

DETERMINING THE COMPOSITION OF HIGH TEMPERATURE COMBUSTION PRODUCTS OF FOSSIL FUEL BASED ON VARIATIONAL PRINCIPLES AND GEOMETRIC PROGRAMMING

by

Velibor V. VUJOVIĆ

Laboratory of Physics, Vinča Institute of Nuclear Sciences, Belgrade, Serbia

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This paper presents the algorithm and results of a computer program for calculation of complex equilibrium composition for the high temperature fossil fuel combustion products. The method of determining the composition of high temperatures combustion products at the temperatures appearing in the open cycle MHD power generation is given. The determination of combustion product composition is based on minimization of the Gibbs free energy. The number of equations to be solved is reduced by using variational principles and a method of geometric programming and is equal to the sum of the numbers of elements and phases. A short description of the computer program for the calculation of the composition and an example of the results are also given.

Key words: *composition high temperature combustion products, chemical and phase equilibrium, minimization Gibbs free energy, variational principles, geometric programming*

Introduction

The analysis and forecast of the development of energy have said that the main sources of primary energy in the foreseeable future remain the fossil fuels. Research and development work on new energy technologies is mainly directed to processes with higher efficiencies. In electric power generation an increase in efficiency can be achieved by increasing the working fluid temperature. High temperature products are obtained in an open magnetohydrodynamic cycle (MHD) facilities, as well as in the high temperature pyrolysis and gasification of coal. In the open cycle MHD power generation [1, 2] the working fluid can reach the values of up to 3100 K. In order to investigate the processes in the components of MHD facilities, it is necessary to know the composition and properties of fossil fuel combustion products. In a general case, combustion products can be a multiphase system of compounds and elements; at higher temperatures of electrons and ions, as well. Due to the large number of combustion product components and to the various chemical reactions and phase changes taking place within them, the determination of the equilibrium composition is a complex task.

* Corresponding author, e-mail: vvejo@vinca.rs

This paper is dedicated to the memory of **Aleksandar Popović** and **Alija Lekić**, the two doyen of the Energoinvests MHD-program (realized in Sarajevo in the period 1979-1991) and which, unfortunately, are not with us any more.

It requires considerable numerical calculations. There are two approaches to the determination of the system of equations describing the equilibrium state: (a) equilibrium constant formulation, and (b) Gibbs free energy minimization. The application of both approaches results in a system of non-linear equations which can be solved by different numerical methods. Some methods for reducing the number of equations to be solved when determining the minimum of the Gibbs free energy have been used [3-8]. Variational principles and the geometric programming method [9] are used in this work.

Definition of combustion product composition

Generally, fossil fuel combustion products represent a mixture which may consist of several phases. The biggest number of the phases usually occurs in the combustion products of coal. The condition for an equilibrium state of the mixture at the constant pressure and the constant temperature is:

$$dG_{T,P} = 0 \quad (1)$$

where G is the Gibbs free energy. The Gibbs free energy for a multiphase system is equal to the sum of the individual phases for which it is assumed to be homogeneous. When expressing the Gibbs free energy of each component through the chemical potential, the equation for the Gibbs free energy of a multiphase system can be written in the following form:

$$G = \sum_k \sum_i \mu_i^k n_i^k \quad (2)$$

where μ_i^k is the chemical potential of one mole of the component i in phase k and n_i^k is the number of moles.

The chemical potential of gaseous components, assuming that the gaseous phase behaves as an ideal mixture of gases, can be determined using the expression:

$$\mu = \mu_i^0 + RT \ln \frac{n_i}{n} + RT \ln p_n \quad (3)$$

where μ_i^0 is the chemical potential in the standard state, R – the universal gas constant, T – the temperature, n – the total number of moles in a phase, and p_n – the pressure with respect to the pressure in the standard state $p_n = p/p^0$ (the standard state for gases is the ideal gas on the $p^0 = 0.101032$ MPa).

With the assumption that the condensed phases behave as ideal solutions, the chemical potential of condensed components can be determined on the basis of the relationship:

$$\tilde{\mu}_i = \tilde{\mu}_i^0 + RT \ln \frac{\tilde{n}_i}{\tilde{n}} \quad (4)$$

where \tilde{n} is the total number of moles of the condensed phases.

