



MODIFYING MATHEMATICAL MODELS FOR CALCULATING OPERATIONAL CHARACTERISTICS OF DIESEL ENGINES BURNING RME BIOFUELS

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Abstract. The article considers and solves the problems of adapting the mathematical models, used in calculating operational characteristics of diesel engines burning mineral diesel oil, to engines converted to RME biofuels. The analysis of mathematical models of calculating the main technical and economic characteristics of diesel engines as well as the parameters of the in-cylinder process and the concentration of toxic substances in the exhaust gases is performed. The need for adjusting the calculation algorithms is also demonstrated. The computer programs based on single-zone thermodynamic models are used in the research. The programs of mathematical modelling are modified, i.e. supplemented with the algorithm for calculating energy characteristics of the combustion products (e.g. specific heat capacity, internal heat, the lower calorific value, etc.). Based on the computer programs, modified for examining diesel engines burning biofuels, the computer-aided mathematical modelling experiment is carried out. The results of modelling are compared with the data obtained in testing the diesel engine 1A41. The mathematical modelling performed demonstrates the accuracy acceptable for solving practical problems: the difference between the obtained calculation results and diesel engine testing data for the load range of $(1.0 \pm 0.5) P_{i\text{nom}}$ does not exceed $\pm 5 \div 7\%$. Higher accuracy of modelling the characteristics of diesel engines, operating in the low- and medium-load modes, may be accounted for by the adjustment of the algorithm for calculating the induction period and the on-set phase of fuel injection.

Keywords: operational characteristics of diesel engines, biofuels, mathematical modelling, in-cylinder process, emission of toxic substances.

1. Introduction

The paper aims to analyse mathematical modelling programs and to modify them. The environmental effects and the in-cylinder process parameters of diesel engines, converted from fossil petroleum-derived diesel fuel to biofuels. To achieve this aim, the following tasks were formulated and performed:

- the analysis of the models of mathematical modelling and their modification for calculating and investigating energy characteristics and environmental effects of diesel engines, burning biofuels;
- structural analysis of the models, aimed at determining the adjustments to be made to the algorithms, used in the investigation of diesel engines burning biofuels;
- modification and validation of mathematical models used in calculations, based on the results obtained in testing diesel engines.

It is well known that mathematical modelling of operational diesel engine characteristics is based on mathematical modelling of the in-cylinder process parameters (e.g. oil supply, the formation and combustion of the fuel-air mixture in the cylinder and the formation of toxic substances).

Depending on the research aims, the analysis and synthesis of diesel engine in-cylinder process are made. In the first case, the characteristics of the processes taking place in the cylinder are calculated using in-cylinder process diagrams obtained in testing. These are heat release characteristics $\frac{dx}{d\varphi} = f(\varphi)$, expressed by differential and integral equations, and the parameters of the in-cylinder process, such as induction phases, a factor of cycle dynamics $(\sigma, \lambda, \frac{dp}{d\varphi_{\text{max}}}; \frac{dp}{d\varphi_{\text{mid}}})$, the characteristic temperature and pressure $(T_{\text{max}}, P_{\text{max}})$, etc.

The results obtained are analysed alongside the parameters of the in-cylinder process, including the excess air coefficient, compression ratio, characteristic injection phases, physical and chemical fuel characteristics, etc.

In considering the in-cylinder process of a diesel engine, the processes, proceeding in the cylinder and operational diesel engine characteristics (e.g. its power, fuel consumption rate, temperature of the exhaust gases, environmental effects, etc.) are modelled.

The mathematical modelling of the in-cylinder process parameters allows us to considerably decrease the material, financial and time expenses because the actual testing of diesel engines is replaced by virtual computer-aided calculations.

The research performed at the Maritime Institute of Klaipėda University (Lebedevas *et al.* 2006, 2007, 2010a, 2010b) helped to obtain a consistent and generalized description of technical, economic and environmental characteristics as well as air pollution, fuel injection and in-cylinder process parameters of diesel locomotives converted to biofuels. The fuels, including certified methyl esters of fatty acids and other biofuels produced in Lithuania, are used.

These investigations are aimed at determining energy characteristics and harmful environmental effects (air pollution) of Lithuanian locomotives converted to biofuels. It is clear that computer-aided modelling based on mathematical models adapted to diesel engines, burning biofuels, should be used in such tests.

2. The Selection and Modification of Models to be Used in Computer-Aided Mathematical Modelling

The stages of analysis and synthesis, supplementing each other, make the inherent parts of investigation. Currently used mathematical modelling of physical processes taking place in the diesel engine cylinder is not formalized. This means that the empirical coefficients are used in calculation methods, irrespective of their complexity level and detailed elaboration. These coefficients should ensure the agreement between the mathematical modelling and engine testing data. In its turn, the validity of synthesis results may be ensured by the experiment, when the empirical coefficients of the mathematical models used are determined and substantiated.

To solve these problems independently, laborious research based on statistical data should be performed. Therefore, most of researchers prefer an experimental study (Schmidt, Van Gerpen 1996; A Comprehensive Analysis of... 2002; Lü *et al.* 2004; Kumar *et al.* 2006; Theobald, Alkidas 1987).

There is a limited number of studies of the particular parameters of engines burning biofuels (Rakopoulos *et al.* 2006, 2007; Rakopoulos, Hountalas 1998; Theobald, Alkidas 1987; Choi *et al.* 1997), based on mathematical modelling. For example, the temperature field of the combustion products in the diesel engine cylinder was investigated at University of Wisconsin, using K1-VA-II, a modern program of modelling the in-cylinder process of a diesel engine burning biofuels (Choi *et al.*

1997). However, the more complicated the mathematical model used, the more difficult the preparation of the initial data for calculation (Иващенко, Горбунова 1989; Кавтарадзе, 2001).

