UDC 662.611.2:662.613.5

A.I. Brunetkin, PhD, Lecturer, Odes. Nat. Polytechn. Un-ty,
A.V. Bondarenko, Engineer, PhD student, Odes. Nat. Maritime Acad.,
A.V. Lysyuk, bachelor, Odes. Nat. Polytechn. Un-ty

DETERMINING THE QUANTITATIVE COMPOSITION OF AN UNKNOWN GASEOUS FUEL AND COMBUSTION PRODUCTS FROM THE MEASURED PROCESS PARAMETERS IN THE FUEL COMBUSTION PROCESS

Introduction. Due to the continuous increase of the main energy sources price (coal, natural gas, oil products), production and application of unconventional hydrocarbon fuels has drawn a lot of attention recently. These gaseous, liquid and solid fuels can have several origins:

— Geological (associated petroleum gas, fracking, firedamp etc.).

— Renewable resources (pyrolysis products of organic residuals: slow pyrolysis yields gaseous fuels, while fast pyrolysis yields mainly liquid ones; fermentation of organic waste products, biofuel etc.).

— Manufacturing waste (blast furnace gas, residual gases during oil processing, fouling gases in garbage etc.).

When conventional fuels using, their composition (standardization), and consecutively their burning capacity, are constant. This allows effective fuel combustion and minimization of pollutant production through modal adjustment of the combustion equipment. Such approach is not suitable for unconventional fuels: their composition, and hence burning capacity, vary during the combustion process. The compositions changes randomly at any time point.

Burning equipment can provide independent control of fuel and oxidizer (air) supply. In such case, combustion of a fuel with unknown composition using a nearly stoichiometric oxidizer ratio can be achieved as follows. For a given fuel supply rate, air supply is controlled by a maximum-temperature feedback control system. Maximum temperature is achieved by oxidizer excess coefficient close to 1.0. Other methods can be used for optimal combustion of a fuel with unknown composition [1]. Planning of the optimal fuel combustion represents a necessary but not sufficient condition for its efficient use. Combustion products are high-temperature multi-component chemically reactive mixtures. Determination of the equilibrium composition and properties of such mixtures is part of many tasks of high-temperature energy generation. This is done mostly using theory and computation. The lack of knowledge of the fuel composition and combustion products does not allow performing such computations.

The composition of an unknown substance or substances mixture, if constant in time, can be determined in different ways: spectroscopy, methods of analytical chemistry, for gas mixtures - using gas analyzers. All these methods share a number of drawbacks: high costs, bulky, large residence times and, hence, delays. This makes them difficult to integrate in an automatic combustion control system. Gas analyzers require a list of gases in the mixture. Application of gas analyzers is additionally complicated by the presence of undesirable components in the secondary energy sources, which leads to additional deterioration and failure of primary equipment. The price of a system grows with the size of this list.

DOI: 10.15276/opu.1.43.2014.22

The present paper exposes a new analytical method developed, which allows determining the composition of a (nearly) arbitrary fuel mixture and its combustion products in real time during the combustion process.

Reference sources review. The problem of combustion gases, which are produced by industrial plants, (or so-called uncertified gases), is actual and open not only in the oil industry, but also in industrial furnaces. It is shown that the use of such gases can save costs on certified fuel natural gas, and avoid overuse [2]. This approach to the issue of non-certified gas burning will follow this article. It should also be noted that the burning of hydrogen-containing gas reduces CO_2 emissions into the environment. Consequently, the ecological aspect is affected. It is analyzed the impact of emissions factories engaged in natural gas combustion [3; 4]. It is shown how the burning of compressed gas by pipe strain increases vapor formation [5]. To be noted is that this does not affect the stack emissions. The model burn natural gas, oil, and gas of an unprotected, and it was taken to reconstruct the heat exchanger in a vertical position, and the output flue gases divided into two streams, one of which leads back to the steam boiler [6]. Flue gas losses, as well as unburned fuel amounts, are estimated at [7]. A model of steam boilers on the total load for natural gas is described [8]. The paper describes the impact of boilers simultaneously loss of energy.

The research goal is to develop a simulation model of the combustion of varying composition hydrocarbon gases in the combustion chamber, output values which are measurement process parameters such as flame temperature, the rate of fuel and oxidizer.

Research essence. Many sources, in particular [9], contain a description of the procedure for calculation of the forward problem of determining burnt gas composition from the known fuel composition. The latter is, generally, a mixture. Based on the known mass or mole fractions of fuel components, as well as their chemical formulas, one writes the pseudo-formula of the fuel as

$$A^{(1)}_{b_{1F}} A^{(2)}_{b_{2F}} \cdots A^{(i)}_{b_{iF}}, \tag{1}$$

where $A^{(i)}$ — symbol of the i$^{\text{th}}$ chemical element;

b_{iF} — number of atoms of the i$^{\text{th}}$ element in one (surrogate) fuel molecule.

