

# NUMERICAL SIMULATION OF AUTOIGNITION AND COMBUSTION PROCESSES IN DIESEL ENGINE WITH NITROGEN OXIDE AND SOOT FORMATION USING “LOGOS” SOFTWARE PACKAGE

I. V. Semenov<sup>1</sup>, R. S. Solomatin<sup>1</sup>, V. V. Elesin<sup>1</sup>, M. Y. Nemtsev<sup>1</sup>, S. M. Frolov<sup>1,2</sup>,  
V. A. Smetanyuk<sup>1,2</sup>, V. S. Ivanov<sup>2</sup>, A. S. Kozelkov<sup>3</sup>, and R. N. Zhuchkov<sup>3</sup>

<sup>1</sup>Scientific Research Institute for System Analysis of the National Research Centre “Kurchatov Institute,” 36-1 Nakhimovskii Prosp., Moscow 117218, Russian Federation

<sup>2</sup>N. N. Semenov Federal Research Center for Chemical and Physics Russian Academy of Sciences, 4 Kosygin Str., Moscow 119991, Russian Federation

<sup>3</sup>Russian Federal Nuclear Center All-Russian Scientific Research Institute for Experimental Physics, 37 Mira Prosp., Sarov 607188, Russian Federation

**Abstract:** Elements of the digital twin of a diesel engine were developed on basis of LOGOS software package for numerical simulation of autoignition and combustion of diesel fuel with regard for nitrogen oxide and soot emission. The gas-phase flow is simulated using the RANS (Reynolds-Averaged Navier–Stokes) approach with the SST (Shear Stress Transport) turbulence model. The dispersed liquid-phase flow is simulated using the Lagrange parcel approach with regard for droplet breakup, evaporation, and collision. Chemical reactions are simulated by the newly developed overall kinetic mechanism (OKM). Formation of nitrogen oxide is modeled using the thermal NO mechanism. Soot formation is simulated using the macrokinetic soot model validated against the detailed kinetic mechanism (DKM) of soot formation and oxidation. The developed computational methodology is validated against a series of experimental and computational data on 14 operation modes of a diesel engine including the data on yields of NO and soot.

**Keywords:** diesel engine; numerical simulation; overall kinetics mechanism; autoignition; combustion; nitrogen oxide; soot; digital twin

**DOI:** 10.30826/CE25190105

**EDN:** TJDQNC

## Figure Captions

**Figure 1** Autoignition delays of *n*-hexadecane–air mixtures (1 – DKM [23]), *n*-hexadecane–air mixtures (2 – DKM [34] and 3 – DKM [23]) and surrogate of diesel fuel with air (4 – OKM in “LOGOS”) at  $\phi = 1$  and various initial conditions: (a)  $P = 4$  MPa; (b) 6; and (c) 8 MPa

**Figure 2** Soot yield for isothermal oxidation of *n*-heptane in highly argon-diluted air at  $P = 10$  atm and  $\phi = 2$  (a), 3 (b), and 4 (c): 1 – DKM [35]; and 2 – OKM in “LOGOS”

**Figure 3** Soot yield for isothermal oxidation of *n*-heptane in highly argon-diluted air at  $P = 50$  atm and  $\phi = 2$  (a), 3 (b), and 4 (c): 1 – DKM [35]; and 2 – OKM in “LOGOS”

**Figure 4** Soot yield for isothermal oxidation of *n*-heptane in highly argon-diluted air at  $P = 100$  atm and  $\phi = 2$  (a), 3 (b), and 4 (c): 1 – DKM [35]; and 2 – OKM in “LOGOS”

**Figure 5** The statement of the problem

**Figure 6** Calculated temperature distributions in the engine cylinder for successive values of crankshaft angle: (a) 719°; (b) 723°; (c) 724°; (d) 726°; (e) 728°; (f) 730°; (g) 735°; (h) 750°; and (i) 770°

**Figure 7** Calculated distributions of the fuel vapor mass fraction in the engine cylinder for successive values of crankshaft angle: (a) 719°; (b) 723°; (c) 724°; (d) 726°; (e) 728°; (f) 730°; (g) 735°; (h) 750°; and (i) 770°

