



Mathematical model of the combustion process for turbojet engine based on fuel properties

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Received: 17 September 2021 / Accepted: 26 February 2022 / Published online: 28 March 2022
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Abstract

This paper presents the impact of the alternative fuels properties on the parameters characterizing the combustion process in a turbojet engine, expressed in the form of a mathematical model. Laboratory tests, bench tests and a regression analysis of the obtained results were conducted. The developed and published combustion process models were briefly described. It has been demonstrated that these models were insufficient in taking into account the impact of fuel properties on the course of the combustion process. The experimental data enabled developing a mathematical model of the combustion process using statistical methods. The developed model, unlike other currently known models, takes into account the chemical composition of the fuel to a greater extent, which is characterized by its physicochemical properties. Mathematical model enables predicting engine operating parameters and the emissions characteristics, based on analysing laboratory test results, and can be used as a tool verifying the environmental impact of new fuels, through predicting the exhaust gas emissions.

Keywords Combustion process model · Exhaust gas emission · Fuel properties · Regression analysis · Turbojet engine

Introduction

The primary fuel used to power gas turbine engines is fossil jet fuel. For decades, the chemical composition of these fuels was modifying together with technological progress and experience in exploitation [1].

The fuels are mainly mixtures of hydrocarbons, obtained from processing of crude oil (conventional fuels), supplemented with enriching additives that improve their operational parameters [2]. Jet fuel is composed primarily of paraffinic and cycloparaffinic hydrocarbons, aromas and olefins [3]. The composition depends on the used crude oil and its refining technology. For this reason, this type of fuel is not defined by the content of individual hydrocarbons, but through regulatory requirements.

Jet fuel chemical composition determines their operational properties. The content of individual hydrocarbons determines fuel properties, such as calorific value, chemical

stability, combustion quality and many other operational properties. This relationship can be expressed as follows [4]:

$$F_p = f(Ch_f) \quad (1)$$

where F_p is the fuel properties and Ch_f is the chemical composition of fuel.

Recently, the petroleum industry has been focused on developing technologies that utilize non-petroleum raw materials in the course of production [5]. This is due to economic, security and environmental factors. Currently, there are seven approved technologies of synthetic components originating from unconventional sources, which can be blended with fossil fuel up to 50%. They are listed in standard ASTM D7655 [6] and are approved for use in aircraft turbine engines.

The complex process of approving fuels containing synthetic hydrocarbons for use in aircraft turbine engines resulted in limiting the previously widespread diversity of hydrocarbon groups within their composition. Changing the hydrocarbon structure of the fuel, besides affecting its properties, also modifies the mechanism of reactions, making up the complex combustion process.

The papers [7–13] were used as a basis to present the relationships between the parameters characterizing the

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combustion process in a turbojet engine and the physicochemical properties of the fuel (Fig. 1). The physicochemical properties of fuel are quantitative variables, since they can adopt specific numerical values. However, a review of the source literature enabled only defining them as qualitative variables. The reason for this is that these relationships were collected based on experiments and observations, without a determined quantitative impact on the combustion process.

Combustion process models

In the case of jet engines, combustion process consists of three stages. The first one involves fuel atomization, which means using the injectors to supply the combustion chamber with a fuel mist, and consists of very finely dispersed fuel droplets [14]. During the second stage, the air stream mixes with the fuel mist (fine fuel droplets increase the evaporation volume of the injected liquid), creating a fuel-air mixture. In the case of older engine designs, fuel is supplied to the combustion chamber via evaporators, where it evaporates in contact with a hot tube (evaporator), and the vapours are lifted with air to the combustion zone. The last stage is the ignition of the fuel-air mixture, resulting from a flame (in the combustion zone), and combustion, which spreads quickly in all areas where air and fuel are mixed within flammability limits [15].