Assuming that combustion products can be considered as a two-phase system, the Gibbs free energy of combustion products is:

$$G = \sum_{i=1}^m n_i \left(\mu_i^0 + RT \ln \frac{n_i}{n} + RT \ln p_n \right) + \sum_{i=m+1}^N \tilde{n}_i \left(\tilde{\mu}_i^0 + RT \ln \frac{\tilde{n}_i}{\tilde{n}} \right) \quad (5)$$

where m is the number of components in the gaseous phase, N – the total number of components, and the symbol \sim refers to the condensed phase.

In order to determine the composition of the above defined two-phase system in the state of chemical equilibrium, in addition to condition (1) a balance of all the elements contained in the combustion products must be fulfilled:

$$\sum_{i=1}^m a_{ij} n_i + \sum_{i=m+1}^N a_{ij} \tilde{n}_i - a_{0j} = 0, \quad j=1,2,\dots,l \quad (6)$$

where a_{ij} is the number of atoms of j -th element in the molecule i -th component, a_{0j} – the total number of atoms of j -th element in combustion products, and l – the number of elements in combustion products.

The condition of the balance of moles in both phases is to be satisfied as well:

$$\sum_{i=1}^m n_i - n = 0 \quad (7)$$

and

$$\sum_{i=1}^m \tilde{n}_i - \tilde{n} = 0 \quad (8)$$

From eqs. (1) and (5)-(8) it follows that it is necessary to solve the system of $N + l + 2$ non-linear equations in order to determine the composition of combustion products. The number of equations to be solved can be reduced by applying the law of mass action [4], or using the Newton-Raphson method and substituting the equations resulting from it [5]. The reduction of the number of equations can be also achieved by applying the geometric programming method.

Algorithm for calculating composition of combustion products

Let us define the function ν as:

$$\nu = \exp\left(-\frac{G}{RT}\right) \quad (9)$$

which, after substituting eq. (5) for the Gibbs free energy becomes:

$$\nu = \prod_{i=1}^N \left(\frac{c_i}{n_i}\right)^{n_i} n^n \tilde{n}^{\tilde{n}} \quad (10)$$

where

$$c_i = \frac{1}{p_n} \exp\left(-\frac{\mu_i^0}{RT}\right) \quad (11)$$

for gaseous components, and

$$\tilde{c}_i = \exp\left(-\frac{\tilde{\mu}_i^0}{RT}\right) \quad (12)$$

for condensed components.

The minimum of the Gibbs free energy with the constraints (6)-(8) corresponds to the maximum of the function ν , as defined by the eq. (10), with the same constraints.

According to the theory of geometric programming [9], the function ν with the constraints (6)-(8) represents a dual function, the direct criterion function which has the form:

$$g_0 = \prod_{j=1}^l t_j^{a_{0j}} \quad (13)$$

where t is the independent variable of the direct criterion function.

The constraints (6)-(8) are then transformed into the two constraints:

$$g_1 = \sum_{i=1}^m c_i \prod_{j=1}^l t_j^{a_{ij}} = 1 \quad (14)$$

and

$$g_2 = \sum_{i=m+1}^N \tilde{c}_i \prod_{j=1}^l t_j^{a_{ij}} = 1 \quad (15)$$

which actually represents the conditions for the balance of molar proportion for the gaseous and condensed phase, respectively:

$$\sum_{i=1}^m x_i = 1 \quad (16)$$

and

$$\sum_{i=m+1}^N \tilde{x}_i = 1 \quad (17)$$

where x_i and \tilde{x}_i are molar part components in the gaseous and condensed phase.

The maximum of the function ν with the constraints (6)-(8) corresponds to the minimum of the function g_0 with the constraints (14) and (15). The determination of the minimum of the function g_0 with constraints (14) and (15) can be transformed to the determination of the minimum of a function:

$$f = g_0 + \lambda_1 g_1 + \lambda_2 g_2 \quad (18)$$

where λ_1 and λ_2 are Lagrangian multipliers.

According to the theory of geometric programming [9], a relationship between the values of the independent variables of the direct criterion function and the corresponding values of the dual function exists in the extreme points.

From that relationship it follows that the mole fraction of components are:

$$x_i = c_i \prod_{j=1}^l t_j^{a_{ij}} \quad (19)$$

for gaseous components, and

$$\tilde{x}_i = \tilde{c}_i \prod_{j=1}^l t_j^{a_{ij}} \quad (20)$$

for condensed components.

In order to determine the fraction of the condensed phase in combustion products, the number of moles of the gaseous and condensed phase is to be calculated by using two corresponding equations of elements balance, *i. e.* any two of eqs. (6).