The choice of mathematical models is based on the following principles:

- internal combustion engines, including diesel engines, are considered to be complex technical systems because they consist of many components, involved in the interrelated mechanical, thermodynamic and chemical processes;
- mathematical description of the processes, taking place in the cylinder, relies on the conceptual models of real physical processes (researchers offered and described a large number of such models, differing in the assumptions made and the considered details);
- there are various approaches to developing mathematical models of the heterogeneous fuel combustion process characteristic of a diesel engine. According to them, there may be zero-dimensional, quasi-dimensional, one-dimensional, two-dimensional and other multidimensional models. In other terms, there are phenomenological, thermodynamic and detailed models;
- the detailed or multidimensional models are based on the numerical calculation of the systems of differential equations, performed at the nodes of the geometrical net of the combustion chamber space. These models provide a spatial or temporal solution to the considered problems;
- phenomenological models are based on the conceptualization of particular processes taking place during the engine's cycle (such as gas exchange, fuel injection, fuel mixing with air, combustion, heat exchange and the formation of toxic substances).

A description of the considered processes, based on phenomenological models, involves both simplified empirical equations and more complicated functional dependences, reflecting actual physical processes. Though the cylinder space may be divided into several zones in a phenomenological model, it cannot provide the detailed spatial description achieved by using multidimensional models.

Phenomenological models may be applied only to the already tested types of diesel engines, otherwise, the testing of the diesel engines used, followed by generalisation of testing results, should be performed, e.g. similar to the testing of high-speed augmented diesel engines made by A. Portnov (Портнов 1963) and S. Pogodin (Погодин 1978).

According to the creators of multizone models (Кавтарадзе, 2001), their practical use would require the solution of the problem of the initial data preparation, which would be actually as difficult as mathematical modelling itself. This particularly applies to the investigation of the currently used diesel engines because many of them either operate in the post-warranty period or are no longer manufactured. The use of multizone

models poses particularly many problems to the investigation of various types of diesel engines.

In the experiments carried out at the Maritime Institute of Klaipėda University, which are based on practical experience (Лебедев, Нечаев 1999; Лебедев и др. 2003), the priority is given to the investigation of physical processes, taking place in the engine's cylinder. The algorithms of these models allow for calculating the operational characteristics of a wide range of diesel engines with practically acceptable accuracy. At the same time, they may be easily adapted to the investigation of the considered diesel engines because the structure of the model allows it.

2.1. The Analysis of Mathematical Models and their Accuracy

Thermodynamics models involve the solution of the systems of differential equations (Иванченко, Балакин 1979).

A mathematical model is based on the system of differential equations, including the equations describing the law of energy conservation and the mass and thermodynamic characteristics of gases in the cylinder of the diesel engine:

$$\left\{ \begin{array}{l} \frac{dT}{d\varphi} = \frac{1}{c_v M} \left(H_u \frac{dg_x}{d\varphi} + \frac{dQ_w}{d\varphi} - c_v T \frac{dM}{d\varphi} - \right. \\ \left. \frac{\pi V_h}{360} pb + i_n \frac{dM_n}{d\varphi} - i_m \frac{dM_m}{d\varphi} \right); \\ \frac{dM}{d\varphi} = g_c \frac{dx}{d\varphi} + \frac{dM_n}{d\varphi} - \frac{dM_m}{d\varphi}; \\ pV = MRT, \end{array} \right. \quad (1)$$

where: $H_u (dg_x / d\varphi)$ is the absolute heat release rate; $dQ_w / d\varphi$ is the heat transferred to the walls of the cylinder of the diesel engine; $i_n (dM_n / d\varphi)$, $i_m (dM_m / d\varphi)$ denote the amount of heat entered and released during the process of the exchange of gases in the cylinder; dM_n , dM_m denote the changes in the elementary mass of fresh air and exhaust gases in the cylinder; M is the mass of the gases in the cylinder of the diesel engine.

The linear differential equations are solved by using the numerical methods.

The 1st and 2nd equations of the systems (1) are 1st order differential equations under the given boundary conditions. These equations are solved by using the numerical mathematical methods of finite differences (Euler, Runge–Kutta, etc.).

The solution of the 1st equation of the system (1) allows us to obtain the values of the temperature (T) of the gases for various values of the crankshaft rotation angle. The values of gas pressure (P) are calculated by using the 3rd equation of the system (1). Based on the results obtained and using the 2nd equation of the system (1), the energy characteristics of an engine are calculated, including the mean indicated pressure and specific indicated fuel consumption.

The components of the equations ($dg_x/d\varphi$, $dx/d\varphi$, $dQ_w/d\varphi$, etc.) are determined by solving the systems of

equations, while $dx/d\varphi$ is the basic parameter describing heat release during the process of fuel combustion in the engine's cylinder. The reliability of the results of mathematical modelling of diesel engine parameters depends on the appropriate setting of $dx/d\varphi$.

The considered solution of a system of differential equations, supplemented with classical relationships describing the internal combustion engine, is aimed at calculating the essential technical and economic indicators of diesel engines (p_{mi} , M_p , p_{me} , b_p , b_e , t_T , P_{max} , etc.).

Depending on the particular tasks of the numerical experiment, the calculation model is supplemented with program modules for calculating fuel injection parameters, the stresses of the parts of the cylinder-piston group and a physical process of the formation of the toxic substances (CO, HC, PM, NO_x) (Theobald, Alkidas 1987; Пусаков 1998).

The following approaches to a more exact definition of the system of differential equations were suggested, based on its analysis:

- using the developed algorithm, to develop a subprogram for calculating energy characteristics of the combustion products in the cylinder, such as specific thermal capacity C_V of the mixture of air and combustion products and their internal energy U . In the original model, the empirical dependences of these parameters on the temperature are only used for calculating the consumption of the conventional fuel (actually, of the constant chemical composition (C, H, O));
- to develop a subprogram for calculating stoichiometric fuel-air ratio L_0 and the lower calorific value H_u (Q_z) of the biofuels used;
- to analyse the algorithms developed for calculating heat release characteristics and the period of combustion induction (modifying them if required).

The following computer programs, using single-zone mathematical models are modified:

- a mathematical modelling program TEPL, aimed at analysing the indicator diagrams obtained in the testing of an actual diesel engine;
- mathematical modelling programs DIAGR and the program IMPULS (Красовский 1983), aimed at creating the indicator diagrams, i.e. calculating energy characteristics, such as diesel engine performance in terms of power and fuel consumption;
- a mathematical modelling program TOXIC, aimed at calculating the concentration of toxic substances in diesel engine exhaust gases (Пусаков 1998).
- The implementation of the program TOXIC involves the following operations:
- mathematical modelling of physical and chemical processes, causing carbon black formation and the release of toxic substances;
- modelling of the impact of operational and fuel injection characteristics of diesel engine on its ecological characteristics.

