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METHOD OF DETERMINING ERROR IN CALCULATED PARAMETERS OF COMBUSTION PROCESS RESULTING FROM ERROR IN THERMODYNAMIC PROPERTIES OF INDIVIDUAL SUBSTANCES

V. E. Alemasov, et al

Foreign Technology Division  
Wright-Patterson Air Force Base, Ohio

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U. S. BOARD ON GEOGRAPHIC NAMES TRANSLITERATION SYSTEM

Block	Italic	Transliteration	Block	Italic	Transliteration
А а	<i>А а</i>	A, a	Р р	<i>Р р</i>	R, r
Б б	<i>Б б</i>	B, b	С с	<i>С с</i>	S, s
В в	<i>В в</i>	V, v	Т т	<i>Т т</i>	T, t
Г г	<i>Г г</i>	G, g	У у	<i>У у</i>	U, u
Д д	<i>Д д</i>	D, d	Ф ф	<i>Ф ф</i>	F, f
Е е	<i>Е е</i>	Ye, ye; E, e*	Х х	<i>Х х</i>	Kh, kh
Ж ж	<i>Ж ж</i>	Zh, zh	Ц ц	<i>Ц ц</i>	Ts, ts
З з	<i>З з</i>	Z, z	Ч ч	<i>Ч ч</i>	Ch, ch
И и	<i>И и</i>	I, i	Ш ш	<i>Ш ш</i>	Sh, sh
Й й	<i>Й й</i>	Y, y	Щ щ	<i>Щ щ</i>	Shch, shch
К к	<i>К к</i>	K, k	Ъ ъ	<i>Ъ ъ</i>	"
Л л	<i>Л л</i>	L, l	Ы ы	<i>Ы ы</i>	Y, y
М м	<i>М м</i>	M, m	Ь ь	<i>Ь ь</i>	'
Н н	<i>Н н</i>	N, n	Э э	<i>Э э</i>	E, e
О о	<i>О о</i>	O, o	Ю ю	<i>Ю ю</i>	Yu, yu
П п	<i>П п</i>	P, p	Я я	<i>Я я</i>	Ya, ya

\*ye initially, after vowels, and after ъ, ь; e elsewhere.  
 When written as ë in Russian, transliterate as yü or ö.  
 The use of diacritical marks is preferred, but such marks may be omitted when expediency dictates.

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GRAPHICS DISCLAIMER

All figures, graphics, tables, equations, etc. merged into this translation were extracted from the best quality copy available.

## RUSSIAN AND ENGLISH TRIGONOMETRIC FUNCTIONS

Russian	English
sin	sin
cos	cos
tg	tan
ctg	cot
sec	sec
cosec	csc
sh	sinh
ch	cosh
th	tanh
cth	coth
sch	sech
csch	csch
arc sin	$\sin^{-1}$
arc cos	$\cos^{-1}$
arc tg	$\tan^{-1}$
arc ctg	$\cot^{-1}$
arc sec	$\sec^{-1}$
arc cosec	$\csc^{-1}$
arc sh	$\sinh^{-1}$
arc ch	$\cosh^{-1}$
arc th	$\tanh^{-1}$
arc cth	$\coth^{-1}$
arc sch	$\operatorname{sech}^{-1}$
arc csch	$\operatorname{csch}^{-1}$
rot	curl
lg	log

### GREEK ALPHABET

Alpha	A	α	•	Nu	N	ν
Beta	B	β		Xi	Ξ	ξ
Gamma	Γ	γ		Omicron	Ο	ο
Delta	Δ	δ		Pi	Π	π
Epsilon	E	ε	•	Rho	Ρ	ρ ϱ
Zeta	Z	ζ		Sigma	Σ	σ ς
Eta	H	η		Tau	Τ	τ
Theta	Θ	θ	ϑ	Upsilon	Υ	υ
Iota	I	ι		Phi	Φ	φ ϕ
Kappa	K	κ	κ ϰ	Chi	Χ	χ
Lambda	Λ	λ		Psi	Ψ	ψ
Mu	M	μ		Omega	Ω	ω

**METHOD OF DETERMINING ERROR IN CALCULATED  
PARAMETERS OF COMBUSTION PROCESS RESULTING  
FROM ERROR IN THERMODYNAMIC PROPERTIES OF  
INDIVIDUAL SUBSTANCES**

