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WORKING PROCESS MODEL DEVELOPMENT OF THE GAS TURBINE ENGINE COMBUSTOR FUELING ON METHANOL

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The use of methanol as a fuel for aircraft and stationary gas turbine engines (GTE) is a priority direction in engine building. It is well known that when modeling the GTE performances using first-level mathematical models, there is an error in calculating specific fuel consumption, which is caused by the simplified description of the GTE combustor working process. The object of the study is the working process in the GTE combustor fueling on methanol. The peculiarity of the developed mathematical model of the working process of the GTE combustor is the use of enthalpy dependencies on temperature, pressure, and mixture composition. Enthalpy dependencies in this form implicitly account for the effect of thermal dissociation and allow for the correct formulation of the equivalent combustion reaction path. For two components (H_2O and CO_2), accounting for pressure leads to the fact that at standard temperature and partial pressures exceeding the saturation pressure, these components exist in a liquid state. This situation, with a constant enthalpy increment in the equivalent process of heating the combustion products from the standard temperature to the temperature at the end of adiabatic heat supply, decreases this temperature.

Clarification of the temperature at the combustor outlet leads to changes in all calculated combustor performances, including the combustor fuel air ratio. The calculation results of the fuel air ratio are compared with known experimental data of the General Electric CF6-80A engine combustor (USA). The average calculation error of the fuel air ratio does not exceed 4 %. The developed model can be implemented in existing and developing mathematical models of gas turbine engines for temperatures at the end of the combustion process below 2,600 K

Keywords: fuel air ratio, combustor, methanol, enthalpy, mathematical model of the combustor

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1. Introduction

One of the primary types of fuel consumed by humanity is natural gas. The continuous growth in energy consumption demands the development of new gas fields, typically located far from consumers. It is not always feasible to transport gaseous fuel via pipelines, so the gas is liquefied and delivered to consumers at cryogenic temperatures (about –160 °C) in tank cars. Alternatively, methane can be converted into methanol at the extraction site and transported as liquid methanol at normal temperatures and pressures.

The main advantages of methanol as a fuel include affordability, environmental friendliness, and a variety of production methods (including renewable energy sources).

It is known that methanol can be used as fuel for both aircraft and stationary gas turbine engines (GTE) [1–5]. Moreover, the conversion of gas turbine engines from one fuel type to another is relatively simple, not requiring significant investment to converting the existing fleet of stationary GTE to methanol fueling.

To design GTE fueling on methanol and to convert the existing fleet of GTE that can use methanol as fuel, it is necessary to have a mathematical model of the combustor working process. This mathematical model should be simple to implement into existing mathematical models of GTE. Therefore, the development of a mathematical model for the gas turbine engine fueling on methanol is a relevant scientific and technical problem.

2. Literature review and problem statement

In [2], a comparison of the performance of three cycles of a gas turbine engine using methanol and n-decane as fuels with pre-combustion chemical cooling was conducted. The calculation results showed that the use of preheated fuel is an effective way to improve engine performance. Moreover, the cycle in which both a rocket turbine and a gas turbine are used can increase the maximum flight Mach number by 7.06 %. In [3], a study was carried out to investigate how different types of fuel (including methanol and ethanol) affect the output performance of industrial gas turbine engines, demonstrating the advantages of using fuels with a higher hydrogen-to-carbon ratio. In [4], a computational study was performed to assess the economic efficiency and carbon dioxide emissions of a regenerative gas turbine engine with thermochemical recuperation operating on methanol and ethanol, as well as their mixtures with steam. At the optimal water-to-methanol ratio, this technology can increase engine efficiency by 3–5 % and reduce carbon dioxide emissions by 12–13 % compared to direct burning of diesel fuel. In [5], an extended environmental and eco-economic study based on exergy and life cycle assessment was conducted on micro GTE using a new iterative method. The following types of fuel were investigated: natural gas, mixtures of natural gas and ammonia, as well as methanol. Methanol demonstrates the best life cycle-based environmental performance compared to other fuel options. A drawback of the works [2–5] is the determination of enthalpy only as a function of temperature, which does not allow for a correct representation of the equivalent chemical reaction path and does not account for the thermal dissociation of combustion products. In [6], a study of a hybrid aircraft engine was conducted using three approaches: exergetic, exergo-economic, and exergo-ecological analysis. Five alternative fuel types with different concentrations were selected for the study. Methanol ranks second after methane in terms of energy production costs and fourth in terms of environmental impact after methane, hydrogen, and ethanol, while still being of the same order of magnitude. It is noted that a mixture of ethanol and hydrogen appears to be a viable option from both an economic and environmental standpoint. In [7], six chemical nonequilibrium models are compared under various conditions encountered in real rocket engines. Unlike [2–5], the works [6, 7] consider thermal dissociation of combustion products but do not accurately describe the equivalent chemical reaction path.

