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Prediction of fuel consumption and carbon dioxide emission when replacing gaseous fuels with renewable hydrogen or their mixture

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Abstract. The paper is devoted to predicting changes in fuel consumption and carbon dioxide emissions when industrial equipment is converted to heating with renewable hydrogen or a mixture of it with other gaseous fuels, such as natural gas. The authors developed a simplified methodology that is appropriate for assessing changes in the energy consumption of equipment and the environmental impact of fuel replacement at the stage preceding the equipment reconstruction. The peculiarity of the methodology is that it allows the calculation of fuel consumption and carbon dioxide emissions when fuel replacement is accompanied by the implementation of measures aimed at improving the energy efficiency of equipment. The methodology can be used for heating and thermal furnaces in metallurgy and mechanical engineering, units for heat treatment of raw materials in the mining and processing industries, heating devices in the food industry, and water and steam boilers. In the example of replacing natural gas with its mixture with renewable hydrogen of different compositions, it is shown that the calculation error using the proposed methodology in comparison with the results obtained by mathematical modeling of fuel combustion, gas flow and heat transfer in this furnace does not exceed 1.5%.

1. Introduction
Carbon dioxide emissions from the fossil fuels combustion are one of the main factors of global warming, which leads to climate change, melting glaciers, rising sea levels, drought in some regions and increased precipitations in others, negative impact on human health and plant development, crop losses, reduced biodiversity, etc. The main goal of the Paris Agreement is to limit the global temperature increase to 2°C relative to the pre-industrial level by the end of the century [1]. This goal can be achieved through the combined efforts of all members of the global community to reduce greenhouse gas emissions.

One of the major sources of carbon dioxide is natural gas, which is used as a fuel in industry, energy and communal services. According to the International Energy Agency, 38% of total natural gas usage

is consumed by the energy sector, 21% - by industry, including 7% by metallurgy [2].

Metallurgy is one of the last stages of iron ore processing. Metallurgy accounts for 2.6 Gt/year of total carbon dioxide emissions, which is approximately 9% of annual global anthropogenic CO_2 emissions [3]. Therefore, this industry significantly affects the achievement of greenhouse gas emission reduction targets. Metallurgy is currently undergoing significant changes related to the development and implementation of green technologies in steel production, the application of carbon capture, use and storage (CCUS) technology, and the use of renewable hydrogen as a fuel in technological processes [3-6].

The reducing natural gas consumption is extremely relevant for Ukraine, as it helps to reduce carbon dioxide emissions and increase the country's energy independence from natural gas imports, the price of which has increased significantly in recent years. In the context of martial law introduced in Ukraine in February 2022, increased economic risks associated with the hostilities, and material losses caused by the destruction in the eastern part of the country, Ukrainian enterprises have limited investment capacity to implement new technologies. Therefore, in recent years, more and more attention has been paid to the reconstruction of existing equipment to improve its energy efficiency. As an alternative to natural gas, renewable hydrogen is increasingly considered.

The authors [7] show that the reconstruction of existing heating equipment can significantly reduce natural gas consumption per unit mass of production by using well-known energy efficiency measures (replacement of lining of the thermal unit using modern thermal insulation materials based on ceramic fibers; increasing the temperature of heating air used for fuel combustion by improving the system of flue gases heat recovery). Using the example of continuous furnace for heating steel slabs, it was determined that the implementation of these measures can reduce natural gas consumption by 26% and reduce carbon dioxide emissions by the same percentage. In this case, the capacity of the furnace's gas pipelines and burners makes it possible to additionally reduce the carbon dioxide emissions by switching the furnace to a gas mixture consisting of 75% natural gas and 25% renewable hydrogen. This measure does not require the replacement gas and air supply lines of the furnace, burners, and other auxiliary equipment and reduces carbon dioxide emissions by 33 % (or 41.1 kg/t of metal) compared to the operation of the furnace before reconstruction when it was heated with natural gas. Work [8] notes that calculating results of fuel consumption and carbon dioxide emissions were obtained by mathematical modeling of fuel combustion, gas flow, and heat transfer in the furnace chamber, taking into account heat transfer processes in heat recovery equipment.