The above model is like a ‘grey box’ because some of subsystems are described by mathematical expressions, while others – by semi-empirical equations and regression dependences.

The modelling of the formation of toxic substances in diesel engine cylinder embraces the following processes: the injection of liquid fuel and air charging in the cylinder; fuel injection and evaporation; gaseous fuel content in the combustion products; fuel combustion and the formation of toxic substances.

The program’s algorithm is a mathematical model of the fuel-air mixture formation and combustion suggested by N. Razleicev (Разлейцев 1980; Разлейцев, Филипповский 1990) supplemented with subprograms for calculating the parameters of gases in the engine’s cylinder, the temperature of the flame, nitric oxides’ formation and the amounts of the emitted hydrocarbons and carbon monoxides.

The model TOXIC allows us to predict carbon black concentration in the exhaust gases and to model hydrocarbon (HC) formation and oxidation of carbon monoxide. The modelling of nitric oxides in diesel engine cylinder is performed using the expressions and equations suggested by academician Y. Zeldovich (1946).

Mathematical programs IMPULS, DIAGR and TEPL, as well as TOXIC, are based on the solution of a system of differential equations (1). The algorithm of the programs analysed was extended by the mathematical model UNIT2. The latter was aimed at calculating energy characteristics of combustion products (e.g. the specific thermal capacity of the mixture of air and combustion products C_V , their internal energy U , stoichiometric air-fuel ratio L_0 and the lower fuel calorific value H_u (Q_w), when the fuel of different chemical compositions is used.

2.2. Developing an Algorithm for Calculating Energy Characteristics of Combustion Products

The original versions of the modified programs are used for investigating the parameters of diesel engines burning conventional fossil fuel:

- 1) The program’s algorithm is based on indices and coefficients, describing mass fraction of elements in the conventional fossil fuel (carbon C = 0.87 kg per one kg of fuel; hydrogen H = 0.126 kg per one kg of fuel; oxygen O = 0.004 kg per one kg of fuel). The calculations involve stoichiometric air-fuel ratio $l_0 = 0.499$ kmol/kg; $L_0 = 14.45$ kg of air per one kg of fuel and the lower fuel calorific value $H_u = 42500$ kJ/kg.

In the modified programs of mathematical calculation (supplemented with UNIT2 subprogram), the following air components are expressed in parts by volume: O_2^v , N_2^v , CO_2^v , H_2O^v and Ar^v .

In this case, taking into account the specified air humidity, the mass fraction of water vapours H_2O^M in the air is calculated, and, then, the values of O_2^M and N_2^M are corrected.

In the initial data set, the chemical composition of the fuel is specified in parts by mass of the

elements as follows: C^M , H_2^M , O_2^M , S^M , H_2O^M , and N_2^M . Otherwise, the standard diesel oil composition $C^M = 0.86$; $H_2^M = 0.13$; $O_2^M = 0.01$ kg per one kg of fuel is considered by default.

Based on the data obtained, the calculation of the stoichiometric constant is performed:

$$l_0 = \frac{8}{3} \cdot C^M + 8 \cdot H_2^M + S^M - O_2^M / O_2^M, \text{ kg air/kg fuel} \quad (2)$$

and the complete combustion fuel mass fractions are determined:

$$CO_2^M = \frac{11}{3} \cdot C + l_0 \cdot r_{CO_2} \cdot \frac{\mu_{CO_2}}{\sum r_i \cdot \mu_i}, \text{ kg/kg fuel}, \quad (3)$$

where: r_{CO_2} and r_i are the mass fractions of CO_2 and the i -th component while μ_{CO_2} and μ_i are molecule mass fractions of CO_2 and the i -th component in the air.

Similarly, the mass fractions of other complete combustion products in the exhaust gases are determined as follows:

$$H_2O^M = 9 \cdot H_2^M + H_2O^M + l_0 \cdot \frac{r_{H_2O} \cdot \mu_{H_2O}}{\sum r_i \cdot \mu_i}, \text{ kg } H_2O/\text{kg fuel}; \quad (4)$$

$$SO_2^M = 2 \cdot S_2^M, \text{ kg } SO_2 / \text{kg fuel}; \quad (5)$$

$$N_2^M = N_2^M + l_0 \cdot \frac{r_{N_2} \cdot \mu_{N_2}}{\sum r_i \cdot \mu_i}, \text{ kg } N_2/\text{kg fuel}. \quad (6)$$

The specific heat and the internal energy of the air, as well as complete combustion products are calculated, using the approximate 3rd degree polynomials:

$$C_V = a_0 + a_1 \cdot T + a_2 \cdot T^2 + a_3 \cdot T^3; \quad (7)$$

$$U = b_0 + b_1 \cdot T + b_2 \cdot T^2 + b_3 \cdot T^3, \quad (8)$$

where: the values of the coefficients $a_0 \div a_3$ and $b_0 \div b_3$ for each component of the air and the combustion products are predetermined by the subprogram UNIT2.

The specific heat C_V and the internal energy U of the air mixture and the combustion products are calculated, taking into account the respective mass fractions of the air and combustion products:

$$C_V = C_V' \cdot \gamma' + C_V'' \cdot \gamma''; \quad (9)$$

$$U_V = U_V' \cdot \gamma' + U_V'' \cdot \gamma'', \quad (10)$$

where: γ' and γ'' are mass fractions of the air and combustion products.

The values of γ' and γ'' are determined by the modelling programs at all stages of the in-cylinder process calculation and transferred to

the UNIT2 subprogram through a common domain.

To find the enthalpy value, the formula $R = \sum R_i \gamma_i$ is used, where R is gas constant of the i -th component of the air and combustion products.

