FOREIGN TECHNOLOGY DIVISION

THERMODYNAMIC AND THERMOPHYSICAL PROPERTIES
OF COMBUSTION PRODUCTS
(Selected Pages)

by


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EDITED TRANSLATION

THERMODYNAMIC AND THERMOPHYSICAL PROPERTIES OF COMBUSTION PRODUCTS (Selected Pages)

By V. Ye. Alemasov, A. F. Dregalin, et al.

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TABLE OF CONTENTS

U. S. Board on Geographic Names Transliteration System........ 11
Forward to Volume II.............................................. 1
Basic Designations Adopted........................................ 5
Chapter I. General................................................ 7
Chapter II. Initial Data for Calculations......................... 10
Chapter III. Accuracy of the Calculation Results............... 38
Chapter IV. Brief Description of Tables and Graphs............ 61
Chapter V. Tables and Graphs of Calculation Results........... 66
Bibliography.......................................................... 109
# U. S. Board on Geographic Names Transliteration System

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*Ye initially, after vowels, and after ё, ё; е elsewhere. When written as ё in Russian, transliterate as ye or ё.*

# Russian and English Trigonometric Functions

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The second volume of the Reference Book begins a series of volumes which present the thermodynamic and thermophysical properties of combustion products of various groups of fuel compounds. As indicated in volume I of the Reference [6], the basis of the grouping of fuel compounds is classification in accordance with related oxidizers since it is namely the oxidizer which usually is the component determining the special features of the fuel compound. Four typical groups of fuels are distinguished.

In the course of working on the Reference it was learned that the presentation of results from the calculation of each typical group of fuels (12-15 fuel compounds) in one volume is inexpedient. Such a volume turns out to be cumbersome, difficult to produce, and inconvenient to use. In this connection, two volumes are devoted to each characteristic group. Thus, the properties of combustion products of fuels based on oxygen and air are presented in Volumes II and III.
The second volume of the Reference presents thermodynamic and thermophysical properties of the combustion products of four fuel compounds in which oxygen is used as the oxidizer. All the data which are presented were obtained by the authors by calculations in accordance with the original methods and programs described in Volume I.

The necessary initial data on the enthalpy of the fuel components were taken primarily from the Reference Book "Termicheskiye konstanty veshchestv" [Thermal constants of substances] [45-48], and the reference data on thermodynamic properties of the components of combustion products - from the reference "Termodinamicheskiye svoystva individual'nykh veshchestv" [Thermodynamic properties of individual substances] [49]. Supplements and refinements obtained by the authors of Reference [49] when preparing its third edition were also used.

The list of properties of combustion products, range and spacing of change of determining parameters (stagnation pressure at the input to the nozzle $p_{CO}$, excess oxidant ratio $\alpha_{m}$, degree of expansion $\varphi$) correspond to those presented in Volume I.

The data obtained by calculation correspond to the liquid state of oxygen with a boiling temperature of $90.188^\circ K$ and a pressure of 1 physical atmosphere. In Volume I of the Reference it was shown that using methods of extrapolation for enthalpy it is possible to re-calculate results to another initial temperature of fuel components or to their different phase state with high accuracy. The derivatives necessary for these recalculations, just as the derivatives for extrapolation in accordance with $p_{CO}$, $\varphi$, and chemical composition of the fuel component (content of admixtures), are presented in the tables of the volume.

The results of the calculation are presented in the form of graphs and tables, a detailed description of which is given in Volume I and a brief one - in this volume.
The basic author and editing work in the preparation of the volume was conducted by members of the Editorial Council under the scientific direction of Academician V. P. Glushko.


Doctor of Technical Sciences V. Ye. Alemasov, Doctor of Technical Sciences A. F. Dregalin, Doctor of Technical Sciences A. P. Tishin, Candidate of Technical Sciences V. A. Khudyakov, and Junior Scientific Associate V. N. Kostin accomplished the basic work - they obtained all calculation data presented in Volume II from the methods and programs which they developed. As regards the tabular material obtained on the BESM-6 computer, the persons mentioned also stepped forth as editors - compilers. They accomplished: the preparation of the initial data for calculation; a check of the results for conformance with initial data; the logical monitoring of the correctness of the calculation's results in accordance with specially developed algorithms; the introduction of special designations into the tables which are absent in the ATsPU EVM [computer alpha-numeric printer]; checking the quality of the printing and necessary completion work.