V. Ye. Alemasov, A. F. Dregalin,  
Z. Kh. Gruzdeva, and A. S. Lyashev  
Kazan'

Thermodynamic calculation is broadly used to determine the parameters of the combustion process. Error in any parameter of the process  $\phi$ , determined as a result of thermodynamic calculation, depends on:

- a) the mathematical error of the calculation method;
- b) error in the original data on the fuel (enthalpy and elementary composition of the fuel);
- c) error from reference data on properties of individual substances - components of combustion products (enthalpy  $I_q^0$ , entropy  $S_q^0$ , and other properties of  $q$ -th substance).

Studied in the work is the effect of error from reference data on the properties of individual substances; errors of type a and b have already been discussed in the literature [1].

In the case of a constant elementary fuel composition (number of atoms of the  $i$ -th chemical element in a molecule of the fuel

$\alpha_1 = \text{const}$ ) any parameter of the combustion process  $\phi$  may represent the function of enthalpy  $i$  and entropy  $s$  of the combustion products. The enthalpy and entropy in turn are determined by the composition of the mixture and by the thermodynamic properties of the individual substances  $I_q^0$  and  $S_q^0$ . Consequently, error  $\Delta\phi$  which develops as a result of errors in the thermodynamic properties of the individual substances can, in the final analysis, be expressed as  $\Delta I_q^0$  and  $\Delta S_q^0$ .

The reference book [2] gives the following expressions for enthalpy  $I_q^0$ , the change in enthalpy  $(H_T^0 - H_0^0)_q$ , and entropy  $S_q^0$  of the  $q$ -th substance:

$$I_q^0 = \Delta H_{293}^0 f_{293, q} + (H_T^0 - H_0^0)_q - (I_{293}^0 - I_0^0)_q; \quad (1)$$

$$(H_T^0 - H_0^0)_q = R_0 T^2 \left( \frac{\partial \ln Q_q}{\partial T} \right)_p; \quad (2)$$

$$S_q^0 = R_0 \ln \frac{Q_q}{N} + R_0 T \left( \frac{\partial \ln Q_q}{\partial T} \right)_p, \quad (3)$$

where  $Q_q$  is the statistical sum with respect to the states of the molecules;  $\Delta H_{293}^0 f_{293, q}$  - the heat of formation.

As we see, errors  $\Delta I_q^0$  and  $\Delta S_q^0$  are determined by the errors of four quantities, which will henceforth be conditionally denoted as:

$$\omega_{qk} = \Delta H_{293}^0 f_{293, q}; \quad (H_{293}^0 - H_0^0)_q; \quad \ln \frac{Q_q}{N}; \quad \left( \frac{\partial \ln Q_q}{\partial T} \right)_p. \quad (4)$$

Consequently, the error of parameter  $\phi$  for small error  $\omega_{qk}$  is the linear functional for  $\Delta\omega_{qk}$

$$\Delta\phi = \sum_q \sum_k \left( \frac{\partial \phi}{\partial \omega_{qk}} \right)_{\alpha_1} \cdot \Delta\omega_{qk}, \quad (5)$$

where quantities  $\Delta\omega_{qk}$  are determined by the reference data of [2];  $\alpha_1$  - the parameters which determine the form of the combustion process.

To calculate  $\Delta\phi$  in the general case we must solve the problem

of linear programming, since for certain components  $\Delta H_{293}^0$  are expressed through the enthalpy of key substances, and errors  $\Delta(H_T^0 - H_0^0)$  and  $\Delta(H_{293}^0 - H_0^0)$  are to a certain extent interrelated.