In the sequence, all calculations use as basis the expression (1), and the knowledge of the specific fuel components is not required. When determining the composition of an unknown fuel, its pseudo-formula can be written in the same manner. The number of each element atoms is unknown in this case. Determining these numbers of atoms and, correspondingly, the composition of gases resulting from its combustion, is the solution of the extended problem considered here.

To resolve that we will use as starting point the model used for its solution in [9], but we have to extend this model with closing equation which would allow finding additional unknowns b_{iF}. O, we shall consider this model.

Matter conservation equation can be written as

$$\sum_q (a_{iq} n_q) = b_{iF} , \tag{2}$$

where q — the number of combustion products;

a_{iq} — the number of atoms of the i$^{\text{th}}$ element in the q$^{\text{th}}$ burnt gas component;

n_q — number of moles of the q$^{\text{th}}$ species in the combustion products.

To obtain a simple formulation of chemical equilibrium equations, the following version of conservation equations is proposed at [10] and used at [9]:

$$\sum (a_{iq} P_q) = M_F b_{iF} . \tag{3}$$

In (3), unlike in (2), M_F moles of fuel is taken into account, which is chosen such that the number (n_q) of moles of the q^{th} burnt gas species is equal to its partial pressure P_q. In this case, M_F is an additional unknown variable and must be defined.

Given (3), the Law of Mass Constancy (chemical equilibrium law for partial pressures) can be written as follows

$$\frac{\prod P_i^{a'_{ij}}}{P_j} = K_j^0 , \tag{4}$$

where P_j, P_i — respectively, the partial pressures of j dependent and i independent burnt gas species, from which the dependent ones can be formed

a'_{ij} — stoichiometric coefficient in the chemical equilibrium reaction;

K_j^0 — chemical equilibrium constant for partial pressures.

Equations 3 and 4 are sufficient for finding q partial pressures of the gases forming the burnt mixture. To determine the value of M_F, Dalton's Law is used:

$$\sum_q P_q = P , \tag{5}$$

where P is the pressure of the burnt gas mixture in the combustion chamber.

Additional closure relations

The model including equations (3), (4), (5) can be used for the solution of the forward problem when the formula 1 of the fuel is known. Consider the solution of the extended problem for a common fuel type, where fuel and oxidizer are in gas phase:

— oxidizer composition is known (air, oxygen etc)

— the fuel is a gas or gas mixture with unknown composition.

In addition to (3), (4), (5) we define the closure relations. In gas phase, molar volumes of any ideal species are equal. Therefore, the ratio of volumetric fuel and oxidizer consumption rates equals their molar ratio in the considered combustion reactions. Thus, using equation (3), an additional balance equation for fuel and combustion products can be written as

$$(I_F + \alpha\chi_0 I_O)M_F = \sum_q I_q P_q , \tag{6}$$

where α — fuel excess coefficient;

χ_0 — molar stoichiometric coefficient

I_F, I_O, I_q — molar enthalpies of fuel, oxidizer and combustion products.

An analogous form of this equation is used for the forward problem, i.e. for determining the burnt gas composition from the known reacting mixture. Temperature and composition of burnt gases are chosen such that the enthalpy balance holds. It is used only once during the calculation, namely to determine one additional unknown (temperature).

To apply eq. 6 for finding several additional variables, one can use the principle of a control system. During one of its steps, volumetric consumption rates of fuel and oxidizer ${}^{(1)}\dot{V}_O, {}^{(1)}\dot{V}_F$ are measured together with the corresponding temperature ${}^{(1)}T$ of the combustion products (upper index ${}^{(1)}$). To equation (6), the following expression can be applied:

$$\alpha \cdot \chi_0 = {}^{(1)}\dot{V}_O \big/ {}^{(1)}\dot{V}_F , \tag{7}$$

where $\dot{V}_O, \dot{V}_F$ are the volumetric consumption rates, and the temperature ${}^{(1)}T$ is related to the enthalpies ${}^{(1)}I_q$ and partial pressures of combustion products.

Thereby, the number of unknowns in the extended problem increases compared to the forward problem: with the known (measured) temperature and fuel and oxidizer consumption, the coefficients in the pseudo-formula (1) are computed, as well as the burnt gas composition such that enthalpy balance is maintained. The list of chemical elements the fuel is composed of must be known (b_{iF}). This poses a limitation of the present model, which is not very strict. Considering a limited number of elements, e.g. $[\mathrm{C}]$, $[\mathrm{H}]$, $[\mathrm{O}]$, $[\mathrm{S}]$, $[\mathrm{N}]$, covers almost all organic substances combustible in ambient air. There is no limitation on the list as such; it can be deduced from the properties of the raw materials, which are processed for production of the unconventional fuel.