On the basis of original calculation data, this same collective prepared all the graphs presented in the second volume except for the graphs on the influence of chemical nonequilibrium (Figs. No. 5.6-5.11, 5.17-5.21, 5.27-5.31). The latter were prepared by Doctor of Technical Sciences U. G. Pirumov from the results of calculations which he conducted jointly with L. F. Kuz'mina, V. S. Chibisova, and A. K. Petrova.

Textual materials of the volume were prepared by: Doctor of Technical Sciences V. Ye. Alemasov and Doctor of Technical Sciences A. F. Dregalin - §§ I, IV, 2.4, 2.5, 3.2-3.5; Doctor of Technical Sciences V. A. Il'inskiy - §§2.1-2.3; Doctor of Technical Sciences U. G. Pirumov - §2.6; Candidate of Technical Sciences V. A. Khudyakov and Junior Scientific Associate V. N. Kostin - §3.1.
Doctor of Technical Sciences A. P. Tishin and Candidate of Technical Sciences V. A. Khudyakov took part in the preparation of materials for §2.1; Z. Kh. Gruzdeva - for §2.5; V. I. Bychenok - for §3.4; and A. S. Lyashev - for §3.5.

The bibliography was prepared by the authors of of the sections from bibliographic sources published primarily prior to 1971.

Scientific editing of the volume was accomplished by Academician V. P. Glushko (responsible editor) and Doctor of Technical Sciences V. Ye. Alemasov. Scientific editing of the volume's sections were conducted by:

Corresponding Member of the Academy of Sciences USSR A. P. Vanichev - sections I, II text, graphs of Figs. 5.1-5.21;
Doctor of Technical Sciences V. A. Il'inskiy - section III of the text;
Doctor of Technical Sciences S. D. Grishin - section IV of the text, graphs of Figs. 5.22-5.35.


The authors express their profound gratitude to all these people.

A review of the manuscript for Volume II was conducted by Doctor of Chemical Sciences Professor L. V. Gurvich, Doctor of Technical Sciences Professor Ye. A. Sivoldoskiy, Doctor of Chemical Sciences
Professor G. B. Manelis, and Candidate of Physical-Mathematical Sciences L. N. Stesik. Doctor of Technical Sciences Ye. V. Samuylov took part in the discussion and review of §§2.5 and 3.3. The authors are grateful to the reviewers for their valuable remarks and advice. The authors mark with special gratitude the work of Doctor of Technical Sciences V. A. Il'inskiy who, without restricting himself to the duties of editor, rendered active creative assistance in the preparation of new materials for section III.

Basic Designations Adopted

- $a$ - speed of sound;
- $\alpha_{ox}$ - excess oxidant ratio;
- $\alpha_p$ - isobaric coefficient of expansion;
- $\beta$ - consumption complex (specific pressure impulse);
- $\beta_T$ - isothermic compression coefficient;
- $c_{p,o}$ - specific heat at constant pressure: molar and weight, respectively;
- $c_{v,o}$ - specific heat at constant volume: molar and weight, respectively;
- $\delta_P$ - degree of pressure expansion;
- $f$ - coefficient of impulse loss;
- $F$ - area;
- $F_P$ - geometric degree of expansion (relative area);
- $f_P$ - specific (unit) area;
- $g$ - per-second flow rate;
- $g$ - weight fraction;
- $\eta$ - coefficient of dynamic viscosity;
- $h_i$ - specific enthalpy: molar and weight, respectively;
- $h_i$ - specific impulse;
- $K$ - equilibrium constant for partial pressures;
- $k_w$ - weighted fuel-air ratio;
- $k_v$ - volumetric fuel-air ratio;
- $\gamma$ - ratio of specific heat;
- $\lambda$ - coefficient of thermal conductivity;
- $M$ - Mach number;
- $m$ - molecular weight;
- $n$ - number of moles, mean index of isentropy;
- $p$ - pressure;
R. - universal gas constant;
\( r \) - radius;
\( \tau \) - relative radius;
\( \rho \) - density;
\( s, s. \) - specific entropy; molar and weight, respectively;
\( T \) - temperature;
\( v \) - specific volume;
\( w \) - rate of flow;
\( x \) - molar fraction;
\( r \) - weight fraction of substance in condensed state.

