat transfer of metal particles with gas]. *Khim. Fiz.* 25(11):17–24.
12. Reitz, R. D. 1987. Mechanism of atomization processes in high pressure vaporizing spray. *Atomisation Spray Technology* 3:309–337.
13. Sergeev, S. S., S. M. Frolov, V. Ya. Basevich, B. Basara, and P. Priesching. 2018. Modelirovanie protsessov smeseobrazovaniya i sgoraniya v dizele s primeneniem detal'nogo kineticheskogo mekhanizma okisleniya goryuchego [Modeling of mixture formation and combustion processes in diesel engine using a detailed kinetic mechanism of fuel oxidation]. *Goren. Vzryv (Mosk.) — Combustion and Explosion* 11(2):88–98. doi: 10.30826/CE18110212.
14. Basevich, V. Ya., A. A. Belyaev, V. S. Posvyanskii, and S. M. Frolov. 2013. Mechanisms of the oxidation and combustion of normal paraffin hydrocarbons: Transition from C_1–C_{10} to C_{11}–C_{16}. *Russ. J. Phys. Chem. B* 7(2):161–169.

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