If the fuel is composed of n elements, then the number of additional unknown values is (n+1), as the enthalpy needs to be determined. Therefore, (n+1) Equations of the type of eq. 6 must be formulated. Each such equation has an associated measurement ${}^{(1)}\dot{V}_O, {}^{(1)}\dot{V}_F, {}^{(1)}T$: In the test mode of the combustor, ${}^{(1)}\dot{V}_O$ is varied. For an assumed number of species in burnt gases, for each equation of type 6 one has to formulate n+1 equations of the main model (3), (4), (5); considering the n+1 new variables, $((q+1)+1)\cdot(n+1)$ equations altogether. So, for instance, for a hydrocarbon fuel consisting of two elements (carbon $[\mathrm{C}]$ and hydrogen $[\mathrm{H}]$)), and when oxygen $[\mathrm{O}]$ is used as oxidizer, $q=9$ species can be considered as combustion products:

$$[\mathrm{CO}],\ [\mathrm{CO_2}],\ [\mathrm{H_2O}],\ [\mathrm{OH}],\ [\mathrm{H_2}],\ [\mathrm{O_2}],\ [\mathrm{H}],\ [\mathrm{O}],\ [\mathrm{C}]. \tag{8}$$

In this case, to solve the forward problem we have to solve a system of $(q+1)=10$ equations and ensure balance in eq. 6. For the solution of the extended problem, a system of $((9+1)+1)\cdot(2+1)=33$ equations must be solved.

Implementation details

To verify the proposed model and to study the associated numerical phenomena, we used the fuel-oxidizer pair $\mathrm{CH_{1,956}}$ (kerosene) + $\mathrm{O_2}$ (liquid oxygen); data on combustion products are given in [11]. When preparing input for computation:

— we chose some value of the coefficient α, computed the corresponding molar fuel/oxidizer ratio, which was considered equal to ${}^{(1)}\dot{V}_O \big/ {}^{(1)}\dot{V}_F$ in the test computations;

— the temperature T of the combustion chamber for the chosen value of α was taken as the measured temperature ${}^{(1)}T$ [11].

The fuel in our test pair consists of $[\mathrm{C}]$ and $[\mathrm{H}]$. This must be known a priori, which is a limitation of the model. In this situation, we need to perform $n+1=3$ measurements of technical parameters for any oxidizer consumption. Therefore we prepared 3 sets of input data V_O, V_F, T for different values of α. The aim of the calculation is to find fuel composition (coefficients b_{iF}) and its enthalpy. In the considered test case, it should be $b_C=1$, $b_H=1.956$, $I_F=-1948\ \mathrm{kJ/kg}=-27237{,}7\ \mathrm{kJ/kmol}$. Fuel enthalpy is provided in two forms, because it is given in the first version while our calculations were performed using molar variables [5]. The molar mass of kerosene used for conversion is $\mu=13{,}9824\ \mathrm{kg/kmol}$.

At the first testing stage, the forward problem based on Equations (3), (4), (5) was solved. The solution method for the initial system of equations and the polynomials for computing enthalpies and entropies of combustion products are adopted as described in [2] and applied in [11]. Enthalpy balance between fresh and burnt gases serves as closure. Therefore, the error of enthalpy approximation was estimated. It is noted that the absolute approximation error for HCl at T=3000 K is ~0,008 kJ/mol compared to [7], which 17 % in relative terms [2]. The computed enthalpy is 0,464 kJ/mol. This is adopted as allowed tolerance, as it leads to an error of not more than 2.2 K when computing temperature. This is realistic. But comparison of enthalpies of our combustion products at T=3000 K computed according to [2] with the data from [7] yields somewhat different values, both the absolute and on the relative scale. The results of the comparison are given in Table 1.

As we can see from the data comparison, the differences are substantial. When formulating enthalpy balance in a combustion equation, the fresh gas enthalpies are taken from tables (exact), while the enthalpy of products is computed using polynomials (with an error) [2]. It is noted that the achieved accuracy, and hence, the point at which a computation can be stopped, was set by the error in determination of combustion products (partial pressures), and the remaining enthalpy misbalance is not discussed [2].

In the present model, enthalpy balance is the main criterion for the computation of the unknown fuel composition. Therefore, the necessity arose to verify, how accurately this balance is maintained during the computations [11]. The possibility of using available data for model verification also needed to be checked. For the chosen fuel-oxidizer pair, a number of computations for different ratios of components were carried out. The results are given in Table 2, together with the results of [11].

Table 1

Comparison of enthalpies of combustion products computed using polynomials from [1] and of the data from the tables in [6][*]

	$\Delta = I_P - I_T$, kJ/mol	$\varepsilon = \frac{I_P - I_T}{I_T} \cdot 100\,\%$
CO	–5,25	+45,2%
CO_2	–9,54	+4,1%
H_2O	–12,60	+12,5%
OH	–8,80	–6,4%
H_2	–8,29	–8,5%
O_2	–31,13	–29,2%
H	–4,23	–1,5%
O	–4,24	–1,4%
C	–2,59	–0,3%

Table 2

Comparison of results from [11] with the solution of the forward problem with enthalpy balance correction