Combustion process chemistry and rate depend on the engine design [16], as well as the properties of used fuel [17]. Fuel must be injected, vaporized and mixed with air in the combustion chamber, before combustion occurs. The extent to which these processes affect combustion greatly depends on the physicochemical properties of fuel. This relationship can be expressed as follows:

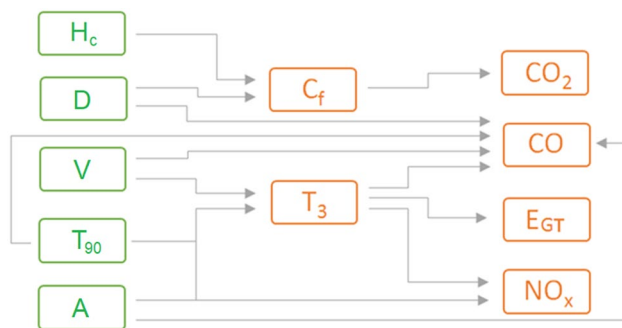


Fig. 1 Dependence of parameters characterizing the combustion process on fuel properties (H_c —neat heat of combustion, D —density, V —viscosity, T_{90} —90% distillation temperature, A —aromatic content, C_f —fuel consumption, T_3 —combustion chamber temperature, E_{GT} —exhaust gas temperature, CO — CO emission, CO_2 — CO_2 emission, NO_x — NO_x emission)

$$E_p = f(F_p) \quad (2)$$

$$E_g = f(F_p) \quad (3)$$

where E_p is the engine operating parameters and E_g is the exhaust gas emission.

Mathematical modelling can be applied for solving problems involving phenomenon repeatability or similarity. However, due to the successive stages of the combustion process (atomization, evaporation and ignition), and the large number of elementary hydrocarbon oxidation reactions, an attempt to describe it using a model is not a simple task.

The following sections present the previously developed combustion process models, together with their limitations.

ARP 1533C model

Hydrocarbon fuel combustion model was presented in ARP 1533C [18]. It includes a methodology for calculating the emission indices of exhaust gas components, fuel-to-air ratio and the combustion efficiency based on carbon monoxide (CO), carbon dioxide (CO_2), hydrocarbon and nitrogen oxides (NO_x) measurements. The combustion process model within the procedure presents an equation for the combustion of a single mole of hydrocarbon fuel and atmospheric air.

This model reduces multi-component hydrocarbon fuels to the form of an averaged chemical formula, e.g. $C_{11.6}H_{22}$ for Jet A fuel. However, hydrocarbons with the same number of carbon atoms exhibit various physicochemical properties. Hence, the conclusion that the averaged chemical formula adopted for various fuels (even petroleum-derived) is a huge simplification. Furthermore, the authors of [19] confirmed that one chemical compound with several isomers, thus the same chemical formula, is characterized by different physicochemical properties, assigned to individual isomers.

CFD model

Computational fluid dynamics (CFD) modelling analyses chemical transformation of hundreds of compounds expressed by thousands of chemical reactions, taking into account the fact that the number of elementary reactions of hydrocarbon oxidation depends on their structure and falls within a range from several hundred to several thousand [20]. However, a detailed numerical simulation of actual fuel combustion is still beyond reach, when it is applied to any fuel that is not a pure component or a mix of more than several components [21].

One of the applied simplifications is the process being represented by a minor number of elementary reactions,

making up a subsequent reaction chain. These so-called global mechanisms are stoichiometric relationships, for which approximated kinetic equations can be determined [22].

Another method is modelling the combustion process using surrogate fuels. They are a simplified equivalent of fuel, composed of one or more selected hydrocarbons that represent the main fuel ingredients. The idea behind minimizing the number of ingredients is obtaining a model fuel that exhibits physicochemical properties and combustion characteristics similar to the conventional jet fuel [7]. Although there are numerous models, such simplification of the mix composition that best mimics real-life fuel being tested remains a significant challenge.

Furthermore, it should be noted that CFD modelling often omits the properties of the tested fuel or takes their values from a library (averaged parameters). The authors of [23] studied the combustion of fuel and its blends with added components, as well as the emission characteristics, describing fuel properties with only two values, i.e., density and viscosity, whereas [24] describes conventional and synthetic fuels only with an average formula C_mH_n , the hydrogen-to-carbon ratio (information derived from the average formula C_mH_n) and net heat of combustion. As highlighted before, fuel composition impacts its physicochemical properties, therefore, adopting average data from libraries or taking into account the minimum number of parameters is a very simplified approach and prevents studying the impact of fuel properties on the combustion process.

Statistical model

During literature review, one publication [25] was found which presents combustion process model for turbojet engine fuel, developed using statistical methods. However, its objective was to statistically analyse the ICAO Aircraft Engine Emissions Databank, in order to estimate the emissions in new turbofan engines. The development of the obtained statistical model did not take fuel properties into account and was based purely on a historical database. Furthermore, no statistical model of the combustion process based on the experimental studies was found.