It should be noted that the mathematical modeling of these processes involves the development of a so-called digital twin of the unit [8, 9], which makes it possible to achieve high accuracy in determining the temperature distribution of flue gases and material in the working chamber, and also requires adaptation and verification of the developed model, which is labor-intensive and time-consuming process. In addition, the equipment of industrial enterprises is characterized by a variety of designs of fuel-consuming units, as well as their auxiliary equipment used for fuel combustion and flue gases heat recovery. This makes it impossible to develop a universal mathematical model that can be used for any type of unit. However, in order to assess the potential for fuel savings and carbon dioxide emissions reduction from the implementation of energy-saving measures and/or replacement of gaseous fuel with its mixture with renewable hydrogen, as well as to select one of a number of units in which the implementation of these measures can be most effective, mathematical modeling, which includes the development of mathematical models of each unit, can be replaced by a simplified methodology for forecasting fuel consumption and carbon dioxide emissions after the implementation of measures. To improve the accuracy of calculations of fuel consumption and CO_2 emissions and to develop the temperature regimes of the unit and ensure the specified technological parameters of its operation, the results obtained using the simplified methodology can be further refined by mathematical modeling on complex models.

Paper [10] proposes a simplified methodology for determining fuel consumption when a unit is switched to heating with gas of a different composition. Its disadvantage is that it does not predict changes in fuel consumption and carbon dioxide emissions with the simultaneous implementation of

measures to improve the energy efficiency of the thermal unit and change the fuel composition. In addition, it does not take into account the existing technical condition of the unit, as it uses only data from the technical passport of the unit and auxiliary equipment to perform calculations. Paper [11] gives an example of applying the methodology [10] to calculate the forecast of fuel consumption when replacing natural gas with its mixture with blast furnace gas and notes that its application leads to an error that increases from 1-2% to 10-25% when the share of blast furnace gas in the mixture increases from 10 to 90%.

The purpose of this study is to develop a simplified methodology for predicting fuel consumption and carbon dioxide emissions when replacing fuel in the unit. The methodology allows to take into account the following:

- change of fuel composition;
- the existing technical condition of the unit and its auxiliary equipment;
- change in the technical performance of the unit due to the implementation of energy-saving measures.

2. Methods

The methodology for predicting fuel consumption and carbon dioxide emissions is based on the laws of mass and energy conservation.

The input data are:

1) maximum productivity of the unit (P, kg/s);

2) parameters characterizing the operation of existing unit when it is heated with fuel 1:

- composition of fuel 1 and conditions of its combustion (air flow rates, oxygen content in the air, air humidity);

- temperature of flue gases leaving the working chamber of the unit (t_{fg1}, °C);

- air temperature before combustion (t_{air1}, °C);

- total heat loss of the unit to the environment (heat loss by heat conduction through the lining, radiation through open windows of the unit, cooling of the unit's structural elements, etc.) - $Q_{\Sigma hl.1}$, W;

- fuel 1 consumption under the maximum productivity (B_{g1}, m^3/s);

3) parameters that characterize the unit operation after implementation of energy saving measures (replacement of lining, use of heat recovery equipment and/or replacement of the existing flue gas heat recovery system with a more efficient one):

- air temperature before combustion (t_{air2}, °C);

- total heat loss of the unit to the environment (heat loss by heat conduction through the lining, radiation through open windows of the unit, cooling of the unit's structural elements, etc.) - $Q_{\Sigma hl.2}$, W;

4) composition of fuel 2 and conditions for its combustion (air flow rates, oxygen content, air humidity).

According to the methodology given in [12], we calculate the combustion of fuels 1 and 2 under the conditions specified in the initial data. The calculations determine the specific air consumption for combustion of 1 m^3 of fuels 1 and 2 (L_{air1} and L_{air2}, m^3/m^3), specific volume of carbon dioxide generated from the combustion of 1 m^3 of fuels 1 and 2 (L_{cd1} and L_{cd2}, m^3/m), specific consumption of flue gases generated from the combustion of 1 m^3 of fuels 1 and 2 (υ_{fg1} and υ_{fg2}, m^3/m^3).