Let us obtain some general relationships for the derivatives  $(\partial\phi/\partial w_{qk})_{\alpha 1}$ . As we know, the thermodynamic description of many processes in closed systems is based on the assumption that a certain function of state  $\psi$  (for example, the enthalpy of the fuel for isobaric combustion, entropy - for isentropic expansion) does not change during the process. For such cases any parameter of the combustion products  $\phi$  may be represented by the functions

$$\left. \begin{aligned} \alpha &= \alpha(p, T, w_{qk}), \\ \beta &= \beta(p, \psi, w_{qk}). \end{aligned} \right\} \quad (6)$$

After we have equated the total differential functions of  $\alpha$  and  $\beta$  for  $p$  and  $\psi = \text{const}$  we get

$$\left(\frac{\partial\alpha}{\partial w_{qk}}\right)_{p, \psi} = \left(\frac{\partial\alpha}{\partial w_{qk}}\right)_{p, T} + \left(\frac{\partial\alpha}{\partial T}\right)_{p, w_q} \left(\frac{\partial T}{\partial w_{qk}}\right)_{p, \psi}. \quad (7)$$

On the other hand, if we write the total differential of the function  $\psi(p, T, w_q)$  for  $p$  and  $\psi = \text{const}$ , we get

$$\left(\frac{\partial T}{\partial w_{qk}}\right)_{p, \psi} = - \frac{\left(\frac{\partial\psi}{\partial w_q}\right)_{p, T}}{\left(\frac{\partial\psi}{\partial T}\right)_{p, w_q}}. \quad (8)$$

Thus, for partial derivatives of the thermodynamic parameters the following expression is valid:

$$\left(\frac{\partial\alpha}{\partial w_{qk}}\right)_{p, \psi} = \left(\frac{\partial\alpha}{\partial w_{qk}}\right)_{p, T} - \left(\frac{\partial\alpha}{\partial T}\right)_{p, T} \cdot \frac{\left(\frac{\partial\psi}{\partial T}\right)_{p, w_q}}{\left(\frac{\partial\psi}{\partial T}\right)_{p, w_q}}. \quad (9)$$

Let us use formula (9) for the case of isobaric combustion, described by the equations

$$\left. \begin{aligned} p &= \text{const}, \\ I &= \text{const} \end{aligned} \right\}, \quad (10)$$

where the subscript "κ" refers to parameters in the combustion chamber.

As a result we get:

for the temperature of the combustion products  $T_k$

$$\left(\frac{\partial T_k}{\partial \omega_{qb}}\right)_{p, T} = \frac{1}{c_p} \left(\frac{\partial i}{\partial \omega_{qb}}\right)_{p, T}, \quad (11)$$

for the molecular weight of the combustion products  $\mu_k$

$$\left(\frac{\partial \mu_k}{\partial \omega_{qb}}\right)_{p, T} = \left(\frac{\partial \mu_k}{\partial \omega_{qb}}\right)_{p, T} - \frac{\mu_k}{c_p T_k} (1 - \alpha_p T_k) \left(\frac{\partial i}{\partial \omega_{qb}}\right)_{p, T}, \quad (12)$$

for the number of moles of the q-th substance in the combustion products

$$\left(\frac{\partial n_q}{\partial \omega_{qb}}\right)_{p, T} = \left(\frac{\partial n_q}{\partial \omega_{qb}}\right)_{p, T} - \frac{1}{c_p} \left(\frac{\partial i}{\partial \omega_{qb}}\right)_{p, T} \left(\frac{\partial n_q}{\partial T_k}\right)_{p, T}, \quad (13)$$

where  $\alpha_p$  is the isobaric expansion coefficient;  $c_p$  - heat capacity at  $p = \text{const}$ .

The derivatives  $(\partial i / \partial \omega_{qk})$  and  $(\partial \mu_k / \partial \omega_{qk})$  are written as the result of differentiating known expressions [1]. For example, for enthalpy we have

$$\left(\frac{\partial i}{\partial \omega_{qb}}\right)_{p, T} = \frac{\sum_n n_n \rho_n \left(\frac{\partial \ln \rho_n}{\partial \omega_{qb}}\right)_{p, T} + n_q \left(\frac{\partial i^0}{\partial \omega_{qb}}\right)_{p, T}}{\mu_T M_T} - i \left(\frac{\partial \ln M_T}{\partial \omega_{qb}}\right)_{p, T}, \quad (14)$$

where  $M_T$  is the number of moles in the fuel, giving us the equality of [1]

$$\left. \begin{aligned} p &= \sum_n \rho_n \\ \left(\frac{\partial \ln p}{\partial \ln x}\right)_p &= \left(\frac{\partial \ln M_T}{\partial \ln x}\right)_p \end{aligned} \right\} \quad (15)$$

where  $\mu_T$  is the molecular weight of the fuel;  $x$  - any parameter.