The presented and characterized combustion process models focus on its various elements; however, in the majority of cases they assume that fuel is the element of the system, the change of which is insignificant or that is not changed at all. This is most probably due to the fact that so far, the modelling process was implemented by turbojet engine engineers. Their primary objective was to improve the engine operating parameters, which was not associated with changing the used fuel as the propulsion source. The process of introducing synthetic fuels to the aviation industry enforced the necessity to conduct work

on modifying fuel physicochemical composition and stop perceiving it as a constant value in modelling the combustion process.

In the light of the above, it seems appropriate to analyse combustion process with greater emphasis on fuel, as a variable within this process, which has been defined as the objective of this paper.

3. Materials and methods

Tested fuels

Conventional jet fuel and its blends with synthetic components form two different technologies approved by ASTM D7566 and biobutanol, which were used in this study and marked as follows:

- Conventional jet fuel (Jet A-1)—Jet;
- Blend of Jet A-1 with synthetic component from hydro-processed esters and fatty acids (HEFA), feedstock: used cooking oil (75:25)—25UCO;
- Blend of Jet A-1 with synthetic component from HEFA, feedstock: used cooking oil (50:50)—50UCO;
- Blend of Jet A-1 with synthetic component from HEFA, feedstock: used cooking oil (25:75)—75UCO;
- Blend of Jet A-1 with synthetic component from HEFA, feedstock: camelina (50:50)—50CAM;
- Blending synthetic component from technology approved by ASTM D7566 (other than HEFA)—S;
- Blend of Jet A-1 with synthetic component from S (75:25)—25S;
- Blend of Jet A-1 with synthetic component from S (50:50)—50S;
- Blend of Jet A-1 with synthetic component from S (25:75)—75S;
- Blend of Jet A-1 with biobutanol (75:25)—25but;
- Blend of Jet A-1 with biobutanol (50:50)—50but;
- Blend of Jet A-1 with biobutanol (25:75)—75but.

HEFA and S components are specified in standard ASTM D7566 and, after blending with fossil fuel in a volume of up to 50%, can be supplied to aviation turbine engines, whereas biobutanol (n-butanol) is an alcohol that was produced through fermenting the C_5 and C_6 sugars. Choosing n-butanol, unlike other components, resulted from the need to increase the range of measured fuel properties, even going beyond the area set out by normative documents. Prepared fuel samples were subjected to selected laboratory tests (Table 1), determined by their impact on the combustion process.



Table 1 Selected fuel properties and their impact on the combustion process

Property	Impact on the combustion process
Density at 15 °C, kg/m ³	Is taken into account during aircraft range calculations—the amount of fuel necessary to secure the combustion process
Viscosity at – 20 °C, mm ² /s	Determines the resistance of fuel flow through filters and nozzles; it also affects the injection process and fuel atomization in the combustion chamber
Net heat of combustion, MJ/kg	Determines the engine efficiency and its characteristics and is taken into account during aircraft range calculations
Aromatic content, % (V/V)	Tendency to incomplete combustion (smoke)
Distillation: 90% v/v at °C, °C	Affects the rate of fuel evaporation, combustion chamber temperature and exhaust gas temperature

Engine

Bench testing was conducted on a Miniature Jet Engine Test Rig (MiniJETRig) with miniature turbojet engine GTM 140 for jet fuels combustion process research. The test rig is used in research and development work, mainly for testing alternative fuels for aviation [26–28]. Its detailed description can be found in [29].