		α=0,4		α=0,7		α=2,0	
		[5]	computation	[5]	computation	[5]	computation
kJ/kmol		$IT = -17588$		$IT = -18523$		$IT = -17112$	
		$I_{CP} = -7625$	$I_{CP} = -7584$	$I_{CP} = -22195$	$I_{CP} = -18520$	$I_{CP} = -25000$	$I_{CP} = -17096$
T, K		2124	2125	3065	3081	2855	2895
Partial pressures	P_{CO}	0,4868	0,4869	0,3458	0,3440	0,0618	0,0594
	P_{CO_2}	0,0181	0,0181	0,1108	0,1131	0,2036	0,2031
	P_{H_2O}	0,0783	0,0784	0,2744	0,2761	0,2127	0,2047
	P_{OH}	—	—	0,0551	0,0592	0,0660	0,0778
	P_{H_2}	0,4143	0,4143	0,1124	0,1094	0,0090	0,0082
	P_{O_2}	—	—	0,0180	0,0130	0,3952	0,3783
	P_H	0,0023	0,0022	0,0645	0,0638	0,0094	0,0098
	P_O	—	—	0,0189	0,0213	0,0422	0,0587
	P_C	—	—	—	—	—	—
	M_F		0,505		0,4571		0,2625

To correct for the enthalpy balance, the computations were performed until relative accuracy of $\sim 10^{-4}$ was reached. The data are provided for combustion chamber pressure of $P_{KC} = 1$ bar. Partial pressures are also measured in bar. As in [2], the computation is done such that partial pressures are equal to mole fractions of combustion products. Consumption rate of the combustion products is 1 kmol/s.

Comparison of results shows that at α=0,4, the computed temperature and enthalpy of products are close to the values provided [11]. For $\alpha = 0,7$ and $\alpha = 2,0$, temperature deviations are insignificant and amount for $\Delta T = 16$ K and $\Delta T = 40$ K, respectively, with relative errors of $\varepsilon \approx 0,5\,\%$ and

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[*] I_P — enthalpy computed using the model from [1]; I_T — looked up enthalpy from [7]

$\varepsilon \approx 1{,}4\,\%$. Enthalpies of combustion products have significant misbalance with fresh gas enthalpies: $20\,\%$ for $\alpha = 0{,}7$, and $\approx 46\,\%$ for $\alpha = 2{,}0$ [11]. Nevertheless, the partial pressures of combustion products are approximately equal in both cases.

We can conclude that

— the proposed model and of the (mathematical) accuracy of its results functionality should be performed using the corrected, compared to [11], temperatures evaluation;

— the data [11] can be considered as a hint for controlling the computed burnt gas composition;

— high sensitivity of the enthalpy of combustion products can lead to numerical instability when solving the system of nonlinear equations arising in the proposed model.

To solve the extended problem, points corresponding to $\alpha = 0{,}4;\ 0{,}7;\ 1{,}0$ are taken. The corresponding ratios of volumetric consumptions (7) are computed. Forward problems are solved, and the corresponding temperatures and burnt gas compositions are computed. With the proposed model being mathematically correct, the numerical solution procedure of the associated system of equations turned out to be numerically unstable, sensitive to initial approximations. To improve stability, one has to find some strong relation between unknown variables, which does not change while combustion products are being computed. To this aim, the ratio between the number of [C] and [H] atoms in the fuel at $\alpha = 1$ (stochiometric ratio of components), on one hand, (7) yields for $\alpha = 1$

$$\dot V_O / \dot V_F = \alpha\chi_0 = \chi_0 . \tag{9}$$

On the other hand, at the stochiometric ratio the maximum number of valences of oxidizing elements equals the maximum number of valences of reducing elements. Therefore, we can write the following balance for hydrocarbons and oxygen

$$C_{b\mathrm{C}}H_{b\mathrm{H}} + \frac{\dot V_O}{\dot V_F}\mathrm{O}_2 = b_\mathrm{C}\mathrm{CO}_2 + \frac{b_\mathrm{H}}{2}\mathrm{H}_2\mathrm{O}\,, \tag{10}$$

and derive from it atomic balance for oxygen:

$$2\frac{\dot V_O}{\dot V_F} = 2b_\mathrm{C} + \frac{b_\mathrm{H}}{2}\,. \tag{11}$$

This equation can be used as this one of the closing equations instead of an enthalpy equations (6). Thereby we can drop the computation of combustion products for one of the measurements, which accounts for 10 equations in the kerosene-oxygen system, so that the total number of equation reduces from 33 to 23. In practice, when maximum-temperature feedback control is used, the ratio of fuel and oxidizer volumetric consumption rates corresponding to the stochiometric ratio can be determined as follows:

— measured volumetric consumption rates at maximum temperature;

— from a few measurements (when possible, on both sides of the temperature maximum) one can establish an approximate dependence of temperature on the ratio between the volumetric consumption rates of fuel and oxidizer; based on this dependence, the ratio of the consumption rates for the maximum temperature is determined;

— combination of the first and the second method, with averaging of the found values provided they are different.