The lower fuel calorific value is specified in the set of the initial data, otherwise, the calculation is performed by applying the well-known Mendeleev dependence:

$$H_u = \left[81 \cdot C^M + 246 \cdot H^M - 30 \cdot (O^M - S^M) - 6 \cdot (W^M + 9 \cdot H^M) \right] / 4.19, \text{kJ/kg}; \quad (11)$$

- 2) In the program TOXIC, a subprogram is used, where gas temperature in the cylinder is determined by the equation (12), rather than by using a subprogram, calculating the pressure P and the temperature T of the combustion products of diesel oil of standard composition ($C^M = 0.86$ kg/kg; $H_2^M = 0.13$ kg/kg; $O_2^M = 0.01$ kg/kg fuel):

$$dT = \left\{ \left[Q_z - (C_V'' - (C_V' - C_V'') \cdot l_0) \cdot T_i \right] \times \frac{dx}{d\varphi} - \frac{dQ_n}{d\varphi} - \frac{pdV}{d\varphi} \right\} / (C_V' \cdot G' + C_V'' \cdot G''), \quad (12)$$

where: $dQ_w/d\varphi$ is the rate of heat transfer to the walls of the diesel engine cylinder, defined using Eichelberg or Woschni equation (Woschni, Flegler 1979; Woschni et al. 1986); $dx/d\varphi$ is the heat release rate in the engine cylinder according to Vibe equation; the pressure p of the combustion products is calculated by Klapeiron-Mendeleev equations.

- 3) The calculation of the concentration of toxic substances in the exhaust gases of diesel engines, burning biofuel, is performed by adjusting semi-empirical dependence constants, which are adapted to the engines burning conventional diesel oil.

For this purpose, the program is provided with visualization and constant value correction facilities, enabling the adjustment of the coefficients' values and ensuring the adequacy of the calculation data and testing results.

2.3. The Analysis of Heat Release Rate in the Engine's Cylinder

Based on the results of the tests, it was determined that the changes in the main heat release rate characteristics of a diesel engine converted to biofuel are mainly related to the following factors:

- a decrease of heat release rate $dx/d\varphi_{I_{max}}$ at the kinetic stage of combustion;
- an increase of heat release rate at the diffusion combustion stage $dx/d\varphi_{II_{max}}$ (Lebedevas et al. 2007).

In all mathematical modelling programs analysed (with some exceptions found in the IMPULS program),

the heat release rate is calculated by using Vibe dependence (Вибге 1962):

$$x = 1 - e^{-c \cdot \left(\frac{\varphi}{\varphi_z} \right)^{m+1}}, \quad (13)$$

where: φ is the crankshaft rotation angle, calculated with respect to the on-set phase of fuel combustion; φ_z is the relative fuel combustion timing; x is the part of the burnt fuel or the respective amount of the heat released; m is the so-called form factor, a characteristic indicator of the fuel combustion process; c is a constant.

The parameters m and φ_z are recalculated for partial loading modes of diesel engines by applying Woschni equations (Woschni, Flegler 1979; Woschni et al. 1986):

$$\frac{m}{m_0} = \left(\frac{\varphi_{i0}}{\varphi_i} \right)^{a_2} \cdot \frac{P_a \cdot T_{a0}}{P_{a0} \cdot T_a} \cdot \left(\frac{n_0}{n} \right)^{a_1}; \quad (14)$$

$$\frac{\varphi_z}{\varphi_{z0}} = \left(\frac{\alpha_0}{\alpha} \right)^{a_3} \cdot \left(\frac{n}{n_0} \right)^{a_4}, \quad (15)$$

where: the index '0' indicates the parameters for the design condition of diesel engine operation; P_a and T_a are the pressure and the temperature of the air in the cylinder.

The equations (12)–(15) are widely used for calculating the operation of diesel engines, burning conventional diesel oil. Their use in calculating $dx/d\varphi$ for a diesel engine burning some kind of biofuel is based on the experimental results obtained by the authors of the paper (Lebedevas et al. 2007):

- the amount of heat $Q_{P_{max}}$, released by the engine burning conventional diesel oil or biofuel before the maximum cycle pressure P_{max} was reached, does not differ considerably when the load of the engine is the same in both cases.
- for different kinds of fuel, similar values of the indicated coefficient of efficiency η_i dependence on the air excess coefficient α were obtained: in the equation $\eta_i = a + b \cdot \alpha$ the values of the coefficient b are similar for different biofuels (see Fig. 1), implying that the values of m and φ_z will also be

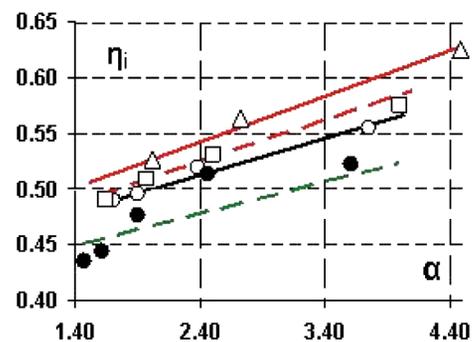


Fig. 1. The dependence of the efficiency factor η_i on the excess air coefficient α of diesel engine A41: \circ is conventional diesel fuel; \square denotes RME biodiesel B30, \triangle denotes RME biodiesel B100

similar. The result obtained shows that Woschni equations (14) and (15) may be also applied to the analysis of the engines burning biofuels.

When the adjustment of the fuel supply phase (angle) is the same, the fuel combustion timing is determined by two factors: the real fuel injection lead angle Φ_{fi} and the induction time φ_i .

The results of testing a diesel engine burning pure biofuel show that the value of Φ_{fi} should be corrected by decreasing it by 2°CA, while the induction period φ_i should be decreased by 1° CA.

2.4. Adjusting the Mathematical Model Used in the Analysis of Indicator Diagrams

The calculation program TEPL is intended for the experimental analysis of the indicator diagrams. In this program, $T = f(\varphi)$, $x = f(\varphi)$, and $dx/d\varphi = f(\varphi)$ are calculated, based on the experimental $p = f(\varphi)$ values.

The modification of this mathematical model is similar to that used in the synthesis-based programs DI-AGR and IMPULS. To calculate α , L_{φ} , H_{φ} , C_V' , C_V'' and R , the algorithm similar to that used in the subprogram UNIT2 was applied.

The main target function, the heat release rate $dx/d\varphi$, is calculated by the following equation:

$$\frac{dx}{d\varphi} = \left[(C_V' \cdot G' + C_V'' \cdot G'') \cdot \frac{dT}{d\varphi} + \frac{dQ_w}{d\varphi} + \frac{pdV}{d\varphi} \right] / \left[Q_z - (C_V'' - (C_V' - C_V'') \cdot l_0) \cdot T \right] \quad (16)$$

where the terms used in the formula (16) are defined above.