From the heat balance equation of the unit

$$Q_f \cdot B_g + Q_{air} \cdot B_g = M_m + Q_{\Sigma hl} + Q_{fg} \cdot B_g \tag{1}$$

we obtain:

$$B_g \cdot \left(Q_f + Q_{air} - Q_{fg}\right) = M_m + Q_{\Sigma hl}, \tag{2}$$

where Q_f – lower working fuel specific energy, J/m^3; B_g – fuel consumption, m^3/s; $Q_{air} = L_{air} \cdot i_{air}^{t_{air}}$ – the heat of the air for fuel combustion, J/m^3; L_{air} – specific consumption of flue gases generated during fuel combustion, m^3/m^3; $\cdot i_{air}^{t_{air}}$ – air enthalpy at temperature t_{air} (°C), with which it is supplied for fuel combustion, J/m^3; M_m – heat absorbed by working chamber material of the unit during its heat treatment, W; $Q_{\Sigma hl}$ – heat losses of the unit to the environment, W; $Q_{fg} = \upsilon_{fg} \cdot i_{fg}^{t_{fg}}$ – heat of flue gases leaving the working chamber of the unit, W; υ_{fg} – specific consumption of flue gases generated during fuel combustion, m^3/m^3; $\cdot i_{fg}^{t_{fg}}$ – enthalpy of flue gases at temperature t_{fg} (°C), with which they exit the working chamber of the unit, J/m^3.

Divide and multiply the left side of the equation by the calorific value of the fuel:

$$B_g \cdot Q_f \left(\frac{Q_f + Q_{air} - Q_{fg}}{Q_f} \right) = M_m + Q_{\Sigma hl}. \tag{3}$$

The value in parentheses on the left side of the equation is known as the coefficient, which characterizes the full utilization of fuel heat in the working chamber of the unit [12, 13]:

$$\eta = \left(Q_f + Q_{air} - Q_{fg} \right) / Q_f = \left(Q_f - (1-r) \cdot Q_{fg} \right) / Q_f, \tag{4}$$

where $r = Q_{air} / Q_{fg}$ – degree of heat utilization of flue gases leaving the unit.

Using (4), equation (3) takes the form:

$$B_g \cdot Q_f \cdot \eta = M_m + Q_{\Sigma hl}. \tag{5}$$

Equation (5) is used to determine the fuel consumption.
Consider two cases:
1) the thermal unit is switched to heating by fuel 2;
2) replacement of fuel in the thermal unit and implementation of energy saving measures.

2.1. Fuel replacement
Since the heat absorbed by the metal during its heat treatment (M_m) and the heat losses by the working chamber to the environment ($Q_{\Sigma hl}$) before and after the fuel replacement are unchanged, using (5), we obtain the equation for determining the fuel 2 consumption:

$$B_{g2} = B_{g1} \cdot \frac{Q_{f1} \cdot \eta_1}{Q_{f2} \cdot \eta_2}, \tag{6}$$

where $\eta_1 = (Q_{f1} - (1-r_1)Q_{fg1}) / Q_{f1}$, $\eta_2 = (Q_{f2} - (1-r_2)Q_{fg2}) / Q_{f2}$, $r_1 = Q_{air1} / Q_{fg1}$, $r_2 = Q_{air1} / Q_{fg2}$, $Q_{air1} = L_{air1} \cdot i_{air}^{t_{air1}}$, $Q_{fg1} = \upsilon_{fg1} \cdot i_{fg1}^{t_{fg1}}$, $Q_{fg2} = \upsilon_{fg2} \cdot i_{fg2}^{t_{fg2}}$; the index "1" means operation of the unit heated by fuel 1, and the index "2 means operation of the unit heated by fuel 2; $i_{fg1}^{t_{fg1}}$ and $i_{fg2}^{t_{fg2}}$ – flue gas enthalpies calculated from the composition of combustion products of fuel 1 and fuel 2 at temperatures t_{fg1} and t_{fg2}, J/m^3.

Usually, the flue gas temperature t_{fg2} is unknown, so during calculation, we assume that the fuel replacement does not significantly change temperature regime of the unit and assume that $t_{fg2} = t_{fg1}$.