Thus, a common drawback of the mathematical models presented in [2–7] is the lack of analysis of the equivalent chemical reaction path at pressure other than standard one. Specifically, the absence of two additional isothermal processes: transitioning from actual pressure to standard one and reversing from standard pressure to actual one. Ignoring these two additional transitions ultimately leads to incorrect determination of the fuel air ratio.

To account for the influence of pressure and thermal dissociation, two approaches can be employed: solving a system of chemical kinetics equations with a large number of equations [6, 7], or utilizing experimental values of enthalpies or specific isobaric heat capacity c_p as functions of temperature T and pressure p [8]. Additionally, by adopting the second approach to determine the enthalpy of combustion products, we obtain a correctly formulated equivalent chemical reaction path. Another significant advantage of the second approach is its simplicity and ease of implementation in existing GTE combustor models [9] and ramjet engines [10].

In [11], a mathematical model for the combustor fueling on aviation kerosene was developed based on the second approach. However, the system of chemical thermodynamics equations for kerosene and methanol differs. Additionally, the work [11] lacks justification for the necessity of considering the equivalent chemical reaction path for non-standard temperature and pressure. Therefore, it is necessary to develop a mathematical model for the working process of a GTE combustor fueling on methanol, taking into account pressure, thermal dissociation of combustion products, and a correctly formulated equivalent chemical reaction path of the combustion process.

3. The aim and objectives of the study

The aim of this work is to develop a mathematical model of the working process of a GTE combustor fueling on methanol, which can be implemented into the existing GTE mathematical models. Such a model will allow obtaining performance of the engine fueling on methanol, considering pressure, thermal dissociation of combustion products, and a correctly formulated equivalent chemical reaction path of the combustion process.

To achieve the aim, the following objectives were set:

– to justify the necessity of considering the influence of pressure when determining the enthalpy of combustion products in the mathematical model of the working process of the GTE combustor;

– based on the determined composition of combustion products and the dependence of the enthalpy of their individual components $h(T, p)$, to develop an algorithm for calculating the fuel air ratio q_f of the GTE combustor fueling on methanol;

– to verify the mathematical model of the working process of a GTE combustor fueling on methanol for calculating q_f by comparing it with known experimental data of GTE combustors.

4. Materials and methods of the study

The object of the study is the working process in a GTE combustor fueling on methanol.

The subject of the study is the influence of pressure and thermal dissociation on the working process in a GTE combustor fueling on methanol.

The study is based on the use of theoretical methods and mathematical modeling of thermodynamic and chemical processes in a GTE combustor.

The hypothesis of the study suggests that the influence of pressure, thermal dissociation of combustion products, and a correctly composed equivalent chemical reaction path can be accounted for by the dependence $h(T, p, q_f)$ during the GTE combustor operation.

The main assumption of the study is the adiabatic reaction occurring in the GTE combustor.

The main simplification of the study is the use of a phenomenological approach.

The study was conducted in the following sequence:

– justification of the necessity to account for the influence of pressure when determining the enthalpy of combustion products was carried out;

– an algorithm was developed for calculating the fuel air ratio, which was implemented in the mathematical model of the working process of the GTE combustor fueling on methanol;

– the mathematical model of the working process of the GTE combustor was verified by comparing the obtained values of q_f with known experimental data of the General Electric CF6-80A engine fueling on methanol [12, 13].