In addition to heat release rate characteristics ($x=f(\varphi)$, $dx/d\varphi=f(\varphi)$), the calculation algorithm models the parameters of heat exchange in the diesel engine cylinder. The mathematical model is based on the works of G. Woschni (Woschni, Fleger 1979; Woschni *et al.* 1986) and the investigation performed in CNIDI (ЦНИДИ – Центральный научно-исследовательский дизельный институт – Central Scientific Research Diesel Institute, Sankt-Petersburg) (Lebedevas, Lebedeva 2004). The heat load of the diesel engine cylinder-piston group is one of the major parameters, determining the reliability of diesel engine operation.

3. Validating the Models Used in Mathematical Modelling Based on the Data of Engine Testing

In testing the programs, the adequacy of their algorithm modification for modelling the major parameters and characteristics of diesel engines burning biofuel was assessed by calculating and evaluating the following items:

- the main energy characteristics of diesel engines (i.e. power and fuel consumption);
- operational characteristics of the diesel engine (the excess air coefficient α , the maximal cycle pressure P_{max} , etc.);
- the concentration of toxic substances (NO_x, CO, HC, carbon black) in the exhaust gases.

The results of computer-based mathematical modelling were compared with the data obtained in stand tests of one-cylinder engine 1A41.

The main parameters of the tested diesel engine are presented in Table 1.

The engine 1A41 was tested when the diesel engine was running at the rated speed of 1750 rpm within the load range P_{mi} (the mean indicated pressure) from 0.25 MPa to 0.85 MPa. The tested fuels are as follows: the fossil diesel fuel (D) and D with rape methyl ester (RME) mixture in the volume proportions from 90% to 10% (B10), 70% to 30% (B30), and pure RME – B100.

Table 1. The main parameters of the diesel engine 1A41

Parameter	1A41
Cylinder diameter, m	0.13
Piston stroke length S, m	0.14
Engine displacement V_h , dm ³	1.115
Compression ratio ϵ	16
Rated power $P_{e\ nom}$, kW	14
Mean indicated pressure p_{mi} , MPa	0.85
Rated speed, rpm	1750
Fuel injection	Direct
Type of combustion chamber	Open

The tests of the engine 1A41 were performed on a certified engine stand which was provided with an electric brake, an automatic fuel consumption gauge, pressure and temperature sensors in the cooling and lubricating systems. The emission of the exhaust gases with harmful components was measured with the ‘Quintox 9106’ automatic gas analyser. In all tested operational modes of the diesel engine, fuel pressure in a high-pressure fuel supply line, gases in the diesel engine cylinder, actual angles at the start and end of fuel injection, averaged with the obtained data within the period of 30÷100 subsequent diesel engine running cycles, were measured by means of the digital station H-2000 and a sensor set of pressure and needle raise of the fuel injector nozzle. The data were averaged over 30÷100 Diesel engine tests.

The analysis of the engine characteristics was made on a certified stand, equipped by modern devices for automated measuring and recording of the main technical-economic parameters (fuel consumption, temperature of exhaust gases, etc.) and the concentration of toxic substances in the exhaust gases.

At the same time, the task of applying the mathematical model to a wide range of operating auto-tractor type diesels was set and performed.

In this paper, the results of computer-aided validation of two out of four modified modelling programs DIAGR and TOXIC are presented.

In the DIAGR program, the validity of modelling results is determined by the heat release rate values which are set by the parameters m and φ_z of Vibe model

(Вибе 1962). This allows for the application of the mathematical model DIAGR to various diesel engine types by setting various combinations of m and φ_z values.

In the TOXIC program, the characteristic dx/dj is not specified directly. It is modelled according to N. Razleicev model (Разлейцев 1980; Разлейцев, Филипковский 1990), depending on the following factors:

- construction and regulation parameters and characteristics of the fuel injection equipment;
- physical and chemical fuel characteristics;
- the statistical parameters of the fuel-air mixture formation in the cylinder.

Therefore, the validation of the TOXIC program is based on the data obtained in testing the diesel engine 1A41.

3.1. Modelling Technical-Economic and In-Cylinder Process Parameters of Diesel Engine

In validating the DIAGR program, the values of the parameters m and φ_z (Вибе 1962; Лебедев, Матиевский 2000) were set in the ranges: $m = 0.5 \div 1.5$; $\varphi_z = 70 \div 100^\circ$ CA, when $V_{cikl} = idem$ (the portion of the fuel injected during the cycle) or $Q_{Pmax} = idem$ are the same.

The German MTU (Motoren Und Turbinen Unijon) 396 series diesel engine was used as a prototype for mathematical modelling.

In the first case, the modelling of diesel engine conversion from fossil diesel fuel D to biofuel was carried out without adjusting its injection system, while in the second case, the modelling was performed, assuring the same operating power of a diesel engine burning various fuels.

In the investigated parameter range of m and φ_z , the changes in diesel engine parameters were practically the same for $V_{cikl} = idem$:

- the conversion from mineral diesel fuel D to RME (B100) resulted in P_{max} decrease by 6÷7 %, while in the case of burning B30 and B10 biofuel, the decrease of P_{max} by 3÷2 % was obtained;
- the excess air coefficient α increased accordingly by 6÷8 % and 4÷3 %;
- the mean indicated pressure P_{mi} decreased by 6÷7 %, when B100 biofuel was used and by 3÷2% when B30 and B10 fuels were burnt;
- the indicated specific fuel consumption b_i increased by 10÷12 % and 3÷2 %, respectively.

Some of the modelling results is presented in Table 2.

In mathematical modelling experiment, a slight effect of peculiarities of engine's operation (the variation of m and φ_z combinations) on the technical-economic diesel engine indicators could be observed, when $Q_{Pmax} = idem$.

In the analysed variation range of m and φ_z , the following changes in the parameters of a diesel engine converted to biofuel were observed:

- the variation of the maximal pressure P_{max} and the mean indicated pressure P_{mi} does not exceed $\pm 1\%$;
- the increase of the specific indicated fuel consumption b_i , including the higher RME biofuel density compared to D, makes 11÷13%.