**Figure 8** Calculated distributions of the NO mass fraction in the engine cylinder for successive values of crankshaft angle: (a) 726°; (b) 728°; (c) 730°; (d) 735°; (e) 750°; and (f) 770°

**Figure 9** Calculated distributions of the soot mass fraction in the engine cylinder for successive values of crankshaft angle: (a) 719°; (b) 723°; (c) 724°; (d) 726°; (e) 728°; (f) 730°; (g) 735°; (h) 750°; and (i) 770°

**Figure 10** Local temperature and equivalence ratio distribution diagram with soot and NO formation zones: 1 — diesel combustion [40]; 2 and 3 — NO formation and soot formation zone boundaries [40]; and 4 and 5 — NO formation and soot formation, “LOGOS” calculation of 5802 diesel operation mode

**Figure 11** Comparison of experimental [19] (1) and calculated (2 — LOGOS and 3 — AVL FIRE [16]) dependencies of the mean pressure on the crankshaft angle for different operation modes of diesel engine: (a) No. 5794; (b) No. 5796; (c) No. 5798; (d) No. 5802; (e) No. 5804; (f) No. 5806; (g) No. 5808; (h) No. 5810; (i) No. 5812; (j) No. 5814; (k) No. 5816; (l) No. 5818; (m) No. 5820; and (n) No. 5822

**Figure 12** Comparison of experimental [19] (1) and calculated (2 — LOGOS and 3 — AVL FIRE) dependencies of the mean temperature on the crankshaft angle for different operation modes of diesel engine: (a) No. 5794; (b) No. 5796; (c) No. 5798; (d) No. 5802; (e) No. 5804; (f) No. 5806; (g) No. 5808; (h) No. 5810; (i) No. 5812; (j) No. 5814; (k) No. 5816; (l) No. 5818; (m) No. 5820; and (n) No. 5822

**Figure 13** Maximum values of mean temperature obtained for different operation modes of diesel engine: 1 — experiment; 2 — AVL FIRE; and 3 — LOGOS

**Figure 14** Calculated dependences of NO (empty signs) and soot (filled signs) mean mass fractions on the crankshaft angle for 5804 (1), 5814 (2), and 5818 (3) regimes

**Figure 15** Calculated pressure (1) and heat release (2) profiles alongside the assigned diesel fuel mass flow rate (3) vs. crank angle for 5802 regime

**Figure 16** Mean NO yields for different operation modes of diesel engine in experiments (1) and by the end of calculations (850°) with AVL FIRE (2) and LOGOS (3)

**Figure 17** Mean soot yields for different operation modes of diesel engine in experiments (1) and by the end of calculations (850°) with AVL FIRE (2) and LOGOS (3)

## Table Captions

**Table 1** Overall kinetic mechanism for autoignition of diesel fuel surrogate in air

**Table 2** Parameters of reaction No. 1

**Table 3** Macrokinetic model of soot formation for OKM

**Table 4** Values of preexponential factor  $A_{\phi p}$  for different conditions in terms of pressure and mixture equivalence ratio

**Table 5** First reaction of the OKM for autoignition of *n*-heptane–air mixtures

**Table 6** Parameters of diesel engine

**Table 7** Initial conditions for each operation mode of diesel engine

**Table 8** Difference in maximum values of mean temperature between experimental and LOGOS calculation results for different operation modes of diesel engine

## Acknowledgments

The study was conducted within the scientific program of the National Center for Physics and Mathematics, section #2 “Mathematical Modeling on Zetta-scale and Exa-scale Supercomputers. Stage 2023–2025.”

