THE MODEL OF THE GAS-DIESEL ENGINE OPERATION PROCESS

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Abstract: Based on the detailed reaction mechanism (DRM) of oxidation and combustion of individual hydrocarbons in air, the overall reaction mechanisms (ORMs) of autoignition and combustion of natural gas (NG) and diesel fuel have been developed for the operating conditions of a gas diesel engine. Using a coupled Flame Tracking – Particle method for simulating volumetric autoignition reactions of a diesel-fuel spray and explicit tracking of the turbulent flame front in an NG–air mixture according to these ORMs, three-dimensional calculations have been performed for the engine operation process with the injection of fuel-lean NG–air mixture as a main charge and pilot injection of a diesel fuel spray for igniting the main charge. The feasibility of using the computational model to develop a digital twin of the gas diesel engine is demonstrated.

Keywords: gas diesel engine; operation process; natural gas; diesel fuel; modeling; digital twin

DOI: 10.30826/CE26190106 **EDN:** OAGDKS

Figure Captions

Figure 1 Typical time histories of temperature T (*1*) and species volume fractions during self-ignition of the NG–air mixture at fuel-to-air equivalence ratio $\Phi = 0.75$, $T_0 = 1250$ K, and $P_0 = 50$ bar obtained using the DRM (*a*) and ORM of Table 2 (*b*)

Figure 2 To the definition of the autoignition delay time t_i for the NG–air mixture at $P_0 = 150$ bar, $\Phi = 0.75$, and $T_0 = 714$ (*a*) and 1818 K (*b*) using the ORM of Table 2

Figure 3 Comparison of autoignition delay times calculated using the DRM (*1*) and ORM (*2*) for the NG–air mixture with $\Phi = 0.50$ at different initial values of temperature and pressure: (*a*) $P_0 = 10$ bar; (*b*) 50; (*c*) 100; and (*d*) $P_0 = 150$ bar

Figure 4 Comparison of autoignition delay times calculated using the DRM (*1*) and ORM (*2*) for the NG–air mixture with $\Phi = 0.75$ at different initial values of temperature and pressure: (*a*) $P_0 = 10$ bar; (*b*) 50; (*c*) 100; and (*d*) $P_0 = 150$ bar

Figure 5 Comparison of laminar flame velocities u_n for NG–air mixtures of different composition calculated based on the DRM [12] (*1*) and ORM of Table 4 (*2*) at $T_0 = 714$ K and $P_0 = 10$ (*a*) and 150 bar (*b*)

Figure 6 Comparison of laminar flame velocities u_n for NG–air mixtures with $\Phi = 0.5$ at different initial temperatures calculated based on DRM [12] (*1*) and ORM of Table 4 (*2*) at $P_0 = 10$ (*a*) and 150 bar (*b*)

Figure 7 Comparison of laminar flame velocities u_n for NG–air mixtures with $\Phi = 0.75$ at different initial temperatures calculated based on DRM [12] (*1*) and ORM of Table 4 (*2*) at $P_0 = 10$ (*a*) and 150 bar (*b*)

Figure 8 Comparison of laminar flame velocities u_n for NG–air mixtures with $\Phi = 0.5$ (*a*) and 0.75 (*b*) at $T_0 = 714$ K and different initial pressures calculated based on DRM [12] (*1*) and ORM of Table 4 (*2*)

Figure 9 Calculated spatial temperature distributions in a planar laminar flame in the NG–air mixture at $\Phi = 0.75$, $T_0 = 714$ K, and $P_0 = 50$ bar: (*a*) DRM [12]; and (*b*) ORM of Table 4

Figure 10 Calculated spatial distributions of species volume fractions in a planar laminar flame in the NG–air mixture at $\Phi = 0.75$, $T_0 = 714$ K, and $P_0 = 50$ bar: (*a*) DRM [12]; and (*b*) ORM of Table 4

Figure 11 Calculated dependences of autoignition delay times of homogeneous (*1*) and droplet (*2*–*6*) mixtures of n-decane (initial air temperature $T_0 = 1000$ K) [15] (*a*) and n-tetradecane ($T_0 = 800$ K) [12, 16] (*b*) with air on Φ at $P_0 = 20$ bar and initial droplet temperature $T_{0d} = 293$ K. Initial droplet diameter d_0: *2* — 60 μm; *3* — 40; *4* — 30; *5* — 20; and *6* — 10 μm