Table 2. Modelling results obtained by using the DIAGR program

Changed values				
Comparison condition $V_{cikl} = idem$	B100	B30	B10	Diesel fuel
Combustion factor m	0.5	0.5	0.5	0.5
Relative fuel combustion timing $\varphi_z, ^\circ CA$	70	70	70	70
Modelling results				
Maximal cycle pressure P_{max} MPa	11.7	11.9	11.9	12
Indicated pressure P_{mi} , MPa	0.94	0.99	1.00	1.01
Maximal cycle temperature T_{max} K	1655	1700	1710	1715
Excess air coefficient α	2.93	2.76	2.72	2.71
Specific indicated fuel consumption b_i , g/kWh	185	169	165.2	162.5

Table 3. Modelling results obtained by using the DIAGR program

Comparison condition $Q_{Pmax} = idem$	B100	B30	B10	Diesel fuel
Combustion factor m	1.5	1.5	1.5	1.5
Relative fuel combustion timing $\varphi_z, ^\circ CA$	100	100	100	100
Modelling results				
Maximal cycle pressure P_{max} MPa	8.00	7.93	7.93	7.90
Indicated pressure P_{mi} , MPa	0.832	0.834	0.833	0.835
Maximal cycle temperature T_{max} K	1390	1395	1395	1395
Excess air coefficient α	2.72	2.71	2.71	2.71
Specific indicated fuel consumption b_i , g/kWh	225	205	200	198

Some of the modelling results are presented in Table 3.

The obtained calculation data (when $Q_{Pmax} = idem$ and $V_{cikl} = idem$) well agree with the real diesel engine power and fuel consumption parameters, when diesel engines are converted to biofuel (Schmidt, Van Gerpen 1996; Lebedevas et al. 2006). For example, when $Q_{Pmax} = idem$, ensuring the same diesel engine power, the specific fuel consumption in the experiment with B100 and B30 increases by 10÷12% and 1÷2 %, respectively, while the variation of the excess air coefficient α reaches 10%.

Therefore, the application of single-zone thermodynamic models ensures the acceptable precision of modelling the parameters (efficiency, fuel consumption and operational characteristics) of a diesel engine burning biofuel.

The obtained data are both of practical and theoretical value because they well agree with the empirically observed results, supporting them when the changes in the parameters of various types of diesel engines converted from D to biofuel (Lebedevas et al. 2006; A Comprehensive Analysis of... 2002; Lü et al. 2004) do not differ considerably.

The comparison of the mathematical modelling results obtained by using the DIAGR program, with the data of testing the diesel engine 1A41, burning the biofuels D, B30 and B100 is presented in Table 4.

Fig. 2 presents the comparison of the mathematically obtained indicator diagrams and those obtained in testing diesel engine 1A41, operating in the high-load mode.

The results obtained indicate that the mathematical model adjusted to the experimental data of the low-load nominal mode ensures the modelling of technical-economic parameters of diesel engine, operating in the low-load mode, with the error not exceeding $\pm 5\%$ for diesel engines burning D. For diesel engines converted to B30 biofuel, the error, except for η_i and α , does not exceed 5% either. In the modes of average loads η_i and α , the modelling error was 6÷8%, while for diesel engines using RME the modelling error in-

creased to 12÷20%. This can hardly be considered acceptable for the solution of practical tasks.

The modelled heat release rate values in the nominal modes are also close to those obtained in testing the engine, though the delay is about 2÷4 °CA. To avoid bigger errors and to use the considered mathematical model for diesel engine's partial load mode modelling, it is recommended:

- to set the real fuel injection phase with great precision as it is relevant for calculating P_{mi} and η_i ;
- to decrease the fuel combustion timing φ_z (calculated for D fuel);
- the value of the combustion factor m can be the same as that used for conventional diesel engine fuel.

The testing results of the TOXIC program are presented in Table 5 and Fig. 3.

Table 4. The comparison of the calculation data obtained by using TEPL program and the results of testing diesel engine 1A41

Fuel	D				B30				RME			
	$P_{mi\ nom}$	0.85 $P_{mi\ nom}$	0.5 $P_{mi\ nom}$	0.25 $P_{mi\ nom}$	$P_{mi\ nom}$	0.85 $P_{mi\ nom}$	0.5 $P_{mi\ nom}$	0.25 $P_{mi\ nom}$	$P_{mi\ nom}$	0.85 $P_{mi\ nom}$	0.5 $P_{mi\ nom}$	0.25 $P_{mi\ nom}$
$P_{max\ exp}$, MPa	7.2	6.7	6.0	5.3	7.3	6.7	6.0	5.5	7.5	6.9	6.2	5.4
$P_{max\ calc}$, MPa	7.1	6.6	6.0	5.4	-	6.7	5.9	5.3	7.2	6.9	-	5.2
δP_{max}	1.4%	1.5%	0%	1.8%	-	0%	1.7%	3.7%	4.1%	0%	-	3.8%
$P_{mi\ calc}$, MPa	0.80	0.73	0.60	0.39	0.83	0.72	0.58	0.38	0.82	0.70	0.54	0.34
$P_{mi\ exp}$, MPa	0.80	0.73	0.61	0.41	0.83	0.73	0.60	0.40	0.83	0.73	0.58	0.39
δP_{mi}	0%	0%	1.6%	4.9%	0%	1.4%	3.3%	5%	1.2%	4.1%	6.9	12.8%
$\eta_{i\ calc}$	0.49	0.49	0.50	0.52	0.47	0.48	0.49	0.51	0.43	0.44	0.45	0.47
$\eta_{i\ exp}$	0.49	0.50	0.52	0.55	0.49	0.51	0.53	0.57	0.49	0.53	0.56	0.63
$\delta \eta_i$	0%	2%	3.8%	5.4%	4%	6%	7.5%	10.5%	12.2%	16.9%	19.6%	25%
α_{calc}	1.94	2.16	2.7	4.25	1.87	2.23	2.81	4.51	1.90	.29	3.08	5.08
α_{exp}	1.94	2.21	2.93	4.77	1.80	2.25	3.04	5.06	1.83	2.21	3.19	5.49
$\delta \alpha$	0%	2.3%	7.7%	10.8%	3.9%	1.1%	7.3%	10.8%	4.2%	3.5%	3.3%	7.3%