In the final version, the test computation was performed for two volumetric ratios: $\dot V_O^{(1)}/\dot V_F^{(1)} = 0{,}5956$ и $\dot V_O^{(2)}/\dot V_F^{(2)} = 1{,}0423$, corresponding to $\alpha^{(1)} = 0{,}4$ and $\alpha^{(2)} = 0{,}7$, and temperatures $T^{(1)} = 2125$ K and $T^{(1)} = 3081$ K (Table 2). The volumetric ratio at the stoichiometric ratio is assumed as $\dot V_O^{(steh)} / \dot V_F^{(steh)} = 1{,}489$.

The choice of m independent components out of the q species in the burnt gas mixture, using which one can formulate l independent reactions of formation of remaining $(q - m)$ species, is substantial for writing down equations (4). The easiest, most convenient and most consistent choice is to consider only the full dissociation of molecular components down to atoms. When solving the considered test problem, out of 9 possible components (8), $m = 3$ where chosen independent $[\mathrm{H}]$, $[\mathrm{O}]$, $[\mathrm{C}]$. From them, $l = 6$ independent reactions (4) of formation of the remaining dependent species were formulated: $[\mathrm{CO}]$, $[\mathrm{CO}_2]$, $[\mathrm{H}_2\mathrm{O}]$, $[\mathrm{OH}]$, $[\mathrm{H}_2]$, $[\mathrm{O}_2]$.

The final system of equation contains:

— two sets with 10 equations each based on (3), (4), (5), corresponding to the two measurements of temperature and volumetric consumption. Each set describes 9 unknown partial pressures (8) and M_F, corresponding to a specific measurement; two equations (6) corresponding to these same dimensions;

— equation (11).

Therefore we have a system of 23 algebraic equations, many of which are nonlinear. The solution should be found numerically. As unknowns, it is useful to take the logarithm of the actual variables. The logarithmic form ensures that the unknowns will not vanish for any temperature of pressure. It also excludes the possibility of appearance of negative partial pressures during the computation, which would have no physical meaning. It also improves numerical stability of the solution, which is found using Newton's method based on Taylor expansion up to power one. The derivatives are also determined with respect to the logarithms of the unknowns, rather than the unknowns themselves. Corrections are also done for the logarithms. To improve numerical stability, special measures are taken. The new approximation is computed by adding only a fraction of the computed correction to the previous value. The value of this fraction is given by the lower relaxation coefficient. It is chosen experimentally in the interval $[0...1]$, and given before the start of the computation. The pressure in the combustion chamber is $P_\Sigma = 1$ bar. The lower relaxation coefficient is $k = 0,4$ in all cases.

Table 3

Results of the extended model computation using equation (11)

	Init. approx.	5 iter.	10 iter.	15 iter.	20 iter.	Exact sol. (forward problem)	Data from Ref. [5]
1	2	3	4	5	6	7	8
$P^{(1)}_{\mathrm{CO}}$	1,0	0,6005	0,4944	0,4872	0,4867	0,4869	0,4432
$P^{(1)}_{\mathrm{CO}_2}$	1,0	0,0314	0,0190	0,0182	0,0181	0,0181	0,0203
$P^{(1)}_{\mathrm{H}_2\mathrm{O}}$	1,0	0,1393	0,0828	0,0789	0,0786	0,0784	0,1011
$P^{(1)}_{\mathrm{OH}}$	0,1	0,0001	0,0001	0,0001	0,0001	0,0001	0,0001
$P^{(1)}_{\mathrm{H}_2}$	0,1	0,5003	0,4208	0,4149	0,4145	0,4143	0,4332
$P^{(1)}_{\mathrm{O}_2}$	0,1	0,0000	0,0000	0,0000	0,0000	0,0000	0,0000
$P^{(1)}_{\mathrm{H}}$	0,1	0,0035	0,0023	0,0022	0,0022	0,0022	0,0023
$P^{(1)}_{\mathrm{O}}$	0,1	0,0000	0,0000	0,0000	0,0000	0,0000	0,0000
$P^{(1)}_{\mathrm{C}}$	0,1	0,0000	0,0000	0,0000	0,0000	0,0000	0,0000
$M^{(1)}_T$	1,0	0,5498	0,5082	0,5051	0,5049	0,5050	0,4910
$P^{(2)}_{\mathrm{CO}}$	1,0	0,4037	0,3480	0,3441	0,3438	0,3440	0,3172
$P^{(2)}_{\mathrm{CO}_2}$	1,0	0,1322	0,1144	0,1132	0,1131	0,1131	0,1042
$P^{(2)}_{\mathrm{H}_2\mathrm{O}}$	1,0	0,3353	0,2807	0,2767	0,2763	0,2761	0,3043
$P^{(2)}_{\mathrm{OH}}$	0,1	0,0622	0,0594	0,0592	0,0592	0,0592	0,0584
$P^{(2)}_{\mathrm{H}_2}$	0,1	0,1316	0,1111	0,1096	0,1095	0,1094	0,1213
$P^{(2)}_{\mathrm{O}_2}$	0,1	0,0128	0,0130	0,0130	0,0130	0,0130	0,0117
$P^{(2)}_{\mathrm{H}}$	0,1	0,0730	0,0645	0,0639	0,0638	0,0638	0,0641
$P^{(2)}_{\mathrm{O}}$	0,1	0,0221	0,0214	0,0213	0,0213	0,0213	0,0191
$P^{(2)}_{\mathrm{C}}$	0,1	0,0000	0,0000	0,0000	0,0000	0,0000	0,0000
$M^{(2)}_T$	1,0	0,4854	0,4591	0,4572	0,4571	0,4571	0,4464
b_{H}	1,0	2,0158	1,9631	1,9578	1,9574	1,9560	2,1808
b_{C}	1,0	0,9773	0,9976	0,9995	0,9996	1,0000	0,9438
I_F	–12000	–79699	–7223	–6567	–6517	–27238	–30527

