IOP Conference Series: Materials Science and Engineering

PAPER • OPEN ACCESS

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To cite this article: V V Sterligov 2020 *IOP Conf. Ser.: Mater. Sci. Eng.* **866** 012028

IOP Conf. Series: Materials Science and Engineering **866** (2020) 012028 doi:10.1088/1757-899X/866/1/012028

Prediction of carbon dioxide emissions from fuel combustion

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Abstract. An objective method for estimating carbon dioxide emissions using specific emissions per 1 kJ of fuel energy is presented. To unify the calculations of the calorific value of gaseous and solid fuels, it is proposed to use a regression calculation model for both coal and gas. The applicability of this approach is proved and on its basis the calculation of possible CO_2 emissions at a given unit power.

1. Introduction

In existing assessments of the environmental situation in the world, pessimistic forecasts are increasingly dominating. And it refers not only to foreign media. In Russia, and even more importantly for us – in Kuzbass, materials appear that predict the disastrous ecology of coal Kuzbass. Written by non-professionals, such publications may provoke a negative reaction from untrained readers.

Meanwhile, the situation is not so tragic and during this period the objectively best information is needed, which, recognizing the difficult situation, would search for and suggest the ways to solve this problem. The basic document created by the international community on climate warming, the so-called "Framework Convention on Climate Change" (UNFCCC) [1], in paragraph 2, contains a precautionary statement that urges mankind to seek funds, even if they are still scientifically and not represented. This determines the relevance of any work aimed at solving the global problem of the greenhouse effect.

In another document created for the implementation of the UNFCCC, the so-called the "Kyoto Protocol" [2], in Art. Section 5 contains the definition of the main measure to combat warming caused by the greenhouse effect, which is energy saving leading to a reduction in greenhouse gas emissions and which can be achieved by direct reduction in the consumption of fuel and especially coal. In our opinion, this is a primitive and even vulgar solution due to the extensive factor. But since society needs energy to function in all areas of life, it is more rational to develop and introduce new ways to use fuel that would give reduced emissions of carbon dioxide – the main representative of greenhouse gases.

The activity of the international society on these energy-ecological problems has not yet reached Russia. It should be said that not all atmospheric experts know that in Russia, as long as the whole world, a fee for carbon dioxide emissions was introduced. But if you look at one of the most authoritative sources on energy-environmental problems [3], then it shows the payment for emissions of SO_2, NO_x, etc., but it does not exist for CO_2.

The Kyoto Protocol also noted the need to introduce accounting for CO_2 emissions, but so far practically nothing was done in Russia in this direction. Since the country has committed itself to continue to reduce CO_2 emissions by signing the Paris Agreement in December 2015 [4], it is necessary to prepare to fulfill these obligations.

2. The unified model for calculation of gas calorific value

This paper presents an attempt to simplify the determination of CO_2 emissions based on the elemental composition (i.e., on the content of individual chemical elements) as opposed to the calculation of the chemical composition, the determination of which is laborious and not always available at any enterprise.

Earlier [5] we proposed the idea of using specific emissions per unit of energy (c). The value of c is defined as follows:

$$c = \frac{m_{CO_2}}{Q_{н}^{р}}, \text{ kg/kJ.} \quad (1)$$

Therefore, it is important to determine quickly and efficiently the values of $Q_{н}^{р}$. Obviously, the model for solid and liquid fuels has its own advantages for the dtermination. In the future, solid fuel will be called coal, and gaseous – gas.

It is hypothesized that the heat from combustion of gaseous fuels and carbon dioxide emissions can be calculated using a simpler model used for coal.

For gaseous fuels from the theory of combustion [5] the equation for determining the calorific value is known:

$$Q_{н}^{р}=39.847CH_4+107.43H_2+122.63CO+63.790C_2H_4+590.59C_2H_4+912.81C_3H_8, \text{ kJ/m}^3, \quad (2)$$

where CH_4, H_2, CO, C_2H_4, C_3H_8 is the percentage content of fuel components.

It should be noted that this equation is deterministic, i.e. defined in strict accordance with the laws of physics and chemistry. Its additive structure is determined by the absence of interaction during the combustion of various components. Numerical coefficients take into account the heat effect of complete oxidation.

For solid and liquid fuels in the source [5] you can find different formulas, but the most used is the so-called "Mendeleev's formula":

$$Q_{н}^{р}=399C^{р}+1030\,H^{р} – 109(O^{р}-S^{р})- 25W^{р}, \text{ kJ/kg,} \quad (3)$$

where $C^р$, $H^р$, $O^р$, $S^р$, $W^р$ – the content per working mass of individual chemical elements.

This is a regression equation that establishes a relationship based on statistical materials. The additive character is also explained by the independent burning of individual elements. Numerical coefficients are obtained by statistically processed observation results.

Unlike the first model, where it is clearly known which element in combination with another is a substance, the amount of which needs to be known exactly, as well as the thermal effect of its oxidation, the second model does not imply knowledge of elements combinations, it does not contain information about their thermal reactions, etc. For this model, there is no need for chemical gas analysis.