## References

1. Kul'chitskiy, A. R. 2000. *Toksichnost' avtomobil'nykh i traktornykh dvigateley* [Toxicity of automobile and tractor engines]. Vladimir: Vladimir State University Publishing House. 256 p.
2. Yin, Z., S. Liu, D. Tan, and B. Wang. 2023. A review of the development and application of soot modelling for modern diesel engines and the soot modelling for different fuels. *Process Saf. Environ.* 178:836–859.
3. Glarborg, P., M. U. Alzueta, K. Dam-Johansen, and J. A. Miller. 1998. Kinetic modelling of hydrocarbon/nitric oxide interactions in a flow reactor. *Combust. Flame* 115:1–27.
4. Glarborg, P., P. G. Kristensen, K. Dam-Johansen, M. U. Alzueta, A. Millera, and R. Bilbao. 2000. Nitric oxide reduction by non-hydrocarbon fuels implications for reburning with gasification gases. *Energ. Fuel.* 14:828–838.
5. Skreiberg, O., P. Kilpinen, and P. Glarborg. 2004. Ammonia chemistry below 1400 K under fuel-rich conditions in a flow reactor. *Combust. Flame* 136:501–518.
6. Klippenstein, S. J., L. B. Harding, P. Glarborg, and J. A. Miller. 2011. The role of NNH in NO formation and control. *Combust. Flame* 158:774–789.
7. Abian, M., M. U. Alzueta, and P. Glarborg. 2019. Formation of NO from N<sub>2</sub>/O<sub>2</sub> mixtures in a flow reactor: Toward an accurate prediction of thermal NO. *Int. J. Chem. Kinet.* 47(8):518–532.