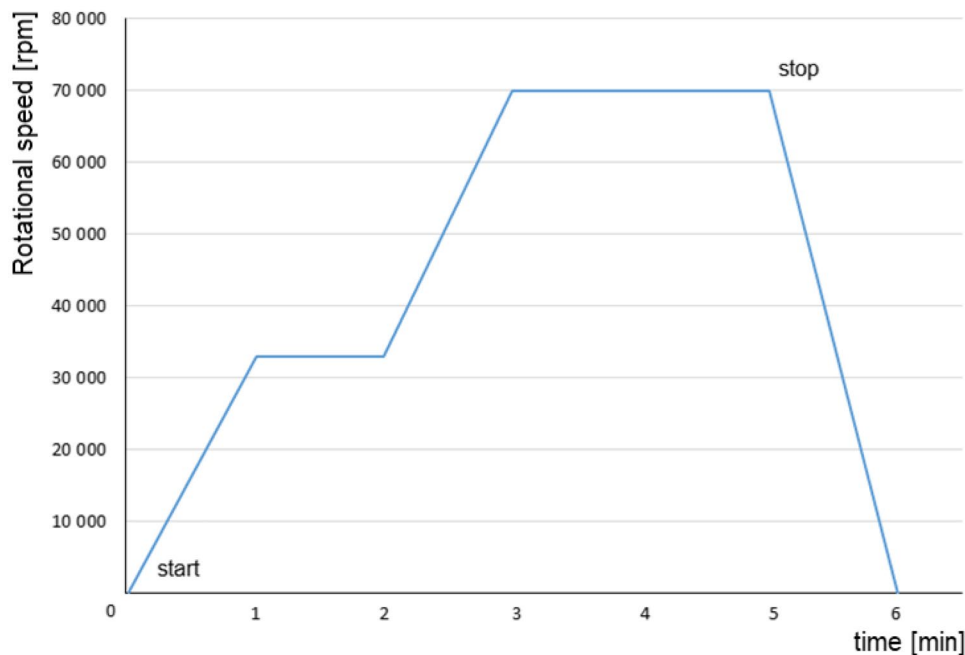
Previous research with the use of the test rig enabled developing a procedure for testing [30]. Nonetheless, given the fact that turbojet engine operating parameters change at various rotational speeds, only one speed, namely 70000 rpm, was selected for the purpose of the paper (Fig. 2). This speed corresponds to 30% of the maximum thrust achieved by the engine and characterizes its lowest thermal load.

Measurement equipment

Each tested fuel was bench-tested at least twice in the course of the research. The parameter results from the last 30 s (stabilization) were taken in the case of each engine test as measurement data sets that were averaged and considered as the measurement result (for T_3 , E_{GT} and C_p) or as a value to calculate EI (for CO , CO_2 and NO_x).

The engine tests involved recording parameters characterizing the combustion process in a turbojet engine:

- Thermodynamic state, namely fuel consumption, mean temperature in the combustion chamber (measured by six thermocouples located circumferentially) and the exhaust gas temperature (measured downstream of the exhaust nozzle),
- Exhaust gas emissions, namely carbon monoxide, carbon dioxide and nitrogen oxides.

Fig. 2 Profile of engine test

The details of the equipment used to measure the exhaust concentration of CO, CO₂ and NO_x are shown in Table 2.

Emissions of gaseous exhaust gas components: CO, CO₂ and NO_x converted and presented in the form of emission indices, according to [31]:

$$EI_i = \frac{X_i}{X_{CO} + X_{CO_2}} \frac{xMW_i}{MW_f} \tag{4}$$

where EI_i is the emission index of species i , $X_{i/CO/CO_2}$ is the mole fractions of species $i/CO/CO_2$, x is the number of moles of carbon in a mole of fuel, and MW_i/MW_f is the molecular weights of species i /fuel.

Results

Selected properties of the fuel samples are presented in Table 3, while Table 4 presents the results of the bench tests.

The impact of synthetic components on the fuel properties, engine operating parameters and exhaust characteristics has been presented in previous works [27, 32, 33]. The obtained results were used as a database for regression analysis.

Development of mathematical model

The main purpose of developing the model was an attempt to describe the relationships presented in Fig. 1 using quantitative features. Multiple regression was used to determine the effect of many independent variables on each dependent variable. During the analysis, the fuel properties were treated as independent variables and the parameters characterizing the combustion process as dependent variables (Fig. 3). Step-wise regression in R software was used to determine their relationship. It involves developing a model, which initially does not contain any explanatory variable, while every successive step expands the model with only such variables that significantly predict the dependent variable.

Data sets are analysed with a certain, predetermined likelihood level, specified by a confidence interval. A confidence interval level of 95% was adopted, which means a 95% probability that the confidence interval will cover an unknown value of the estimated parameter.

The development of a regression model for each explained variable (parameter characterizing the combustion process) took into account only explanatory variables (fuel properties) shown in Fig. 1. Nonetheless, this figure only shows their qualitative relationships, and applying the regression will enable their quantitative correlations.

Each constructed model was rated and verified through checking the significance of all explanatory variables (using Snedecor’s F distribution), significance of partial regression coefficient (using Student’s t distribution), matching of the theoretical and experimental curves (using the R^2 determination coefficient), lack of collinearity between independent variables (using the variance inflation factor), and conformity of the residuum and normal distributions (using the Shapiro–Wilk test).