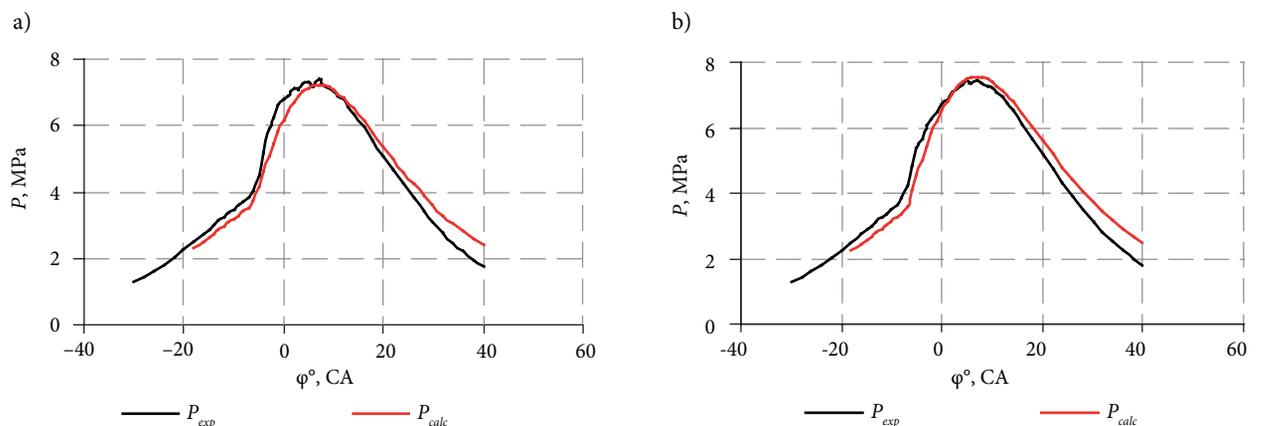


Fig 2. The comparison of the calculation data obtained by using DIAGR program and the results of testing diesel engine 1A41 ($n = 1750\ min^{-1}$; $P_{mi\ nom}$) shown by indicator diagrams: a – burning conventional diesel fuel; b – burning RME

Table 5. The comparison of TOXIC program calculation results and the data obtained in testing diesel engine 1A41

Fuel	D				B30				RME			
	$P_{mi\ nom}$	0.85 $P_{mi\ nom}$	0.5 $P_{mi\ nom}$	0.25 $P_{mi\ nom}$	$P_{mi\ nom}$	0.85 $P_{mi\ nom}$	0.5 $P_{mi\ nom}$	0.25 $P_{mi\ nom}$	$P_{mi\ nom}$	0.85 $P_{mi\ nom}$	0.5 $P_{mi\ nom}$	0.25 $P_{mi\ nom}$
Operation mode												
$P_{max\ calc}$, MPa	7.0	6.5	6.0	6.2	7.1	6.6	6.1	6.2	7.0	6.5	6.0	5.0
$P_{max\ exp}$, MPa	7.1	6.6	6.0	5.4	–	6.7	5.9	5.3	7.2	6.9	–	5.2
δP_{max}	1.4%	1.5%	0%	14.8%	–	1.5%	3.3%	17%	2.7%	5.7%	–	3.9%
$T_{b\ calc}$, K	1000	942	774	681	1053	927	787	663	1038	928	747	543
$T_{g\ exp}$, K	763	723	638	533	783	703	623	523	783	703	613	518
$e_{NOx\ calc}$, g/h	217.6	173.4	138.4	142.7	225.4	190.6	151.1	150.0	240.8	202.8	164.8	80.5
$e_{NOx\ exp}$, g/h	203.2	171.1	117.9	65.6	208.3	169.7	103.3	58.95	207.8	193.6	100.4	48.3
δe_{NOx}	7.1%	1.3%	17.5%	118%	8.2%	12.4%	46%	154%	16%	47%	64%	67%
$\varphi_{i\ calc}$, °avpk	–7.0	–6.0	–5.0	–4.0	–7.0	–6.0	–5.0	–5.0	–8	–8	–7	–6
$\varphi_{i\ exp}$, °avpk	–6.5	–5.5	–4.5	–3.5	–6.5	–6.0	–5.0	–5.0	–8.0	–7.5	–	–5.5
α_{calc}	1.86	2.09	2.62	4.2	1.79	2.1	2.74	4.45	1.83	2.21	3.00	5.03
α_{exp}	1.94	2.21	2.93	4.77	1.80	2.25	3.04	5.06	1.83	2.21	3.19	5.50
$\delta\alpha$	4.1%	5.9%	10.4%	12.1%	0.5%	4.7%	9.8%	12.1%	0	0%	5.7%	0.7%

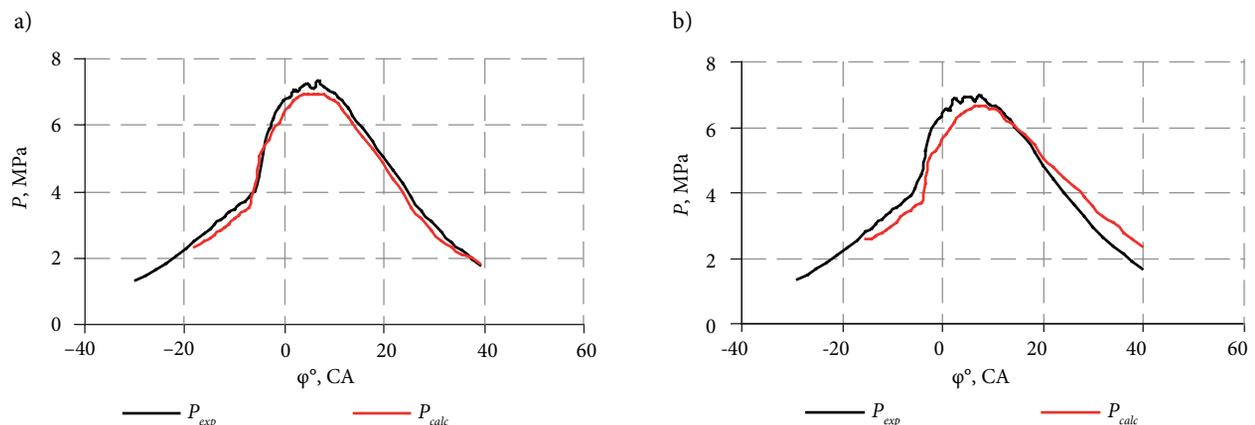


Fig. 3. The comparison of TOXIC program calculation results and the data obtained in testing diesel engine 1A41. Indicator diagrams of the diesel engine 1A41 ($n=1750\ min^{-1}$): a – burning B100 (RME), $P_{mi\ nom}$; b – burning B30 (D70/RME30); 0.85 $P_{mi\ nom}$

The comparison of mathematical modelling results and the data obtained in testing a real diesel engine shows that:

- in the main load modes ($P_{mi\ nom}$, 0.85 $P_{mi\ nom}$, 0.5 $P_{mi\ nom}$), the agreement between the operational parameters P_{max} and α is satisfactory. The significant deviation of P_{max} and α (up to 12÷14%) in the low load mode can be explained by the significant decrease of the actual fuel supply angle, which was not adjusted during modelling. This trend can be clearly observed in Fig. 3b).