Taking into account that:

$$n_i = x_i n \quad (21)$$

and

$$\tilde{n}_i = \tilde{x}_i \tilde{n} \quad (22)$$

from the balance of any two elements it is obtained:

$$n \sum_{i=1}^m a_{ij1} x_i + \tilde{n}_i \sum_{i=m+1}^N a_{ij1} \tilde{x}_i - a_{0j1} = 0 \quad (23)$$

and

$$n \sum_{i=1}^m a_{ij2} x_i + \tilde{n}_i \sum_{i=m+1}^N a_{ij2} \tilde{x}_i - a_{0j2} = 0 \quad (24)$$

Solving the eqs. (23) and (24) we have obtained the expressions for the numbers of moles in the gaseous and condensed phase:

$$n = \frac{a_{0j1} \sum_{i=m+1}^N a_{ij2} \tilde{x}_i - a_{0j2} \sum_{i=m+1}^N a_{ij1} \tilde{x}_i}{\sum_{i=1}^m a_{ij1} x_i \sum_{i=m+1}^N a_{ij2} \tilde{x}_i - \sum_{i=1}^m a_{ij2} x_i \sum_{i=m+1}^N a_{ij1} \tilde{x}_i} \quad (25)$$

and

$$\tilde{n} = \frac{a_{0j2} \sum_{i=1}^m a_{ij1} x_i - a_{0j1} \sum_{i=1}^m a_{ij2} x_i}{\sum_{i=1}^m a_{ij1} x_i \sum_{i=m+1}^N a_{ij2} \tilde{x}_i - \sum_{i=1}^m a_{ij2} x_i \sum_{i=m+1}^N a_{ij1} \tilde{x}_i} \quad (26)$$

On the basis of the previous considerations it follows that the problem of determining the Gibbs free energy minimum (5), with the constraints of (6), (7) and (8), which requires the solution of $N + l + 2$ non-linear equations, has been reduced to the determination of the minimum of the functions f (18) with $l + 2$ non-linear equations. In case of a MHD open cycle working fluid this means solving a system of 6-14 non-linear equations instead of a system of 50-60 non-linear equations.

Different methods can be used for the computation of the minimum of function f . In this paper the Newton-Raphson method has been used.

Computer programme

Based on the methodology and equations given in the previous chapter, a computer program for the calculation of the composition has been developed [10]. A slightly modified Blau program [11] for geometric programming is used for computation of the minimum of the direct criterial function with the constraints (14) and (15), *i. e.* for the computation of the values of the independent variables of that function at the point of the minimum. When applying the Newton-Raphson method, the initial values for all the independent variables are taken to be $10^{-5.5}$. Those values are selected on the basis of the numerous calculations of the composition of gaseous, liquid, and solid fuel combustion products, and are used for the calculation of the composition of gaseous combustion products, *i. e.* for the gaseous phase in multiphase combustion products, for the first value of temperature.

When calculating the composition of combustion products with the condensed phase, the values of the independent variables obtained by the calculation for the gaseous

phase only for the same temperature and pressure are used as the initial values of the independent variables for the first value of temperature. The resulting values from the preceding calculations are used as the initial values of the independent variables for other temperatures.

The initial Lagrangian multipliers ($\lambda_1 = -2.45$ and $\lambda_2 = 0.0003$) are selected on the basis of the analysis of the number of iterations required for determining the minimum criterial function.

Existing programs can, with minor modifications, be used to estimate the composition of the system that contains more than two phases. In this case you should increase the number of constraints on the direct criterial function and the number of equations for determining the number of moles of different phases. The maximum number of phases, including gaseous, with which it can be counted is equal to the number of elements contained in the combustion products.

The input data necessary for determining the composition of combustion products form an integral part of the program. The program entered the data for the 139 components in gaseous and 38 components in the condensed state. The components comprise 19 elements. Input data for the components and elements may be updated, *i. e.* can be increased the number of components that account.

Result of calculation

As already stated, the program can be used for the calculation of the products of the combustion of fossil fuels in the case of the gaseous products of combustion or of the two phase products of combustion. The value of Lagrangian multipliers λ_2 points to the existence of the condensed phases, *i. e.* if λ_2 has a negative value in the combustion products, it is the condensed phases, and if λ_2 has a positive value in the combustion products the condensed phase can not exist.

The paper gives a comparative analysis of the calculation results obtained by this computer program with the results obtained by a similar computer program which has been developed at the Institute of High Temperatures (IVTAN), Moscow, Russia [12].