Computation results are provided in Table 3. It contains:

Column 1:

P — partial pressure (bar);

M_F — number of kmol of fuels in the reaction required to obtain 1 kmol of combustion products;

$^{(1)}, ^{(2)}$— upper indices indicate the number of the measurement, to which the considered parameter belongs;

$b_{\mathrm{H}}, b_{\mathrm{C}}$ — number of hydrogen and carbon atoms in the fuel;

I_F — fuel enthalpy (kJ/mol).

Column 2: initial approximations.

Columns (3...6): computation data for the extended problem after 5, 10, 15, 20 steps, respectively.

Column 7: corrected data, obtained when solving the forward problem (Table 2), used for accuracy estimation of the considered problem (reference values).

Column 8: computation results for the extended problem obtained with the initial data (temperatures) from [11].

Results. The comparison results analysis provides the following issues:

— comparison of columns 6 and 7 shows that the solution is obtained with a high level of mathematical accuracy, i.e. the model does not yield any distortions related to assumptions or numerical errors. Insignificant deviations (in the fourth digit) can be explained by the fact that the reference values (column 7) were obtained with the same accuracy;

— fast convergence of computation results (columns 3...6) allows an indirect conclusion that the numerical solution is highly stable

— test computations and comparison of results (columns 7 and 8) demonstrate high sensitivity and significant error when determining quantitative fuel composition and enthalpy. But the error in the determined burnt gas composition is not that large (it is observed when solving the forward problem), and in this case they do not exceed half of the second significant digit, which corresponds to relative error of ~ 0,05 (engineering accuracy).

Conclusions.

— the mathematical model based on equations of the type (3...6), (11) for gaseous fuel allows determining its quantitative composition, enthalpy, burnt gas composition using as input variables some measured technical parameters (consumption rates of fresh gases and corresponding temperatures in the combustion chamber) and the known elemental (qualitative) composition of the fuel ([C], [H], [O], etc.);

— the mathematical accuracy of the model allows applying the obtained data to estimate the sensitivity of computation results on the inaccuracy of the measurement channel of initial technical parameters;

— when solving real technical problems, enthalpies and entropies of combustion products must be determined based on tables of type [12] or using software packages, tabulating databases of similar type. Polynomial dependencies for calculation of enthalpy and entropy of combustion products described cannot be used for solving the extended problem due to substantial approximation error [2].

Literature

1. Brunetkin, A.I. Identification of quantitative composition of an unknown gaseous fuel and its combustion products based on the measured parameters of technological process of fuel combustion / A.I Brunetkin, M.V. Maximov, A.V. Bondarenko // Вісник НТУ “ХПІ”. Сер.: Енергетичні та теплотехнічні процеси й устаткування. — 2014. — № 12(1055). — С. 131 — 142.
2. Boisvert, P.G. Fuel sparing: Control of industrial furnaces using process gas as supplemental fuel / P.G. Boisvert, A. Runstedtler // Applied Thermal Engineering. — 2014. — Vol. 65, Iss. 1-2. — PP. 293 — 298.
3. The major sources of gas flaring and air contamination in the natural gas processing plants: A case study / M. Davoudi, M.R. Rahimpour, S.M. Jokara et al // Journal of Natural Gas Science and Engineering. — 2013. — Vol. 13 — PP. 7 — 19.
4. Berghout, N. Techno-economic performance and challenges of applying CO_2 capture in the industry: A case study of five industrial plants / N. Berghout, M. van den Broek, A. Faaij // International Journal of Greenhouse Gas Control. — 2013. — Vol. 17. — PP. 259 — 279.