- the difference between the actual and the calculated temperature of the exhaust gases up to 200÷300 K can be explained by the fact that the program calculates the temperature (T_b) at the end of the expansion process, while the experiment fixes the temperature (T_g) of the diesel engine exhaust gases. In this case, it is important that the relative temperature changes are actually alike (see Table 6). For the same reasons as in the case of P_{max} and α , a considerable deviation can be observed for the temperatures $T_{b\ calc}$ and $T_{g\ exp}$ in the range of low-load modes.

Table 6. The comparison of the characteristic temperature changes in the calculation by a mathematical and in testing data

	D				B30				B100			
	$P_{mi\ nom}$	0.85 $P_{mi\ nom}$	0.5 $P_{mi\ nom}$	0.25 $P_{mi\ nom}$	$P_{mi\ nom}$	0.85 $P_{mi\ nom}$	0.5 $P_{mi\ nom}$	0.25 $P_{mi\ nom}$	$P_{mi\ nom}$	0.85 $P_{mi\ nom}$	0.5 $P_{mi\ nom}$	0.25 $P_{mi\ nom}$
$T_{b\ calc}$, %	100	94	77	68	105	93	79	66	104	93	75	54
$T_{g\ exp}$, %	100	95	84	70	103	92	82	68	103	92	80	68
δT , %	0	–1	–9	–1	+2	+1	–3.8	–3	+1	+1	–6.7	–26

3.2. Determining the Concentration of Toxic Substances in the Exhaust Gases of Diesel Engines by Mathematical Models

The amount of NO_x, the most toxic component of the exhaust gases, largely depends on the parameters and characteristics of the engine's operation.

It is known (Лебедев, Нечаев 1999) that the dynamics of NO_x formation is affected by the processes of the fuel-air mixture formation and its combustion in the diesel cylinder, which are characterized by the induction period (φ_i) and heat release rate in the kinetic combustion phase ($dx/d\varphi_{I_{max}}$). Therefore, the assessment of e_{NO_x} and φ_i as interlinked quantities is appropriate. On the other hand, the calculation of the absolute NO_x value is exceptionally complicated because it is associated with the precise determination of the temperature fields and air-fuel concentration in the field.

For this purpose, the 3-D mathematical models rather than single-zone thermodynamic models were used (e.g. KIVA-II) (Choi et al. 1997). Presentation of the initial data in the form required for this type of models is an equally complicated task as the calculation of the mathematical model itself. Therefore, in practice, for calculating the effect of the particular parameters or factors on NO_x emission, its relative variation is assessed. A similar procedure was made in testing the TOXIC program.

To assess NO_x emission modelling results (for diesel engines burning RME), the relative percentage value of the parameter was applied.

In Table 5, the absolute values obtained in testing the engine and mathematical modelling is presented, while, in Table 7, the estimates of their relative variation (assuming the calculation and the experimental e_{NO_x} values in the $P_{mi\ nom}$ mode to be 100%) are given.

The values of NO_x obtained by modelling in the range of $(1.0 \div 0.5)P_{mi\ nom}$ demonstrate the need for setting the fuel supply angle with the utmost precision at the beginning of the process and to calculate the induction period φ properly.

4. Conclusions

Based on the analysis of mathematical modelling programs, used in calculating various diesel engine parameters, the programs' algorithms were adjusted. The validation of the modified programs, based on the data obtained in testing diesel engines burning biofuels, allowed the authors to make the following conclusions:

1. Thermodynamic (single-zone) mathematical models, used for describing the major parameters of diesel engines burning RME biofuels (e.g. their power, fuel consumption, temperature of the exhaust gases, etc.), show the acceptable accuracy of calculation (with the error of $\pm 5\%$). The algorithms for calculating energy characteristics of the combustion (C_V , H_U , U) of diesel engines, burning fuels of different chemical compositions, should be adjusted.
2. The equations, used for calculating the characteristics $dx/d\varphi$ in the original models, provide the acceptable accuracy of calculation of energy and ecological characteristics of diesel engines, operating in full- or medium-load modes. The use of mathematical models for describing the operation of diesel engines in the low-load modes (lower than $0.5 P_{mi\ nom}$) requires further research to render more precise parameters of the kinetic combustion phase and algorithms for calculating the characteristics $dx/d\varphi$.
3. The analysed and modified mathematical modelling programs TEPL, TOXIC, IMPULS and DIAGR, are used now in the examination of energy and ecological characteristics of diesel engines burning RME and other biofuels, carried out at the Maritime Institute of Klaipėda University.

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Table 7. The comparison of relative variation of e_{NO_x} emission values obtained by using the TOXIC program and in testing the engine

	D				B30				RME			
	$P_{mi\ nom}$	0.85 $P_{mi\ nom}$	0.5 $P_{mi\ nom}$	0.25 $P_{mi\ nom}$	$P_{mi\ nom}$	0.85 $P_{mi\ nom}$	0.5 $P_{mi\ nom}$	0.25 $P_{mi\ nom}$	$P_{mi\ nom}$	0.85 $P_{mi\ nom}$	0.5 $P_{mi\ nom}$	0.25 $P_{mi\ nom}$
$e_{NO_x\ calc}$	100	79	63	66	1.03	0.87	0.69	0.69	1.1	0.93	0.76	0.37
$e_{NO_x\ exp}$	100	84	58	33	1.03	0.84	0.51	0.29	1.03	0.96	0.49	0.24
δe_{NO_x}	0	-6.3	+8	+100	0	+3.6	+35	+138	+6.8	-3.1	+55	+54

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