The significant differences between these methods concern the mathematical setting of the problem and the methods used in solving it.

The IVTAN method includes a group expansion for the pressure, balance relation to the initial atoms and conditions of the heterogeneous chemical equilibrium for the components of the condensed phases. The gaseous phase is treated as a chemically reacting mixture of ideal gases, while for describing of the condensed phases uses the model of mutually insoluble pure substances. The basic mathematical problem of the IVTAN methodology is related to the solution of non-linear equations. For solving systems of equations they use the Newton's modified method of linearization.

As an example of the calculations, the combustion products of Kuznetskii coal are selected.

For the calculation of the composition of high temperature combustion products Kuznetskii coal was used, with the following results of the technical analysis (weight parts): C = 0.700, H = 0.050, S = 0.050, O = 0.079, N = 0.019, ash = 0.117, and humidity = 0.030; and the composition of the ash: SiO₂ = 0.476, Fe₂O₃ = 0.146, Al₂O₃ = 0.243, CaO = 0.054, MgO = 0.019, SO₃ = 0.029, Na₂O = 0.017, and K₂O = 0.016. As an oxidizer, the air without preheating was used, where the surplus oxidizer was $\alpha = 1$.

Since it is a high-temperature product to be used in the process of MHD energy conversion, it is assumed that dry potassium carbonate (K_2CO_3) was added to the combustion products so that the mass content of potassium (K) in all products is 1%. It is also assumed that the products during the combustion process allocate 80% of the ash in the form of liquid slag.

The relative content of the atoms of certain elements in such a mixture amounted to: C = 0.07689, H = 0.06827, O = 0.18908, N = 0.65738, Ar = 0.00426, K = 0.00347, S = 0.00021, Al = 0.00014, Si = 0.00019, Ca = 0.00003, Fe = 0.00005, Mg = 0.00001, and Na = 0.00001.

It is taken that 48 gaseous components can occur in the products of combustion, and they are: e^- , C, S, H, N, Al, Si, Ca, Fe, O, Mg, Na, K, Ar, O_2 , OH, NO, NO_2 , AlO, Al_2O , N_2 , H_2 , H_2O , CO, CO_2 , HO_2 , H_2O_2 , N_2O , S_2 , SO, SO_2 , SO_3 , SiO, SiO_2 , MgO, CaO, KO, KOH (KOH) $_2$, NaOH, $Fe(OH)_2$, O^- , Na^+ , K^+ , O_2^- , OH^- , NO_2^- , and AlO_2^- ; 7 components in the condensed state: Al_2O_3 , Fe_2O_3 , CaO, MgO, K_2SiO_3 , K_2SO_4 , and KOH.