8. Xi, J., G. Yang, J. Cai, and Z. Gu. 2021. A review of recent research results on soot: The formation of a kind of carbon-based material in flames. *Frontiers Materials* 8:695485. doi: 10.3389/fmats.2021.695485.
9. Glarborg, P., J. A. Miller, B. Ruscic, and S. J. Klippenstein. 2018. Modelling nitrogen chemistry in combustion. *Prog. Energ. Combust.* 67:31–68.
10. Gleason, K., F. Carbone, A. J. Sumner, B. D. Drollette, D. L. Plata, and A. Gomez. 2021. Small aromatic hydrocarbons control the onset of soot nucleation. *Combust. Flame* 223:398–406. doi: 10.1016/j.combustflame.2020.08.029.
11. Martin, J. W., M. Salamanca, and M. Kraft. 2022. Soot inception: Carbonaceous nanoparticle formation in flames. *Prog. Energ. Combust.* 88:100956. doi: 10.1016/j.pecs.2021.100956.
12. Frolov, S. M., V. S. Ivanov, F. S. Frolov, P. A. Vlasov, R. Axelbaum, P. H. Irace, G. Yablonsky, and K. Waddell. 2023. Soot formation in spherical diffusion flames. *Mathematics* 11:261. doi: 10.3390/math11020261.
13. Zhao, F., W. Yang, and W. Yu. 2020. A progress review of practical soot modelling development in diesel engine combustion. *J. Traffic Transportation Engineering – English Edition* 7(3):269–281.
14. Zhao, F., W. Yang, D. Zhou, W. Yu, J. Li, and K. L. Tay. 2017. Numerical modelling of soot formation and oxidation using phenomenological soot modelling approach in a dual-fueled compression ignition engine. *Fuel* 188:382–389.
15. Zhou, H., X. Li, and F. Liu. 2019. Soot formation and oxidation mechanisms in a diesel engine separated swirl combustion system. *Fuel* 257:115955.
16. AVL FIRE: Computational fluid dynamics for conventional and alternative powertrain development. Available at: <https://www.avl.com/> (accessed February 20, 2026).
17. Richards, K. J., P. K. Senecal, and E. Pamraning. 2025. CONVERGE 5\*. Madison, WI: Convergent Science.
18. ANSYS Forte Theory Guide, Release 2024 R1. 2024. Canonsburg, PA: ANSYS, Inc.
19. Basevich, V. Ya., S. N. Medvedev, S. M. Frolov, F. S. Frolov, B. Basara, and P. Priesching. 2016. Makrokineticheskaya model' dlya rascheta emissii sazhi v diezele [Macrokinetic model for calculation of soot emissions in diesel engine]. *Goren. Vzryv (Mosk.) – Combustion and Explosion* 9(3):36–46.
20. 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 the detailed kinetic mechanism of fuel oxidation]. *Goren. Vzryv (Mosk.) – Combustion and Explosion* 11(2):88–98.
21. Basevich, V. Ya., S. M. Frolov, V. S. Ivanov, F. S. Frolov, and I. V. Semenov. 2023. The effects of multistage fuel-oxidation chemistry, soot radiation, and real gas properties on the operation process of compression ignition engines. *Engineering* 4(12):2682–2710.
22. Frolov, S. M., K. A. Avdeev, V. S. Ivanov, P. A. Vlasov, F. S. Frolov, I. V. Semenov, and M. S. Belotserkovskaya. 2023. Evolution of the soot-particle size distribution function in the cylinder and exhaust system of piston engines. Simulation. *Atmosphere – Basel* 14(1):13. 20 p.
23. Basevich, V. Ya., A. A. Belyaev, V. S. Posvyanskii, and S. M. Frolov. 2013. Mechanisms of oxidation and combustion of normal paraffinic hydrocarbons: Transition from C<sub>1</sub>–C<sub>10</sub> to C<sub>11</sub>–C<sub>16</sub>. *Russ. J. Phys. Chem. B* 7(2):177–185.
24. Kozelkov, A., A. Kurkin, A. Puzan, V. Kurulin, N. Tarasova, and N. Gerasimov. 2025. Application features of a VOF method for simulating boiling and condensation processes. *Algorithms* 18:604.
25. Korotkov, A. V., A. S. Kozelkov, V. V. Kurulin, and M. A. Shishlenin. 2025. Applying a synthetic turbulence generator to an unmatched RANS–LES interface. *J. Comput. Appl. Math.* 475:116223.
26. Menter, F. R. 1993. Zonal two-equation  $k$ – $\omega$  turbulence models for aerodynamic flows. AIAA Paper No. 1993-2906.
27. Burcat, A., and B. Ruscic. 2005. Third Millennium Ideal Gas and Condensed Phase Thermochemical Database for Combustion with updates from Active Thermochemical Tables. Argonne, IL, USA: Argonne National Laboratory. Technical Report ANL-05/20. 258 p.
28. Reitz, R. D. 1987. Modelling atomization process in high-pressure vaporizing sprays. *Atomization Spray Technology* 3(4):309–337.
29. Dukowicz, J. K. 1980. A particle–fluid numerical model for liquid sprays. *J. Comput. Phys.* 35:229–253.
30. Basevich, V. Ya., and S. M. Frolov. 2006. Global kinetic mechanisms for modeling multistage autoignition of hydrocarbons in reacting flows. *Russ. J. Phys. Chem. B* 25(6):524–532.
31. Basevich, V. Ya., P. A. Vlasov, A. A. Skripnik, and S. M. Frolov. 2008. Modelirovanie sazheobrazovaniya v dvigatelyakh vnutrennego sgoraniya [Modeling of soot formation in internal combustion engines]. *Goren. Vzryv (Mosk.) – Combustion and Explosion* 1:40–43.
32. Zeldovich, Ya. B. 1946. The oxidation of nitrogen in combustion and explosions. *Acta Physicochim. URS* 21:577–628.
33. Hanson, R. K., and S. Salimian. 1984. Survey of rate constants in H/N/O systems. *Combustion chemistry*. Ed. W. C. Gardiner, Jr. New York, NY: Springer-Verlag. 361–422.
34. Bogin, G. E., Jr., K. C. Dehoff, R. L. McCormick, and M. A. Ratcliff. 2014. Experiments and computational fluid dynamics modelling analysis of large  $n$ -alkane ignition kinetics in the ignition quality tester. *Energ. Fuel* 28(7):4781–4794.
35. Agafonov, G. L., I. Naydenova, P. A. Vlasov, and J. Warnatz. 2007. Detailed kinetic modelling of soot formation in shock tube pyrolysis and oxidation of toluene and  $n$ -heptane. *P. Combust. Inst.* 31:575–583.
36. Agafonov, G. L., A. A. Borisov, N. V. Smirnov, K. Ya. Troshin, P. A. Vlasov, and J. Warnatz. 2008. Soot formation during pyrolysis of methane and reach methane/oxygen mixtures behind reflected shock waves. *Combust. Sci. Technol.* 180(10):1876–1899.

37. Agafonov, G. L., V. N. Smirnov, and P. A. Vlasov. 2011. Shock tube and modelling study of soot formation during the pyrolysis and oxidation of a number of aliphatic and aromatic hydrocarbons. *P. Combust. Inst.* 33:625–632.
38. Agafonov, G. L., I. V. Bilera, P. A. Vlasov, Y. A. Kolbanovskij, V. N. Smirnov, and A. M. Tereza. 2015. Soot formation during the oxidation and pyrolysis of acetylene and ethylene in shock waves. *Kinet. Catal.* 56(1):12–30.
39. NIST Chemistry Webbook. Available at: <https://webbook.nist.gov/chemistry/> (accessed February 20, 2026).
40. Dempsey, A. B., S. J. Curran, and R. M. Wagner. 2016. A perspective on the range of gasoline compression ignition combustion strategies for high engine efficiency and low NO<sub>x</sub> and soot emissions: Effects of in-cylinder fuel stratification. *Int. J. Engine Res.* 17(8):897–917.