The developed and positively verified linear regression equations presented together show the model of combustion process in a turbojet engine:

$$T_3 = 424.2 + 0.49 T_{90} \pm 3.2 \tag{5}$$

$$E_{gt} = 396.8 + 0.49 T_{90} \pm 2.4 \tag{6}$$

$$C_f = 2.822 - 0.0155 W_o \pm 0.025 \tag{7}$$

$$EI_{CO} = 2025.4 - 2.01 G_{15} - 1.69 T_{90} + 2.47 A \pm 6.6 \tag{8}$$

$$EI_{CO_2} = 82.4 W_o + 4.0 G_{15} - 3740 \pm 28 \tag{9}$$

This analysis did not allow to build a regression equation for NO_x. This may be due to the fact that fuel is not part of the NO_x formation process and the nitrogen oxide formation rate might indirectly depend on fuel properties. These oxides are formed primarily as a result of atmospheric nitrogen oxidation at very high temperatures, encountered in the combustion chamber.

The regression equations of the dependence of combustion process characterizing parameters on fuel properties are shown in Fig. 4.

The regression Eqs. (5)–(9) allow for the verification of qualitative relationships identified by the literature review. In addition, significant independent variables can be quantified using regression coefficients. Collected Eqs. (5)–(9) were treated as a combustion process mathematical model, taking

Table 2 Details of measurement equipment for gas emissions

Parameter	Sensor type	Range	Least count	Accuracy
CO	Electrochemical	0–2 000	0.1 ppm	±5% of the measured value
CO ₂	Infrared	0–25	0.01%	±5% of the measured value
NO	Electrochemical	0–500	0.1 ppm	±5% of the measured value
NO ₂	Electrochemical	0–100	0.1 ppm	±5 ppm

Table 3 Selected properties of the fuel samples

Property	Test method	Requirements ASTM D1655/ASTM D7566	Test result											
			Jet	25but	50but	75but	25UCO	50UCO	75UCO	50CAM	25S	50S	75S	S
Density at 15 °C, kg/m ³	ASTM D 4052	775–840	790.1	794.0	800.1	806.5	779.8	770.7	761.4	779.9	782.9	773.8	766.0	758.6
Viscosity at -20 °C, mm ² /s	ASTM D 445	Max 8.0	3.069	4.070	6.320	8.092	3.227	3.481	3.754	4.968	3.312	3.699	4.155	4.766
Net heat of combustion, MJ/kg	ASTM D 3338	Min 42.8	43.31	40.73	38.18	35.63	43.54	43.74	43.95	43.69	43.49	43.67	43.84	44.02
Aromatic content, % (V/V)	ASTM D1319/calculative	Max 25.0	15.1	11.3	7.6	3.8	11.3	7.6	3.8	9.1	11.3	7.6	3.8	0
Distillation: 90% v/v at °C, °C	ASTM D 86	Report	213.5	205.2	200.5	184.2	224.7	235.1	241.7	230.0	213.0	211.9	209.7	206.6

into account the fuel properties to a greater extent than the previously known models.

However, this model has limitations, which include:

- Input data falling within a range of fuel property intervals or in its close vicinity;
- Output data falling within a range of the intervals of obtained test bench results or in its close vicinity;
- The ability to apply the developed model for predicting results obtained only for the GTM 140 engine (used to conduct bench tests);
- The ability to apply the model for predicting results obtained for specific engine operating conditions (pre-defined rotational speed).

Conclusions

The objective of the research was to develop a mathematical model of combustion process using regression analysis. In order to implement the above laboratory and bench tests of conventional jet fuel and its blends with alternative components were carried out.

The obtained results were used as a database to conduct a regression analysis of data resulting in regression models covering the impact of fuel physicochemical properties on selected parameters characterizing the combustion process. Compiled regression equations were treated as a combustion process mathematical model, taking into account the fuel composition characterized by its properties to a greater extent than the previously known models. Furthermore, the created linear regression model is enabled to quantitatively describe qualitative relationships, identified by the source literature review.