5. Results of the working process study of the gas turbine engine combustor fueling on methanol

5. 1. Justification of the necessity to account for pressure influence when determining the enthalpy of combustion products

The peculiarity of determining the average specific isobaric heat capacity of water vapor and carbon dioxide in combustion products lies in accounting for the heat of phase transition. The classical approach does not consider this heat [14] because the standard thermal effect of the chemical oxidation reaction ΔH^0_{comb} is tied to standard conditions for the reactants: normal atmospheric pressure p_0=760 mm·Hg=101,325 Pa and temperature T_0=25 °C=298 K. The deviation of the initial temperature of the oxidizer and fuel in calculations is taken into account by a well-known formula based on Kirchhoff's equation [15]. For adiabatic oxidation reaction:

$$\Delta H_{C-A}+\Delta H_{A-B}+\Delta H_{B-D}=0, \tag{1}$$

where $\Delta H_{A-B}=\Delta H_{298}^{0}$ – standard thermal effect of reaction at T_0 and p_0; ΔH_{C-A} – change in enthalpy of reactants (starting substances) reflecting the thermal effects accompanying the transition of reactants from the initial parameters T_1 and p_1 to the standard T_0 and p_0:

$$\Delta H_{C-A}=\sum_{n=1}^{n_1}\nu\cdot\int_{T_0,\,p_0}^{T_1,\,p_1}\int\left(c_p(T,p)\mathrm{d}p\mathrm{d}T+r_0\right); \tag{2}$$

where ΔH_{B-D} – change in enthalpy of reaction products reflecting the thermal effects accompanying the transition of reaction products from the final parameters T_2 and p_2 to the standard T_0 and p_0:

$$\Delta H_{B-D}=\sum_{n=1}^{n_2}\nu\cdot\int_{T_0,\,p_0}^{T_2,\,p_2}\int\left(c_p(T,p)\mathrm{d}p\mathrm{d}T+r_0\right); \tag{3}$$

where r_0 – in both cases, the latent heat of phase transition of a substance, which can be represented as a function of the partial pressure of that substance.

The essence of expression (1) is better illustrated graphically: the first figure (Fig. 1, *a*) refers to the oxidation reaction occurring at normal atmospheric pressure, and hence at low partial pressures of carbon dioxide and water vapor, where the phase transition temperature lies below the standard 25 °C. The second figure (Fig. 1, *b*) pertains to situations with high partial pressures of water vapor and carbon dioxide, where the phase transition temperature exceeds 25 °C. As the comparison showed, ignoring this fact leads to a noticeable deterioration in the combustor calculation results.

5. 2. Algorithm for calculating the fuel air ratio

The stoichiometric amount of moist air L_0, for the complete combustion of 1 kg of methanol of a given composition is determined:

$$L_0=\frac{\mu_{O_2}}{g_{O_2}}\left(\frac{g_C}{\mu_C}+\frac{1}{4}\frac{g_H}{\mu_H}-\frac{1}{2}\frac{g_O}{\mu_O}\right), \tag{4}$$

where g_i – mass fraction of the component; μ, kg/kmol – molar mass of the component.

The chemical reaction of methanol (CH_4O) combustion in air with excess of oxidizer λ can be represented by equation (5):

$$CH_4O+1.5\lambda\left(\begin{array}{l}\frac{x_{N_2}}{x_{O_2}}\cdot N_2+O_2+\frac{x_{Ar}}{x_{O_2}}\cdot Ar+\\+\frac{x_{CO_2}}{x_{O_2}}\cdot CO_2+\frac{x_{H_2O}}{x_{O_2}}\cdot H_2O\end{array}\right)=$$

$$=\left(1+1.5\lambda\cdot\frac{x_{CO_2}}{x_{O_2}}\right)\cdot CO_2+\left(2+1.5\lambda\cdot\frac{x_{H_2O}}{x_{O_2}}\right)\cdot H_2O+$$

$$+1.5\lambda\cdot\frac{x_{N_2}}{x_{O_2}}\cdot N_2+1{,}5(\lambda-1)\cdot O_2+1.5\lambda\cdot\frac{x_{Ar}}{x_{O_2}}\cdot Ar, \tag{5}$$