5. Liu, H. Optimization of PEM fuel cell flow channel dimensions—Mathematic modeling analysis and experimental verification / H. Liu, P. Li, K. Wang // International Journal of Hydrogen Energy. — 2013. — Vol. 38, Iss. 23. — PP. 9835 — 9846.
6. Possibilities for reconstruction of existing steam boilers for the purpose of using exhaust gases from 14 MW or 17 MW gas turbine / D. Tucakovic, G. Stupar, T. Zivanovic et al. // Applied Thermal Engineering. — 2013. — Vol. 56, Iss. 1-2. — PP. 83 — 90.
7. Rusinowski, H. Hybrid model of steam boiler / H. Rusinowski, W. Stanek // Energy. — 2010. — Vol. 35, Iss. 2. — PP. 1107 — 1113.
8. Bujak, J. Optimal control of energy losses in multi-boiler steam systems / J. Bujak // Energy. — 2009. — Vol. 34, Iss. 9. — PP. 1260 — 1270.
9. Бондаренко, А.В. Моделирование образования продуктов сгорания газообразного углеводородного топлива / А.В. Бондаренко // Судовые энергетические установки. — 2014. — Вып. 31. — С. 178 — 186.
10. Давыдов, В.О. Метод расчета температуры горения произвольной смеси газообразного углеводородного топлива при произвольном избытке воздуха / В.О. Давыдов, А.В. Бондаренко // Пр. Одес політехн ун-ту. — 2013. — Вып. 3(42). — С. 98 — 101.
11. Максимов, М.В. Модель и метод определения условной формулы углеводородного топлива при сжигании / М.В. Максимов, А.И. Брунеткин, А.В. Бондаренко // Восточно-Европейский журнал передовых технологий. — 2013. — Т. 6, № 8(66). — С. 20 — 27.
12. Математическая модель сжигания несертифицированных видов топлива / Т.С. Добровольская, М.В. Максимов, В.Ф. Ложечников, А.В. Бондаренко // Восточно-Европейский журнал передовых технологий. — 2014. — Т. 2, № 8(68). — С. 44 — 51.

References

1. Brunetkin, A.I. Identification of quantitative composition of an unknown gaseous fuel and its combustion products based on the measured parameters of technological process of fuel combustion / A.I Brunetkin, M.V. Maximov, A.V. Bondarenko // Visnyk NTU “KhPI”. Ser.: Enerhetychni ta teplotekhnichni protsesy y ustatkuvannia [Bull. NTU “KhPI”. Series: Energy and Thermal processes and equipment]. — H.: NTU “KhPI” 2014. — № 12 (1055). — pp. 131 — 142. (in Russian).
2. Boisvert, P.G. Fuel sparing: Control of industrial furnaces using process gas as supplemental fuel, Canada [Text] / P. G. Boisvert, A. Runstedtler// Applied Thermal Engineering. — 2014. — Vol. 65. — pp. 293 — 298.
3. The major sources of gas flaring and air contamination in the natural gas processing plants: A case study, Iran [Text] / M. Davoudia, M. R. Rahimpoura, S. M. Jokara, F. Nikbakhtb, H. Abbasfard // Journal of Natural Gas Science and Engineering. — 2013. — Vol. 13 — pp. 7 — 19.
4. Berghout, N. Techno-economic performance and challenges of applying CO2 capture in the industry: A case study of five industrial plants, the Netherlands [Text] / N. Berghout, M. Broek, A. Faaij // International Journal of Greenhouse Gas Control. — 2013. — Vol. 17. — pp. 259 — 279.
5. Liu, H. Optimization of PEM fuel cell flow channel dimensions—Mathematic modeling analysis and experimental verification, USA [Text] / H. Liu, P. Li, K. Wang // International Journal of Hydrogen Energy. — 2013. — Vol. 38. — pp. 9835 — 9846.
6. Possibilities for reconstruction of existing steam boilers for the purpose of using exhaust gases from 14 MW or 17 MW gas turbine, Serbia [Text] / D. Tucakovica, G. Stupara, T. Zivanovica, M. Petrovica, S. Belosevic // Applied Thermal Engineering. — 2013. — Vol. 56. — pp. 83 — 90.
7. Rusinowski, H. Hybrid model of steam boiler, Poland [Text] / H. Rusinowski, W. Stanek // Energy. — 2010. — Vol. 35. — pp. 1107 — 1113.
8. Bujak, J. Optimal control of energy losses in multi-boiler steam systems, Poland [Text] / J. Bujak // Energy. — 2009. — Vol. 34. — pp. 1260 — 1270.
9. Bondarenko, A.V. Modelirovanie obrazovaniya produktov sgoraniya gazoobraznogo uglevodorodnogo topliva [Simulation of formation of combustion products of gaseous hydrocarbon fuel] / A.V. Bondarenko // Sudovye energeticheskie ustanovki [Ship Power Plants]. — Odessa, 2013. — Vol. 31. — pp. 178 — 187. (in Russian).
10. Davydov, V.O. Metod rascheta temperatury goreniya proizvol’noy smesi gazoobraznogo uglevodorodnogo topliva pri proizvol’nom izbytke vozdukha [Method of calculating the combustion temperature of any mixture of gaseous hydrocarbon fuel for arbitrary excess air] / V.O. Davydov, A.V. Bondarenko //

Pratsi Odeskoho politekhnichnoho universytetu [Proc. Odesa Polytechnic. Univ.] — Odessa, 2013. — Iss. 3 (42), — pp. 98 — 101. (in Russian).