Figure 12 Comparison of autoignition delay times for a stoichiometric air mixture of n-tetradecane (a diesel fuel surrogate) calculated based on the DRM [12] (*1*) and ORM (*2*) at different temperatures and pressures: (*a*) 10 bar; (*b*) 50; (*c*) 100; and (*d*) 150 bar

Figure 13 Calculated dependences of pressure (*a*) and maximum temperature (*b*) on the crank angle in the cylinder of a diesel engine with injection of liquid n-tetradecane (diesel fuel surrogate) (*1*, $d_0 = 20$ μm, and $\Phi = 0.2$), in an HCCI engine with the NG–air mixture (*2*, $\Phi = 0.75$), and in a gas diesel engine (*3*); $T_0 = 473$ K; $P_0 = 1$ bar; compression ratio $\varepsilon = 17$; and rotation speed $n = 1800$ rpm

Figure 14 Calculated dependence of the average pressure in the cylinder of a gas diesel engine on the crank angle (CA)

Figure 15 A calculation example illustrating the efficiency of the coupled Flame Tracking – Particle method for simulating injection and autoignition of the diesel fuel spray followed by flame propagation in the NG–air mixture: (*a*) 719° CA; (*b*) 720°; (*c*) 721°; (*d*) 722°; (*e*) 725°; (*f*) 730°; (*g*) 735°; (*h*) 740°; (*i*) 745°; and (*j*) 750° CA

Figure 16 A calculation example illustrating the low sensitivity of temperature distributions in a gas diesel engine to the selected ignition parameters: ignition temperature $T_{\rm ign}$ and ignition source radius $r_{\rm ign} = 730°$ CA: (*a*) $T_{\rm ign} = 2000$ K, $r_{\rm ign} = 3$ mm; (*b*) $T_{\rm ign} = 1800$ K, $r_{\rm ign} = 3$ mm; (*c*) $T_{\rm ign} = 1800$ K, $r_{\rm ign} = 6$ mm; and (*d*) $T_{\rm ign} = 1800$ K, $r_{\rm ign} = 1{,}5$ mm

Figure 17 Calculated dependences of the average pressure in a gas diesel engine for different values of ignition parameters $T_{\rm ign}$ and $r_{\rm ign}$: *1* — $T_{\rm ign} = 2000$ K, $r_{\rm ign} = 3$ mm; *2* — $T_{\rm ign} = 1800$ K, $r_{\rm ign} = 3$ mm; *3* — $T_{\rm ign} = 1800$ K, $r_{\rm ign} = 6$ mm; and *4* — $T_{\rm ign} = 1800$ K, $r_{\rm ign} = 1{,}5$ mm

Table Captions

Table 1 Composition of NG (%(vol.))

Table 2 Overall kinetic mechanism of NG–air mixture autoignition

Table 3 Kinetic parameters of reaction No. 1 at $T_0 = 714$–1818 K, $P_0 = 10$–150 bar, and $\Phi = 0.50$–0.75

Table 4 Overall reaction mechanism of combustion reactions of NG–air mixtures (P_0 in bar)

Table 5 Preexponential factor for reaction No. 1 in Table 4 at $P_0 = 10$ bar

Table 6 Calculated and measured relative autoignition delays $t_i/t_{i,\rm st}$ for homogeneous n-decane–air mixtures of different compositions

Table 7 Rate-limiting reaction in the ORM of autoignition for homogeneous air mixtures of n-tetradecane (a diesel-fuel surrogate)

Table 8 The optimized values of the kinetic parameters of the rate-limiting reaction in the ORM of autoignition for the homogeneous air mixtures of n-tetradecane (a diesel-fuel surrogate) with $\Phi = 1.0$ at $P_0 = 10$–150 bar and $T_0 = 714$–1818 K

Table 9 A fragment of the look-up table for the laminar flame velocity u_n (cm/s) in the NG–air mixture with $\Phi = 0.65$ and $\Omega = 0$ (exhaust gas recirculation) in the temperature and pressure ranges of 450–900 K and 1–100 bar, respectively

Table 10 Parameters and operating conditions of a gas diesel engine (courtesy of AVL LIST GmbH)

Acknowledgments

The work was carried out within the framework of the state task of the NRC "Kurchatov Institute" — SRISA on the topic No. FNEF-2024-0002 "Mathematical modeling of multiscale dynamic processes and virtual environment systems" (1023032900401-5-1.2.1). The authors are grateful to V. Ya. Basevich for assistance in developing overall kinetic mechanisms.

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Received October 30, 2025
After revision January 15, 2026
Accepted January 19, 2026

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