NUMERICAL MODELING OF COMBUSTION AND POLLUTANTS FORMATION IN CYLINDER OF DIESEL USING A DETAILED KINETIC MECHANISM OF N-HEPTANE OXIDATION

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Abstract: Based on three-dimensional unsteady Reynolds averaged Navier–Stokes equations coupled with different semiempirical turbulence models ($k-\varepsilon$, $k-\xi-f$, and hybrid turbulence model), Lagrangian model of liguid-fuel spray and quasi-laminar combustion model with a detailed kinetic mechanism of fuel vapor oxidation and NOx formation, the calculations of diesel in-cylinder rotating flow with and without liquid fuel injection, with and without fuel combustion, are performed. The results of calculations are compared with the results of large eddy simulation and advantages and disadvantages of different semiempirical turbulence models were highlighted. The best prediction of such an important parameter of flow motion in the combustion showed slightly overestimated values of wall heat flux, which is a reason for some disagreement between calculated and experimental curves for in-cylinder pressure and calculated and measured NOx concentrations.

Keywords: diesel; computational fluid dynamics (CFD); large eddy simulation (LES); detailed kinetic mechanism

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References

- Liu, Y., A. Ali, and R. D. Reitz. 2004. Simulation of effects of valve pockets and internal residual gas distribution on HSDI diesel combustion and emissions. SAE Paper No. 2004-01-0105. 19 p.
- 2. Borisov, A.A., V.A. Smetanyuk, K.Ya. Troshin, and I.O. Shamshin. 2016. Samovosplamenenie v gazovykh vikhryakh [Self-ignition in gas vortices]. *Goren. Vzryv* (*Mosk.*) – *Combustion and Explosion* 9(1):4–13.
- 3. Kavtaradze, R. Z. 2008. *Teoriya porshnevykh dvigateley*. *Spetsial'nye glavy*. Moscow: Izd-vo MGTU im. N. E. Baumana. 720 p.
- 4. Launder, B. E., and D. B. Spalding. 1974. The numerical computation of turbulent flows. *Comput. Method. Appl. Mech. Eng.* 3(2):269–289.
- Hanjalić, K., M. Popovać, and M. Hadziabdić. 2004. A robust near-wall elliptic relaxation eddy-viscosity turbulence model for CFD. *Int. J. Heat Fluid Flow* 25:897–901.
- Basara, B., and S. Jakirlic. 2003. A new turbulence modeling strategy for industrial CFD. *Int. J. Numer. Meth. Fluids* 42:89–116.

- 7. Dukowicz, J. K. 1980. A particle–fluid numerical model for liquid sprays. *J. Comp. Phys.* 35:229–253.
- Basevich, V. Ya., A. A. Belyaev, S. N. Medvedev, V. S. Posvyanskiy, F. S. Frolov, and S. M. Frolov. 2016. A detailed kinetic mechanism of multistage oxidation and combustion of isooctane. *Russ. J. Phys. Chem. B* 10(5):801–809.
- Chemical-kinetic mechanisms for combustion applications. San Diego mechanism web page. Mechanical and Aerospace Engineering (Combustion Research), University of California at San Diego. http:// combustion.ucsd.edu.
- Smagorinsky, J. S. 1963. General circulation experiments with the primitive equations. I: The basic experiment. *Monthly Weather Rev.* 91(3):99–164.
- Medvedev, S. N., V.A. Smetanyuk, S. M. Frolov, and I. O. Shamshin. 2013. Metody uskoreniya mnogomernykh gazodinamicheskikh raschetov s detal'nymi kineticheskimi mekhanizmami okisleniya i goreniya motornykh topliv [Acceleration of multidimensional gasdynamic calculations with detailed reaction mechanisms of oxidation and combustion of motor fuels]. *Goren. Vzryv (Mosk.) – Combustion and Explosion* 6:45–50.

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