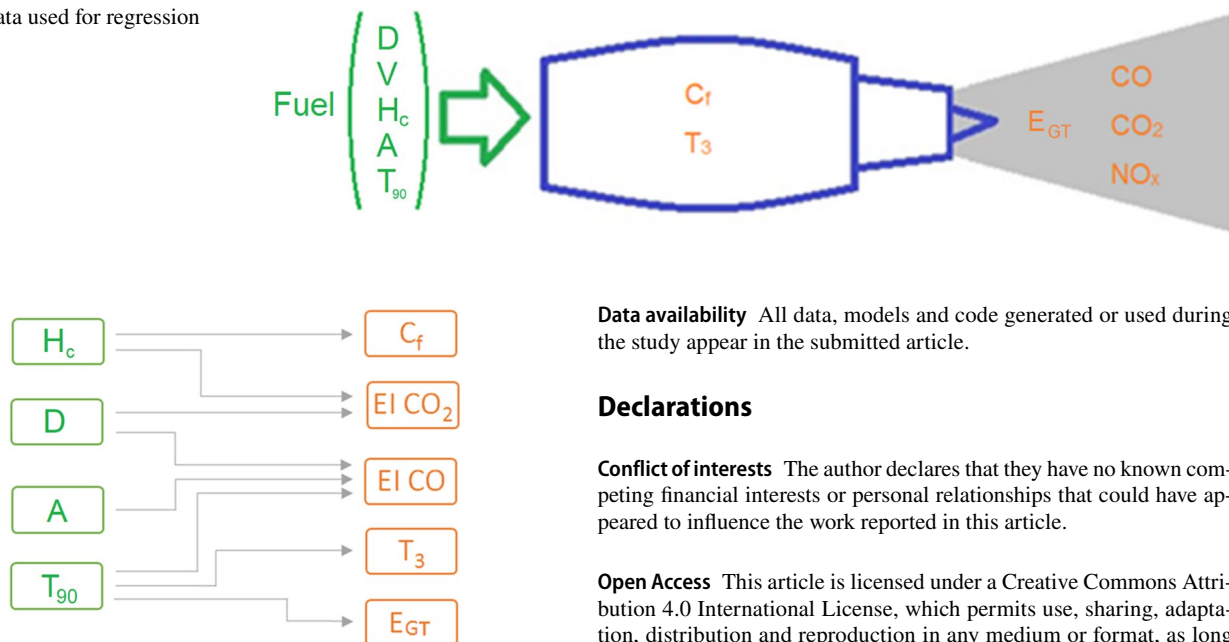
The developed combustion process mathematical model enables predicting engine operating parameters and the emissions characteristics, based on analysing laboratory test results. This model can be used as a tool verifying the environmental impact of new fuels, through predicting the exhaust gas emissions. The developed model relates only the engine used in bench tests, while the use of the methodology implemented in this research allows to extend the model to other engines. However, statistical data analysis and the resulting model are aimed at facilitating and extending the scope of inference about the impact of fuel properties on the combustion process.

The author further plans to conduct laboratory and test bench tests of other alternative fuels, with their results supplementing input data, in order to constantly update the combustion process model for a GTM 140 engine. A perspective to continue the research is conducting test rig studies involving other engines, including full-sized ones, in order to verify the obtained relationships within the developed



Table 4 Bench test results

Fuel sample	Number of measurements	T_3	E_{GT}	C_f	EI_{CO}	EI_{CO_2}	EI_{NO_x}
Jet	300	531.8	503.4	2.154	113.3	2990	1.63
25but	450	518.6	495.5	2.204	113.0	2793	1.026
50but	450	518.9	490.2	2.214	102.5	2614	0.866
75but	450	516.7	489.5	2.278	96.6	2422	0.750
25UCO	300	537.2	509.0	2.133	97.9	2998	1.46
50UCO	300	540.2	513.5	2.133	94.2	2987	1.54
75UCO	300	542.0	514.2	2.132	93.3	2971	1.62
50CAM	300	537.4	510.5	2.096	103.5	2973	1.84
25S	300	530.9	503.8	2.155	121.6	2964	1.64
50S	300	529.4	501.0	2.139	130.8	2936	1.63
75S	300	530.4	500.9	2.167	141.4	2906	1.63
S	300	530.0	501.4	2.187	154.0	2896	1.66

Fig. 3 Data used for regression analysis**Fig. 4** Dependence of parameters characterizing the combustion process on fuel properties from regression equations from regression equations

mathematical model and to attempt to develop a general model that enables assessing the impact of fuel chemical composition on the parameters characterizing the combustion process.

Acknowledgements This research was funded by the Ministry of Science and Higher Education (Poland) for the project financed within the framework of the statutory activity. The author would like to thank Prof. Andrzej Kulczycki DSc, PhD Eng. and Wojciech Dziegielewski for their support as thesis advisers.

Data availability All data, models and code generated or used during the study appear in the submitted article.

Declarations

Conflict of interests The author declares that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this article.

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