Specific emissions of carbon dioxide (kg$_{CO2}$/kg$_{material}$) when heating the furnace with fuel 1

($b_{\mathrm{CO_2}_1}$) and after replacement the fuel ($b_{\mathrm{CO_2}_2}$) are determined by following formulas:

$$b_{\mathrm{CO_2}_1} = B_{\mathrm{g1}} \cdot L_{\mathrm{cd1}} \cdot \frac{\rho_{\mathrm{CO2}}}{P}, \quad b_{\mathrm{CO_2}_2} = B_{\mathrm{g2}} \cdot L_{\mathrm{cd2}} \cdot \frac{\rho_{\mathrm{CO2}}}{P}, \tag{7}$$

where $\rho_{\mathrm{CO_2}} = 1.98$ kg/m^3 is density of carbon dioxide under normal conditions.

2.2. Fuel replacement with simultaneous implementation of energy saving measures
If the proposed measures, in addition to fuel replacement, improve flue gas heat recovery systems or reduce heat losses in the furnace working space, then, using (5), we obtain the equation for fuel 1 consumption after the implementation of energy saving measures (B_{g1}^*, m^3/s):

$$B_{\mathrm{g1}}^* = \frac{B_{\mathrm{g1}} \cdot Q_{\mathrm{f1}} \cdot \eta_1 - (Q_{\Sigma\mathrm{hl.1}} - Q_{\Sigma\mathrm{hl.2}})}{Q_{\mathrm{f1}} \cdot \eta_1^*}, \tag{8}$$

where $\eta_1^* = \left(Q_{\mathrm{f1}} - (1 - r_1^*) \cdot Q_{\mathrm{fg1}}^*\right)/Q_{\mathrm{f1}}$, $r_1^* = Q_{\mathrm{air1}}^* / Q_{\mathrm{fg1}}^*$, $Q_{\mathrm{air1}}^* = L_{\mathrm{air1}} \cdot i_{\mathrm{air}}^{t_{\mathrm{air2}}}$, $Q_{\mathrm{fg1}}^* = \upsilon_{\mathrm{fg1}} \cdot i_{\mathrm{fg}}^{t_{\mathrm{fg2}}}$ – performance indicators of the unit when it is heated with fuel 1 after the implementation of energy saving measures; t_{fg2} – temperature of flue gases at which they leave the working chamber of the unit after the implementation of the measures, °C. If the flue gas temperature t_{fg2} is unknown, it is assumed that $t_{\mathrm{fg2}} = t_{\mathrm{fg1}}$.

Next, fuel consumption is determined when switching the unit to fuel 2 heating:

$$B_{\mathrm{g2}} = B_{\mathrm{g1}}^* \cdot \frac{Q_{\mathrm{f1}} \cdot \eta_1^*}{Q_{\mathrm{f2}} \cdot \eta_2}, \tag{9}$$

where $\eta_2 = \left(Q_{\mathrm{f2}} - (1 - r_2)Q_{\mathrm{fg2}}\right)/Q_{\mathrm{f2}}$, $r_2 = Q_{\mathrm{air2}} / Q_{\mathrm{fg2}}$, $Q_{\mathrm{air2}} = L_{\mathrm{air2}} \cdot i_{\mathrm{air}}^{t_{\mathrm{air2}}}$, $Q_{\mathrm{fg2}} = \upsilon_{\mathrm{fg2}} \cdot i_{\mathrm{fg2}}^{t_{\mathrm{fg2}}}$; the index "2" means the unit operation after implementation of energy saving measures and fuel replacement; $i_{\mathrm{fg2}}^{t_{\mathrm{fg2}}}$ – flue gas enthalpies calculated from the composition of fuel 2 combustion products at temperature t_{fg2}, J/m^3. If t_{fg2} is unknown, we accept $t_{\mathrm{fg2}} = t_{\mathrm{fg1}}$, and $r_2 = r_1^*$.

Specific carbon dioxide emissions (kg$_{\mathrm{CO2}}$/kg$_{\mathrm{material}}$) when heating the furnace with fuels 1 and 2 are determined by equations (7).

3. Results and discussion
Paper [7] presents the initial data and results of mathematical modeling of fuel combustion and heat exchange processes in the working chamber of continuous furnace for heating slabs. The paper also determines fuel consumption and carbon dioxide emissions when implementing the following measures:

1) switching the furnace from natural gas heating to heating with a mixture of natural gas and renewable hydrogen with its content in the mixture 25, 50, 75% and 100%;

2) replacement of natural gas with a mixture of natural gas and hydrogen with the simultaneous implementation of the following measures:

- replacement of a lining made of refractory bricks with a lining made of modern refractory ceramic materials with low thermal conductivity coefficients. The measure reduced heat losses from the furnace's working chamber to the environment from 21.911 to 13.410 MW.