11. Maximov, M.V. Model' i metod opredeleniya uslovnoy formuly uglevodorodnogo topliva pri szhiganii [Model and method for determining the conditional formula of hydrocarbon fuel combustion] / M.V. Maximov, A.I. Brunetkin, A.V. Bondarenko // Vostochno-Evropeyskiy zhurnal peredovykh tekhnologiy [East Eur. Journal of Advanced Technologies]. — 2013. — Vol. 6, # 8 (66). — pp. 20 — 27. (in Russian).
12. Matematicheskaya mofel' szhiganiya nesertifitsirovannykh vidov topliva [Mathematical model of burning uncertified fuels] / M.V. Maksimov, V.F. Lozhechnik, T.S. Dobrovol'skaya, A.V. Bondarenko // Vostochno-Evropeyskiy zhurnal peredovykh tekhnologiy [East Eur. Journal of Advanced Technologies]. — 2014. — Vol. 2. — pp. 44 — 51. (in Russian).

АНОТАЦІЯ / АННОТАЦИЯ / ABSTRACT

О.І. Брунеткін, А.В. Бондаренко, О.В. Лисюк. **Визначення кількісного складу невідомого газоподібного палива і продуктів згоряння на основі виміряних технологічних параметрів в процесі горіння.** Існує широкий спектр і значний потенціал альтернативних (несертифікованих) видів газового палива. Невизначеність і гнучкість складу нетрадиційних видів палива серйозно обмежує можливі експлуатації цих джерел енергії. Запропоновано математичну модель, засновану на рівняннях хімічної термодинаміки, що дозволяють обчислити склад продуктів згоряння в умовах неоптимального співвідношення паливо — окислювач, і обчислювальний метод визначення складу палива в процесі згоряння, тим самим дозволяючи визначити оптимальні параметри горіння. Обговорюються обмеження підходу. Також запропоновано розв'язання зворотного завдання, а саме: визначення кількісного складу та калорійності (ентальпії) продуктів згоряння на підставі відомого якісного складу продуктів згоряння, а також виміряного обсягу їх потоку і температури (виміряних технологічних параметрів). Проведено оцінку запропонованої моделі, встановлено її обмеження.

Ключові слова: нетрадиційні палива, гнучкість палива, продукти згоряння, математична модель, рівняння хімічної термодинаміки.

А.И. Брунеткин, А.В. Бондаренко, А.В. Лысюк. **Определение количественного состава неизвестного газообразного топлива и продуктов сгорания на основе измеренных технологических параметров в процессе горения.** Существует широкий спектр и значительный потенциал альтернативных (несертифицированных) видов газового топлива. Неопределенность и гибкость состава нетрадиционных видов топлива серьезно ограничивает возможные эксплуатации этих источников энергии. Предложены математическая модель, основанная на уравнениях химической термодинамики, позволяющих вычислить состав продуктов сгорания в условиях неоптимального соотношения топливо — окислитель, и вычислительный метод определения состава топлива в процессе сгорания, что позволяет определить оптимальные параметры горения. Также предложено решение следующей обратной задачи: определение количественного состава и калорийности (энтальпии) продуктов сгорания на основании известного качественного состава продуктов сгорания, а также их измеренного объема потока и температуры (измеренных технологических параметров). Проведена оценка предложенной модели, установлены её ограничения.

Ключевые слова: нетрадиционные топлива, гибкость топлива, продукты сгорания, математическая модель, уравнения химической термодинамики.

A.I. Brunetkin, A.V. Bondarenko, A.V. Lysyuk. **Determining the quantitative composition of an unknown gaseous fuel and combustion products from the measured process parameters in the fuel combustion process.** There exists a wide range and a considerable potential of alternative (non-certified) gas fuel types. Uncertainty and flexibility of non-conventional fuels' composition seriously limits the possible exploitation of these energy sources. Therefore developed are both a mathematical model based on the chemical thermodynamics equations, allowing to calculate the composition of the combustion products in terms of suboptimal ratio of fuel — oxidizer, and a computational method for determining the composition of fuel in the combustion process, thus allowing to determine the optimal parameters of combustion. The limitations of the approach are being discussed. Also suggested is the solution of the inverse problem, namely, the determination of the composition and caloric content (enthalpy) of combustion products on the basis of combustion products and their measured volume known qualitative composition flow and temperature (measured process parameters). An assessment of the proposed model being effected, its limitations have been found.

Keywords: unconventional/alternative fuel, fuel flexibility, combustion products, mathematical model, equations of chemical thermodynamics.

Reviever Dr. techn. sciences, Prof. of Odesa nat. polytechnic univ. Maksimov M.V.

Received May 6, 2014