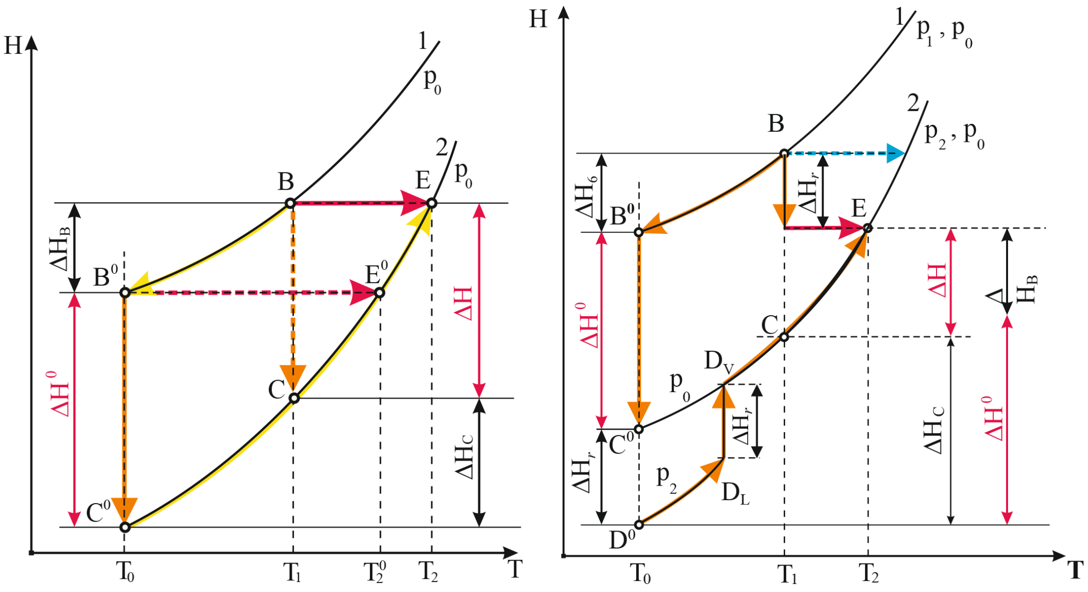
where x_i – molar fraction of the component. The factor of 1.5 preceding the oxidizer excess coefficient corresponds to the stoichiometric ratio of fuel to oxidizer.

Air is considered a mixture of five gases – nitrogen, oxygen, water vapor, carbon dioxide, and argon.

From the law of conservation of energy in [11], the equation for the fuel air ratio q_f was obtained:

$$q_f=\frac{G_f}{G_{air}}=\frac{1}{\dfrac{H_u\cdot\eta_g}{h_g^*-h_{air}^*}-1}, \tag{6}$$

where G_f and G_{air}, kg/s – fuel consumption and air mass flow rate; H_u, kJ/kg – the specific lower calorific value of the fuel, given its known composition, is determined, for example, by Mendeleev's formula; η_g – the fuel combustion efficiency coefficient; h_{air}^*, kJ/kg – the specific enthalpy of air at temperature and pressure at the inlet to the combustor; h_g^*, kJ/kg – the specific enthalpy of combustion products at temperature and pressure at the outlet of the combustor.



a *b*

Fig. 1. To derive the equation for the general thermal effect in an adiabatic oxidation reaction: *a* – without phase transition of the reaction products; *b* – with phase transition of the reaction products

The specific enthalpy of combustion products at the outlet of the combustor is determined as [11]:

$$h_g^* = \sum_{i=1}^{n} g_i h_i^*, \tag{7}$$

$$\Delta h_i^* = c_{p_{aa_i}} \cdot \left(T_i^* - T_0\right) = \frac{1}{p_i - p_0} \int_{p_0}^{p_i} \left(\int_{T_0}^{T_i^*} c_p(T, p) \mathrm{d}T \right) \mathrm{d}p, \tag{8}$$

where $c_{p_{aa_i}}$, kJ/kg K – the average integral specific isobaric heat capacity of a component within the specified range of temperatures from T_0 to T_i^* and pressures from p_0 to p_i; T_i^*, K – outlet temperature T_{ex}^* or inlet temperature T_{in}^* of the combustor; T_0=298 K – the temperature commonly used as a reference one in thermochemistry problems, for which the standard enthalpies of substances formation are known; p_i and p_0 – partial pressures of the mixture component at the end and at the beginning of the integration process.

Partial pressures are determined through the molar fractions of the components:

$$p_i = \sum_{i=1}^{n} x_i \cdot p_{mix}, \tag{9}$$

where p_{mix} – mixture pressure.

Based on the partial pressures and temperatures at the inlet and outlet of the combustor, the heat capacities of air and combustion products are determined:

$$c_{p_{aa.mix_i}} = \sum_{i=1}^{n} x_i \cdot c_{p_{aa_i}}. \tag{10}$$

The dependencies $c_{pa}=f(T, p)$ for the main components of air and combustion products, averaged over pressure and temperature, obtained in [11] are used in the study.