- improvement of the flue gas heat recovery system, which increased the combustion air heating temperature from 352 to 450°C when the furnace was heated with natural gas;

- adjusting the temperature regime of the furnace, which led to a change in the temperature of flue

gases from 915 to 860 °C when the furnace was heated with natural gas.

Based on the initial data of [7] and the developed methodology, we calculated fuel consumption and specific carbon dioxide emissions, the results of which are shown in tables 1 and 2. To compare the results and determine the calculation error, tables 1 and 2 also show the results of calculating the same values obtained using the mathematical modeling method previously published in [7].

Tables 1 and 2 show that satisfactory results were obtained for predicting fuel consumption and carbon dioxide emissions for both cases under consideration. The maximum relative calculation error was 1.3% (table 2, hydrogen fraction in the mixture is 0.75), which corresponds to a fuel consumption of 125 m^3/h and specific carbon dioxide emissions of 0.64 kg/(t_{metal}).

Table 1. The results of calculations by developed methodology and the results of mathematical modeling of the furnace during the implementation of measure 1.

Fuel	Natural gas	Mixture of natural gas and hydrogen			Renewable hydrogen
Content of hydrogen in mixture	0.00	0.25	0.5	0.75	1.00
Results of mathematical modeling of the furnace [7]					
Fuel consumption, m^3/h	6151	7439	9405	12790	20253
Specific emissions of CO_2, kg/(t_{metal})	125.84	114.14	96.20	65.41	0.00
Results obtained by the proposed methodology					
Fuel consumption, m^3/h	-	7445	9430	12857	20199
Specific emissions of CO_2, kg/(t_{metal})		114.23	96.46	65.76	0.00
Relative calculation error of fuel consumption (specific emissions of CO_2), %	-	0.1 (0.1)	0.3 (0.3)	0.5 (0.5)	0.3 (0.0)

Table 2. Results of calculations by developed methodology and results of mathematical modeling of the furnace when implementing measures 1-3.

Fuel	Mixture of natural gas and hydrogen			Renewable hydrogen
Content of hydrogen in mixture	0.25	0.5	0.75	1.00
Results of mathematical modeling of the furnace [7]				
Fuel consumption, m^3/h	5523	6956	9466	15166
Specific emissions of CO_2, kg/(t_{metal})	84.74	71.15	48.41	0.00
Results obtained by the proposed methodology				
Fuel consumption, m^3/h	5529	7013	9591	15161
Specific emissions of CO_2, kg/(t_{metal})	84.84	71.74	49.05	0.00
Relative calculation error of fuel consumption (specific emissions of CO_2), %	0.1 (0.1)	0.8 (0.8)	1.3 (1.3)	0.03 (0.00)

The developed methodology, in contrast to the known methodology [10], predicts the fuel consumption and carbon dioxide emissions with satisfactory accuracy, and takes into account the technical condition of the unit and the efficiency of heat recovery devices during calculations. Methodology disadvantage is a need to collect additional data - the parameters of the unit's operation: flue gas temperature, air heating temperature, changes in heat losses from the unit's working space to the environment.

4. Conclusions

A simplified methodology has been developed that predicts fuel consumption and specific carbon dioxide emissions when replacing fuel in technological units and implementing energy-saving measures without mathematical modeling of fuel combustion, gas flow, and heat exchange in working chamber of continuous furnace. It is determined that when replacing natural gas with its mixture with renewable hydrogen or when the unit is completely converted to renewable hydrogen, the maximum error in calculating the predicting data does not exceed 1.5%.

The methodology can be used to assess changes in fuel consumption and environmental impact at the stage preceding the reconstruction of the unit, as well as to justify the selection of units where the implementation of energy-saving measures and/or fuel replacement can provide the greatest benefit. The application of the methodology is recommended for heating and thermal furnaces in metallurgy and mechanical engineering, units for heat treatment of raw materials in the mining and processing industries, heating devices in the food industry, water heating and steam boilers.

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