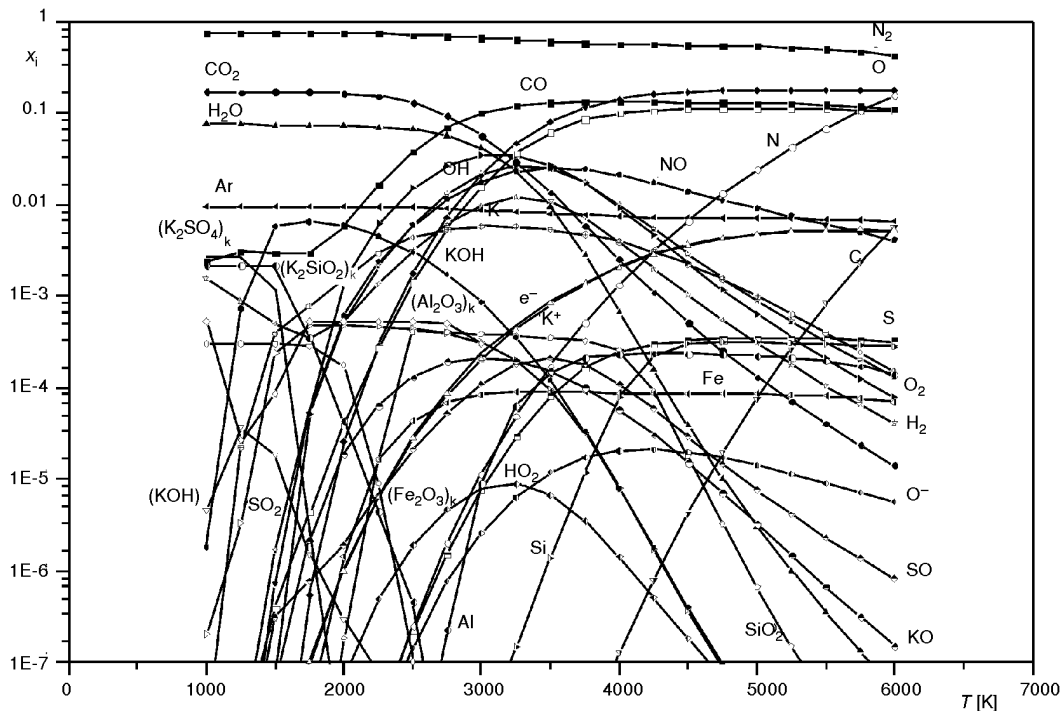


Figure 1. The computer results of the calculation of the combustion product composition of Kuznetskii coal (with the addition of ionizing seed) in the air, for the field temperature of 1000-6000 K at the pressure of 0.1 MPa

Figure 1 provides an overview of the calculation results of the combustion product composition of Kuznetskii coal (with the addition of ionizing seed) in the air for the field temperature of 1000-6000 K at the pressure of 0.1 MPa – obtained by our computer program.

A detailed comparison of the calculation results obtained by this program with the results obtained by IVTAN realized for the pressure 0.1 MPa and 1.0 MPa and temperature range of 1000-3500 K is given in [10].

The results of calculation for the gas phase composition, for the pressure of 0.1 MPa and the reference temperature of 3500 K and 1500 K are given in tab. 1. Table 2 presents the composition of the condensed phase for temperatures of 1500 K and 1000 K.

Table 1. Composition of the gaseous components of Kuznetskii coal combustion products for $p = 0.1$ MPa (mole fractions)

Components	3500 K		1500 K	
	This paper	IVTAN [10]	This paper	IVTAN [10]
e ⁻	8.37-04	8.37-04	5.66-09	5.77-09
C	1.94-09	1.94-09	7.22-25	6.39-25
S	8.23-05	8.22-05	2.73-10	4.44-10
H	6.17-02	6.17-02	4.11-07	3.98-07
N	1.71-04	1.71-04	5.21-14	5.21-14
Al	6.09-05	6.09-05	1.97-21	4.44-21
Si	3.43-08	3.43-08	1.22-26	2.12-26
Ca	4.62-05	4.62-05	1.16-15	1.55-14
Fe	9.32-05	9.32-05	2.48-10	9.36-10
O	8.10-02	8.10-02	1.02-09	1.09-09
Mg	1.44-05	1.44-05	1.73-13	6.94-12
Na	1.87-05	1.83-05	9.40-06	9.23-06
K	5.34-03	5.34-03	4.28-04	4.44-04
Ar	7.94-03	7.94-03	9.56-03	9.56-03
O ₂	2.70-02	2.70-02	6.39-08	7.23-08
OH	2.46-02	2.46-02	1.57-06	1.62-06
NO	2.51-02	2.51-02	6.53-07	6.95-07
NO ₂	3.93-06	3.93-06	1.94-12	2.20-12
AlO	1.99-04	1.99-04	1.51-18	3.62-18
Al ₂ O	4.23-07	4.23-07	6.22-27	3.35-26
N ₂	6.00-01	6.00-01	7.37-01	7.37-01
H ₂	1.09-02	1.09-02	5.43-04	5.09-04
H ₂ O	9.53-03	9.53-03	7.30-02	7.28-02
CO	1.30-01	1.30-01	3.27-03	3.08-03
CO ₂	1.36-02	1.36-02	1.69-01	1.70-01
HO ₂	6.68-06	6.68-06	5.00-12	2.98-12
H ₂ O ₂	5.27-08	5.27-08	3.88-12	4.12-12
N ₂ O	1.29-06	1.29-06	3.88-11	4.13-11
S ₂	8.62-09	8.62-09	4.44-11	1.18-10
SO	2.14-04	2.14-04	3.70-07	6.40-07
SO ₂	9.54-05	9.55-05	2.55-04	4.71-04
SO ₃	8.44-09	8.44-09	2.40-09	4.70-09
SiO	3.45-04	3.45-04	2.15-14	3.96-14
SiO ₂	8.77-06	8.78-06	1.53-14	3.00-14
MgO	4.22-06	4.22-06	6.79-15	2.90-13
CaO	9.73-06	9.73-06	1.34-16	1.91-15
KO	1.52-04	1.52-04	5.71-08	6.31-08
KOH	1.21-04	1.21-04	6.02-03	6.44-03
(KOH) ₂	3.60-12	3.60-12	1.90-05	2.17-05
NaOH	1.22-07	1.25-07	1.30-05	1.32-07
Fe(OH)	8.07-09	8.05-09	2.42-07	9.59-07
O ⁻	1.20-05	1.21-05	5.60-15	6.07-15
Na ⁺	2.14-07	2.15-07	2.61-13	2.51-13
K ⁺	8.54-04	8.54-04	5.72-09	5.83-09
O ₂ ⁻	4.43-07	4.43-07	3.64-16	4.20-16
OH ⁻	4.46-08	4.46-08	5.25-11	5.51-11
NO ₂ ⁻	1.09-08	1.10-08	1.09-14	1.26-14
AlO ₂ ⁻	3.19-07	3.19-07	1.85-17	4.81-17