5. 3. Mathematical model verification of the working process of the GTE combustor fueling on methanol

Verification of the mathematical model for calculating q_f was carried out by comparing the calculation results with experimental data obtained during testing the CF6-80A engine combustor in various modes [12].

The combustor test results for different engine operating modes are presented in Table 1.

The total pressure losses of the CF6-80A engine combustor are presented in [13].

Table 1

Operating conditions of the combustor fueling on methanol [12]

Conditions	Combustor inlet			Gas average outlet temperature, K	Combustion efficiency, %	Fuel consumption (methanol), g/s
	Air temperature, K	Air pressure, MPa	Mass flow rate, kg/s			
Approach, 30 % thrust	614	1.102	7.09	1,036	99.9	216
Climb	772	2.426	13.42	1,360	99.9	650
Takeoff	805	2.789	15.02	1,434	99.8	789.1
Minimum cruise	608	0.621	3.96	995	99.8	127.9
Normal cruise	686	0.936	5.49	1,194	99.9	231.8
Maximum cruise	726	1.132	6.4	1,289	99.9	300

For the calculations, methanol CH_4O was used as fuel, whose elemental composition is provided in Table 2.

Table 2

Chemical composition of CH_4O

Component	Molar fraction x_i	Mass fraction g_i
Carbon C	1/6=0.16667	0.3749
Hydrogen H	2/3=0.6667	0.1258
Oxygen O	1/6=0.16667	0.4993

Atmospheric air was represented as a mixture of gases described in Table 3.

Table 3

Chemical composition of atmospheric air*

Component	Chemical formula	Molar fraction x_i	Mass fraction g_i
Nitrogen	N_2	0.768484	0.747711
Oxygen	O_2	0.206161	0.229120
Argon	Ar	0.009217	0.012788
Carbon Dioxide	CO_2	0.000314	0.000480
Water Vapor	H_2O	0.015824	0.009901

*Note: *p_{atm}=101,325 Pa; t_{atm}=27 °C; d=10 g/kg of dry air, molar mass of wet air is 28.792 kg/kmol*

The fuel air ratio was calculated in two ways:

– with the developed model based on the use of enthalpy $h(T, p, q_f)$, which is calculated using the specific isobaric heat capacity $c_{paa}(T, p, q_f)$ averaged over temperature and pressure;

– with the model presented in [14]. In that model, the enthalpy dependence is represented as $h(T, q_f)$.

The relative calculation error of q_f was calculated by the equation:

$$\delta q_f = \frac{\left(q_f\right)_{calculated} - \left(q_f\right)_{test}}{\left(q_f\right)_{test}} 100\,\%, \tag{11}$$

where $(q_f)_{calculated}$ – calculated fuel air ratio; $(q_f)_{test}$ – experimental fuel air ratio.

Comparison of the calculation results with the experimental data is shown in Fig. 2.

Fig. 2 illustrates that the average relative calculation error:

– when using enthalpy values in the form of $h(T, q_f)$ [14], is δq_f=5...22 %;

– when using enthalpies calculated with the specific heat capacity c_{paa} averaged over temperature and pressure, is δq_f=0.79...7.45 %.

The error of δq_f=7.45 % is maximum during the approach condition. In [11], when comparing calculation results with experimental data obtained during tests of the CF6-80A engine combustor fueling on kerosene, the maximum error also corresponded to the approach condition. This behavior could be explained by measurement errors during this condition in the experiment.

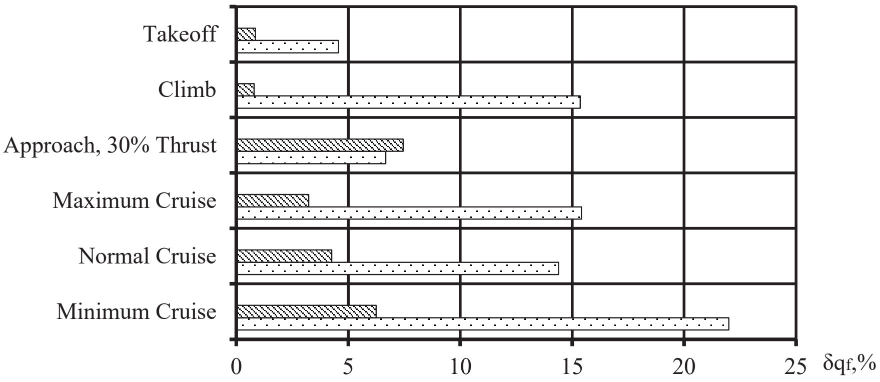


Fig. 2. Comparison of calculation results with experimental data: ▨ — the relative calculation error taking into account temperature and pressure changes $c_{paa}(T, p, q_f)$; ░ — the relative calculation error using dependencies $h(T, q_f)$