To determine partial derivatives  $(\partial \ln n_q / \partial \omega_{qk})_{p, T}$  and  $(\partial \ln M_T / \partial \omega_{qk})_{p, T}$  we differentiate the system of equations for thermodynamic equilibrium [1] with respect to  $\omega_{qk}$  at  $p$  and  $T = \text{const}$ .

As a result we get a closed equation system for calculating the derivatives

$$\left(\frac{\partial \ln n_j}{\partial \omega_q}\right)_{p,T} = \sum_i a_{ij} \left(\frac{\partial \ln n_i}{\partial \omega_q}\right)_{p,T} - \delta_{j,q} R_j + \delta_{j,q} R_i; \quad (15)$$

$$\sum_j a_{ij} n_j \left(\frac{\partial \ln n_j}{\partial \omega_q}\right)_{p,T} + n_i \left(\frac{\partial \ln n_i}{\partial \omega_q}\right)_{p,T} - B_i \left(\frac{\partial \ln W_i}{\partial \omega_q}\right)_{p,T} = 0; \quad (17)$$

$$\sum_n n_n \left(\frac{\partial \ln n_n}{\partial \omega_q}\right)_{p,T} = 0, \quad (18)$$

where  $\delta_{jq}$  and  $\delta_{ij}$  are the Kronecker symbols;  $i$  - atomic component;  $j$  - molecular component; quantities  $R_1$  and  $R_j$  are determined by differentiating the logarithm of the equilibrium constant, and are given in Table 1.

Table 1

$\omega_q$	$\Delta H_{k,q}^0$	$H_{293}^0 - H_0^0$	$\ln \frac{Q}{N}$	$\left(\frac{\partial \ln Q}{\partial T}\right)_p$
$R_i$	$\frac{a_{ij}}{R_j T}$	$-\frac{a_{ij}}{R_j T}$	$-a_{ij}$	0
$R_j$	$-\frac{1}{R_j T}$	$\frac{1}{R_j T}$	1	0
$\left(\frac{\partial \ln Q}{\partial \omega_q}\right)_{p,T}$	1	-1	0	$R_j T$

The values of quantity  $\Delta \omega_{k,q}$  can be selected on the basis of published data. For the calculations below the data of [2] were used along with materials from the 3rd edition of this handbook, which is being prepared.

We took errors  $\Delta(\Delta H_{293,q}^0)$  and  $\Delta(H_{293}^0 - H_0^0)_q$  directly from the tabulated data of [2]; error in  $Q/N$  was determined from the ratio

$$\Delta \ln \frac{Q}{N} = \frac{\Delta \phi_T^0}{R_0}. \quad (19)$$

where  $\phi_T^0$  is the reduced thermodynamic potential, whose error is given in [2].

To calculate errors  $\Delta(\partial \ln Q / \partial T)_p$  we used the approximate estimate recommended in [2]

$$\Delta S_p^* \approx (2 - 3) \Delta \Phi_{T_0}^* \quad (20)$$

Consequently, the greatest error equals

$$\Delta \left( \frac{d \ln Q}{dT} \right)_p = 4 \frac{\Delta \Phi_p^*}{R_0 T} \quad (21)$$

The presented method of estimating the errors in parameters  $\Delta \Phi$  was used to determine errors  $\Delta T_k$  and  $\Delta \mu_k$ , which arise in calculating the combustion process of several fuels. Characteristic quantities for relative errors  $\delta T_k \%$  and  $\delta \mu_k \%$  are given in Table 2 (pressure  $p_k$  - MN/m<sup>2</sup>,  $\alpha_{ox}$  - excess oxidant ratio).

Table 2

Fuel	$\alpha_{ox}$	$p_k$	$\delta T_k, \%$	$\delta \mu_k, \%$
O <sub>2</sub> +H <sub>2</sub>	0.6	15	0.27	0.22
N <sub>2</sub> O <sub>4</sub> +(CH <sub>3</sub> ) <sub>2</sub> NNH <sub>2</sub>	0.8	15	1.16	0.37
O <sub>2</sub> +kerosene	0.8	15	0.14	0.78

When  $\psi=s$  the given method can also be used to estimate errors in the calculated parameters of isentropic expansion, particularly to determine error in specific pulse.

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