Table 2. Composition of the condensed components of Kuznetskii coal combustion products for $p = 0.1$ MPa (mass fractions)

Components	1500 K		1000 K	
	This paper	IVTAN [10]	This paper	IVTAN [10]
Al ₂ O ₃	5.18-04	5.27-04	5.24-04	5.27-04
Fe ₂ O ₃	2.89-04	2.92-04	2.93-04	2.95-04
CaO	1.22-04	1.24-04	1.23-04	1.24-04
MgO	2.90-05	2.97-05	2.90-05	2.97-05
K ₂ SiO ₃	2.13-03	2.16-03	2.15-03	2.16-03
K ₂ SiO ₄	1.21-03	0	2.69-03	2.70-03
KOH	2.50-05	0	8.96-03	8.24-03

As seen from tab. 1, at the temperature of 3500 K and pressure of 0.1 MPa at high temperature gaseous products only the gaseous phase exists and the matching of the calculation results for both calculations is full for basic components which have significant molar shares, and for the components whose mole fraction is very small. Somewhat worse agreement of the results was present at lower temperatures, the temperature of 1500 K in this case, especially for the components whose mole fraction of components was small. This can be explained by different models for the condensed phase. It should be noted that this difference increases with reducing the presence of these components in the gaseous phase.

From tab. 2 it is also seen that there is a difference in the calculation results obtained with one and the other programs, which is, as noted above, a consequence of different models for the condensed phase.

Conclusions

It has been shown that it is possible to considerably reduce the number of equation to be solved, when determining the composition of fossil fuel combustion products based on minimization of the Gibbs free energy, by applying the variational principles and geometric programming.

For the system of non-linear equations obtained in this way may be solved by some of the numerical procedures – in our case the Newton-Raphson method is used. The initial values of the independent variables and the Lagrangian multipliers used in the calculations are determined on the basis of a numerous calculations of the composition of gaseous, liquid, and solid fuel combustion products.

We have developed a computer program for calculating the composition of the monophase and two-phase combustion products of the fossil fuels. This program can, with minor modifications, be used to estimate the composition of the systems that contain more than two-phases.

The paper gives a comparison of the calculation results obtained by this computer program with the results of calculations of the combustion products of the Kuznetskii coal obtained in the Institute of High Temperatures (IVTAN), Moscow, Russia. As was expected, different methods and programs to calculate the composition for the same initial data and the same models of gaseous and condensed phases does not lead to significant differences in the results of calculations.

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Nomenclature

a_{ij}	– number of atoms of j -th element in the molecule i -th component, [–]	p_n	– pressure with respect to the pressure in the standard state, [MPa]
a_{0j}	– total number of atoms of j -th element in combustion products, [–]	T	– temperature, [K]
f	– dual function defined with eq.(18), [–]	t	– independent variable of the direct criterion function, [–]
G	– Gibbs free energy, [kJkmol]	R	– universal gas constant, [kJkmol ⁻¹ K ⁻¹]
g_0	– direct criterion function, [–]	x_i	– mole fraction of components in the gaseous phase, [–]
l	– number of elements in combustion products, [–]	\tilde{x}_i	– mole fraction of components in the condensed phase, [–]
m	– number of components in gaseous phase, [–]	<i>Greek letters</i>	
N	– total number of components, [–]	λ_1, λ_2	– Lagrangian multipliers, [–]
n	– total number of moles of the gaseous phase, [–]	μ_i^0	– chemical potential in the standard state, [kJkmol]
n_i^k	– number of moles of component i in phase k , [–]	μ_i^k	– chemical potential of one mole of component i in phase k , [kJkmol]
\tilde{n}	– number of moles of condensed phase, [–]		

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