*Received June 23, 2025*

*After revision October 3, 2025*

*Accepted October 13, 2025*

## Contributors

**Semenov Ilya V.** (b. 1973) — Candidate of Science in physics and mathematics, head of department, leading research scientist, Scientific Research Institute for System Analysis of the National Research Centre “Kurchatov Institute,” 36-1 Nakhimovskii Prosp., Moscow 117218, Russian Federation; [ivsemenov@niisi.ras.ru](mailto:ivsemenov@niisi.ras.ru)

**Solomatin Roman S.** (b. 1994) — Candidate of Science in physics and mathematics, senior research scientist, Scientific Research Institute for System Analysis of the National Research Centre “Kurchatov Institute,” 36-1 Nakhimovskii Prosp., Moscow 117218, Russian Federation; [solomatin@niisi.ras.ru](mailto:solomatin@niisi.ras.ru)

**Elesin Vladimir V.** (b. 1982) — research scientist, Scientific Research Institute for System Analysis of the National Research Centre “Kurchatov Institute,” 36-1 Nakhimovskii Prosp., Moscow 117218, Russian Federation; [elesin@niisi.ras.ru](mailto:elesin@niisi.ras.ru)

**Nemtsev Maksim Y.** (b. 1991) — Candidate of Science in physics and mathematics, senior research scientist, Scientific Research Institute for System Analysis of the National Research Centre “Kurchatov Institute,” 36-1 Nakhimovskii Prosp., Moscow 117218, Russian Federation; [nemtsev@niisi.ras.ru](mailto:nemtsev@niisi.ras.ru)

**Frolov Sergey M.** (b. 1959) — Doctor of Science in physics and mathematics, head of department, head of laboratory, N. N. Semenov Federal Research Center for Chemical Physics for the Russian Academy of Sciences, 4 Kosygin Str., Moscow 119991, Russian Federation; professor, National Research Nuclear University MEPhI (Moscow Engineering Physics Institute), 31 Kashirskoe Sh., Moscow 115409, Russian Federation; leading research scientist, Scientific Research Institute for System Analysis of the National Research Centre “Kurchatov Institute,” 36-1 Nakhimovskii Prosp., Moscow 117218, Russian Federation; [smfrol@chph.ras.ru](mailto:smfrol@chph.ras.ru)

**Smetanuk Victor A.** (b. 1978) — Candidate of Science in physics and mathematics, leading research scientist, N. N. Semenov Federal Research Center for Chemical Physics for the Russian Academy of Sciences, 4 Kosygin Str., Moscow 119991, Russian Federation; senior research scientist, Scientific Research Institute for System Analysis of the National Research Centre “Kurchatov Institute,” 36-1 Nakhimovskii Prosp., Moscow 117218, Russian Federation; [smetanuk@chph.ras.ru](mailto:smetanuk@chph.ras.ru)

**Ivanov Vladislav S.** (b. 1986) — Doctor of Science in physics and mathematics, deputy director, N. N. Semenov Federal Research Center for Chemical Physics of the Russian Academy of Sciences, 4 Kosygin Str., Moscow 119991, Russian Federation

**Kozelkov Andrey S.** (b. 1980) — Doctor of Science in physics and mathematics, head of department, leading research scientist, Russian Federal Nuclear Center All-Russian Scientific Research Institute for Experimental Physics, 37 Mira Prosp., Sarov, 607188, Russian Federation; [askozelkov@mail.ru](mailto:askozelkov@mail.ru)

**Zhuchkov Roman N.** (b. 1983) — Candidate of Technical Science, leading research scientist, Russian Federal Nuclear Center All-Russian Scientific Research Institute for Experimental Physics, 37 Mira Prosp., Sarov, 607188, Russian Federation; [rnzhuchkov@vniief.ru](mailto:rnzhuchkov@vniief.ru)