Indices

\( r \) - fuel;
\( ox \) - oxidizer;
\( t \) - propellant;
\( n \) - parameters in a vacuum (superscript);
\( 0 \) - deceleration parameters;
\( l \) - parameters of nonreacting mixture;
\( k \) - parameters at input to chamber;
\( e \) - parameters at input to nozzle;
\( \bullet \) - parameters in nozzle throat (subscript);
\( \ast \) - parameters in exit section of nozzle.
CHAPTER I

GENERAL

1.1. Brief Survey of Published Data

Oxygen as an oxidizer is widely used in various chemical fuels. The most widespread fuel combinations are a combination of oxygen with liquid hydrocarbon fuels of the gasoline and kerosene type.

Some information on the properties of the combustion products of such fuels are presented in [22, 37].

The wide use of natural gas as a fuel required a determination of the properties of the products of natural gas combustion with oxygen and hydrogen. These properties are presented in Soviet and foreign works [20, 55, 76] as applicable to various thermotechnical devices.

Fuel based on natural gas and air-oxygen oxidizers with easily ionized additives are employed to generate electric power by the magnetohydrodynamic method. Some information on the properties of the combustion products from such fuels is contained in [8, 13, 25, 91].

The successful development and employment of jet propulsion systems substantially expanded the list of fuels being employed and investigated. In addition to conventional hydrocarbon fuels, ammonia, asymmetrical dimethylhydrazine, pentaborane, and other fuels are employed in combination with oxygen or are being studied.
One of the most effective fuels is employed with liquid oxygen-liquid hydrogen which was first proposed for ZhRD's [liquid-fuel rocket motors] in 1930 by K. E. Tsiolkovskiy [33].

Calculation data on the properties of combustion products of such fuel combinations are presented in many works.

Usually, information on the properties of combustion products is presented in the form of IS-diagrams [20, 69] or in the form of tables and graphs. The range of change of the determining parameters and the list of properties to be calculated differ substantially in different works. The majority of works encompass narrow intervals of change in the composition of the fuel ($\alpha_{ok}$), pressure on the input to the nozzle ($p_{co}$), and degree of gas expansion in the nozzle ($\varepsilon$). As a rule, only the basic thermodynamic properties of the combustion products are determined. Transfer properties are presented in a few sources [4, 15, 40, 87]. The most complete and systematized information on the properties of the combustion products of a number of fuels is contained in the works of authors [2-4, 10-12]. They present a broad list of thermodynamic properties and examine different versions in the accomplishment of the processes. These data were obtained in a broad range of determining parameters. Thus, the calculations of the fuels of liquid oxygen + kerosene [10] and liquid oxygen + asymmetrical dimethylhydrazine [11] encompass a range of change of the excess oxidant ratio $\alpha_{ok} = 0.1-10$, pressure at the input to the nozzle $p_{co} = 2-25 \text{ MN/m}^2$, and degree of expansion $\varepsilon = 20-5000$. For the liquid fuel of oxygen + liquid hydrogen [2, 12], information on combustion products was obtained in the range of $\alpha_{ok} = 0.05-10$, $p_{co} = 1-30 \text{ MN/m}^2$, and $\varepsilon = 10-10,000$.

Of foreign works, we can note a summary of data on the fuel of liquid oxygen + liquid hydrogen [83] as well as a few works containing fragmentary information on the combustion products of several fuels, for example, [43, 71, 82].

A systematic generalized impression of the materials mentioned above in the form, for example, of a compiled reference book is
inexpedient. This is hindered by many circumstances: the differences in initial data in various works, different completeness of information, different intervals of change in determining parameters, the absence of accuracy estimates, and so forth.

1.2. Fuels Presented in Volume II

Volume II presents thermodynamic and thermophysical properties of combustion products of fuel groups which are of interest for contemporary and promising thermoenergy engineering and engine building. They are liquid two-component fuels based on oxygen as an oxidizer:
liquid oxygen + liquid hydrogen,
liquid oxygen + kerosene,
liquid oxygen + asymmetrical dimethylhydrazine,
liquid oxygen + liquid ammonia.

The list of properties determined by calculation is the same for all fuels. The range of change in the determining parameters \( \alpha, \theta, P, \phi \) varies in accordance with two types of grids: "large" (B) and "small" (M). More detailed information on the list of properties and grids of parameters are presented in Chapter XIII of Volume I.