6. Discussion of calculation results of the combustor performance by the proposed model

By using the dependencies $h(T, p)$ for air and $h(T, p, q_f)$ for combustion products, it is possible to account the influence of pressure, thermal dissociation of combustion products, and a correctly formulated equivalent chemical reaction path. Neglecting these factors leads to a significant error in determining the temperature at the end of the combustion process (Fig. 1), and consequently, the fuel air ratio.

Traditionally, it is believed that the enthalpy of combustion products does not depend on pressure [2–7]. However, at high pressures of the gas mixture, its individual components (water and carbon dioxide) may have partial pressures exceeding the saturation pressure value at standard temperature T_0. This means that at standard temperature, they exist not in the gaseous state, but in the liquid state. Therefore, the initial reference level of the combustion products enthalpy shifts downward from point C^0 to point D^0. Accounting for this circumstance ultimately leads to obtaining a lower combustion temperature T_2. The equivalent chemical oxidation reaction path for high-boiling components is increased by two additional isothermal processes. The first is the transition from pressure p_1 to pressure p_0 for the reactants, and the second is the transition from pressure p_0 to pressure p_2 for the combustion products (in the Brayton cycle, p_1 and p_2 coincide). In the works [2–7], which assume the independence of enthalpy from pressure, this circumstance is not taken into account, leading to a systematic error in determining the temperature at the end of the combustion process. Moreover, its discrepancy with the experiment is entirely attributed to the phenomenon of thermal dissociation [6, 7]. Unlike [2–7], the use of $h(T, p, q_f)$ allows for the correct formulation of the equivalent combustion reaction path and accounts for the effect of thermal dissociation implicitly. This ultimately reduces the average calculation error of the fuel air ratio from δq_f=13.1 % to 3.8 % (Fig. 2).

Thus, the proposed algorithm for calculating q_f for GTE fueling on methanol can be utilized in both developing and existing mathematical models of GTE combustors. Moreover, the approach proposed for the development of the combustor mathematical model can be applied to any chemical fuels.

A limitation of the developed model is the existence of a working range for the specific heat capacity c_{paa} (upper range of pressure p=200 bar and temperature T=2,600 K) [16]. If pressures and temperatures exceed these operational ranges, extrapolation is actually used, which may lead to calculation error accumulation.

One of the study drawbacks is the lack of comparison of the calculation results with a model based on solving a system of chemical kinetics equations.

A promising direction for future research is further development of the method for calculating the fuel air ratio in GTE combustors fueling on hydrogen and its mixture with methane.

7. Conclusions

1. The necessity of accounting for the influence of pressure when determining the enthalpy of combustion products is justified when the partial pressure of a component exceeds the saturation pressure at temperature T_0=298 K.

2. Based on the determined composition of combustion products and the dependence of the enthalpy of their individual components $h(T, p)$, an algorithm for calculating the fuel air ratio was developed. The peculiarity of this algorithm is the implicit consideration of processes occurring in the GTE combustor fueling on methanol. This allows for increased accuracy in calculating fuel air ratio both in existing mathematical models of the GTE combustor and in those under development.

3. Comparison of the calculation results with the outcomes of experimental tests conducted on the CF6-80A engine combustor fueling on methanol revealed a reduction in the calculation error in determining the fuel air ratio. The average calculation error for the combustor operation modes does not exceed δq_f=3.8 %.

Conflict of interest

The authors declare no conflict of interest regarding this study, whether financial, personal, authorship or otherwise, that could affect the study and its outcomes presented in this paper.

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Data availability

The manuscript has no associated data.

Use of artificial intelligence tools

The authors confirm that they did not use artificial intelligence technologies in creating the presented paper.

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