3. Hypothesis proof

For this purpose, calculations were carried out for three flammable gases according to the periodic formula for solid fuel. The calculation results are presented in table 1.

Table 1. Comparative calculation of the calorific value of burnt gases by the formula for solid fuel.

Fuel (gas)	Mass composition, %	Calorific value $Q_{н}^{р}$, MJ		
		according to the equation (2)		according to the equation (3)
		MJ/m^3	MJ/kg	MJ/kg
Methane CH_4, ρ=0.714 kg/m^3	C=75.00 % H=25.00 %	35.847	51.776	51.206
Propane CH_4,	C=81.81 %	912.281	46.969	46.929

ρ=1.96 kg/m^3	H=18.19 %			
Natural gas (volumetric composition) CH_4 =85 %, C_2H_4=10 %, CO=2 %, ρ=0.7585 kg/m^3	C=71.05 % H=24.12 % N=4.34 % CO=0.49 %	37.094	48.900	48.927

The base value in the calculation of $Q_н^Р$ was the value determined by the adopted for gas equation (2), MJ/m^3. By dividing this value by density, the quantity $Q_н^Р$ MJ/kg was determined, which was compared with the calculation results by the proposed method using the elementary mass composition of the gas and equation (3) for solid fuel.

For all three cases, the approximation error was determined by formula (4):

$$\Delta Q=\frac{(Q_н^р)_1-(Q_н^р)_2}{(Q_н^р)_1}\cdot 100\ \%. \quad (4)$$

For the base, we took the value $Q_н^Р$ calculated by formula (1).

For all three cases, the error was: ±1.0%, which is an acceptable error level for the proposed simplified methodology for calculating $Q_н^Р$ and is comparable to the error when using basic equations (1) and (2).

4. Methodology for determining emissions

Since the hypothesis of the applicability of the elementary composition for calculation of the calorific value can be accepted for gaseous fuels, it can be used to estimate the carbon dioxide emission potential and determine the specific emission value m_{CO_2} per unit of released energy, i.e.

$$m_{CO_2}=\frac{M_{CO_2}}{Q_н^Р}. \quad (5)$$

This expression is the key one, and on its basis the following algorithm is proposed for the existing heat engineering unit.

1. The production capacity of the unit *G*, t/h is determined. As a rule, it is known even at the design stage, therefore, the proposed methodology for CO_2 emissions can be used both for forecasting emissions and for studying existing units;

2. The required amount of energy is calculated on the basis of regulatory or practical data according to the performance of unit G:

$$N = eG \text{ kW}, \quad (6)$$

where *e* is the normative specific indicator of energy consumption per unit of production, J/t (unit/s),

G – unit capacity, t/h (unit/s).

The choice of fuel is carried out if there is the possibility of different options, and its consumption is determined *B*, kg/s (t/h):

$$B=\frac{N}{Q_н^Р} \text{ kg/s (m}^3\text{/s)}; \quad (7)$$

here $Q_н^Р$ – is the heat from fuel combustion, kJ/kg (kJ/m^3);

4. The composition of the fuel (coal) is determined by the mass of carbon M_C

$$M_C = B\cdot\%C \text{ kg/s}; \quad (8)$$

By formula (2) we determine the value of $Q_н^Р$.

IOP Conf. Series: Materials Science and Engineering **866** (2020) 012028 doi:10.1088/1757-899X/866/1/012028

In the case of using gas fuel, the carbon mass is calculated by summing the contributions of all carbon-containing fuel components, i.e.

$$M_{\mathrm{C}} = \sum_{i=1}^{n} M_{\mathrm{C}_i}, \tag{9}$$

which is possible with knowledge of the fuel composition.

6. The calculation is based on the material balance of combustion of any carbon-containing fuel component, for example

$$C+O_2=CO_2;$$
$$CO_2+1/2O_2=CO_2;$$
$$CH_4+2O_2=CO_2+2H_2O, \text{ etc.}$$

From these reaction equations it follows that for any hydrocarbon with complete combustion (and in the existing heat engineering unit it is certainly necessary to achieve complete combustion of fuel) 1 atom C generates 1 CO_2 molecule; mass ratio $m_{\mathrm{CO}_2}/m_{\mathrm{C}}$ = 44/12 = 3.67 = const. This makes it possible to determine the predicted carbon dioxide emission:

$$M_{\mathrm{CO}_2} = 3.67 \cdot M_{\mathrm{C}}, \text{ kg/s.} \tag{10}$$

To determine the carbon content (% by mass in the fuel) it is enough to burn the fuel and determine the carbon content in the fuel and its mass from the CO_2 content in the combustion products.

5. Conclusion

Using the proposed methodology, it is possible not only to predict the amount of greenhouse gas CO_2 emissions, but also the amount of fees for these emissions, as well as to abandon the costly analysis of gas composition and determine CO_2 emissions based on the fuel and energy balance of the enterprise.

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