Table 1.1 presents a list of fuels which are examined in Volume II and indicates a grid of parameters in accordance with which the calculation was accomplished.

Table 1.1. Fuels examined in Volume II of the Reference Book.

<table>
<thead>
<tr>
<th>№</th>
<th>Топливо ( \Theta )</th>
<th>( \alpha, \theta )</th>
<th>( P, \phi )</th>
<th>Сетка (B)</th>
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<tr>
<td>1</td>
<td>( O_2 + H_2 )</td>
<td>0.3-5.0</td>
<td>0.1-50</td>
<td>Б</td>
</tr>
<tr>
<td>2</td>
<td>( O_2 + \text{керосин} )</td>
<td>0.4-5.0</td>
<td>0.1-50</td>
<td>Б</td>
</tr>
<tr>
<td>3</td>
<td>( O_2 + (\text{CH}_3)_2NNH_2 )</td>
<td>0.3-5.0</td>
<td>0.1-50</td>
<td>Б</td>
</tr>
<tr>
<td>4</td>
<td>( O_2 + \text{NH}_3 )</td>
<td>0.6-2.0</td>
<td>0.2-50</td>
<td>М</td>
</tr>
</tbody>
</table>

KEY: (1) Fuel; (2) Grid; (3) Kerosene.
CHAPTER II

INITIAL DATA FOR CALCULATIONS

2.1. Chemical Composition of Fuel Components

Fuel components are technical products and admixtures are present in them along with the basic substance. The admixture content is regulated in the Standards for a number of technical substances which serve as fuel components.

If the chemical composition of an admixture is close to the composition of the basic substance and its content is low, then in a number of cases the admixture can be identified with the basic substance introducing, where necessary, a correction for heat of formation.

2.1.1. Oxidizers

Liquid oxygen $O_2$. The composition is standardized in accordance with GOST [All-Union State Standard] 6331-68, "Liquid oxygen, technical and medical." This standard is extended to liquid oxygen which is obtained from the air by deep freezing.

Depending upon the content of oxygen and admixtures technical liquid oxygen is produced in three varieties. The composition is presented in Table 2.1. In accordance with GOST 6331-68 the content of carbon monoxide, gaseous acids, bases, ozone, and other gas oxidizers is not standardized. However, the quantity of these substances is low and they can be disregarded.
The basic admixture in liquid technical oxygen is nitrogen whose weight content in liquid oxygen does not exceed 0.8%. When performing calculations for the Reference Book only liquid nitrogen was considered as an admixture for liquid oxygen.

Table 2.1. Liquid oxygen, technical and medical.

<table>
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<tr>
<th>Наименование показателей</th>
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<tr>
<td>1. Содержание кислорода в объемных % не менее</td>
<td>99.7</td>
</tr>
<tr>
<td>2. Содержание метанола в 1 л жидкого кислорода в мл при 20°C и 760 мм рт. ст. не более</td>
<td>—</td>
</tr>
<tr>
<td>3. Содержание масла в 1 л жидкого кислорода в мг не более</td>
<td>—</td>
</tr>
<tr>
<td>4. Содержание двукиси углерода в 1 л жидкого кислорода в мл при 20°C и 760 мм рт. ст. не более</td>
<td>3</td>
</tr>
<tr>
<td>5. Содержание влаги и механических примесей</td>
<td>—</td>
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</tbody>
</table>

KEY: (1) Name of indices; (2) Standard for varieties; (3) Oxygen content in volume %, no less than; (4) Acetylene content in 1 liter of liquid oxygen in ml at 200°C and 760 mm Hg, no more than; (5) Oil content in 1 liter of liquid oxygen in mg, no more than; (6) Content of carbon dioxide in 1 liter of liquid oxygen in ml at 200°C and 760 mm Hg, no more than; (7) Content of moisture and mechanical admixtures; (8) Not standardized.

2.1.2. Fuels

Liquid hydrogen H₂. Liquid hydrogen is obtained from commercial gaseous hydrogen whose chemical composition is regulated in accordance with GOST 3022-61.

In gaseous hydrogen which is obtained by the electrolysis of water and chloride salts as well as by the iron vapor method, oxygen, nitrogen, and water may be present in noticeable quantities; also carbon monoxide in hydrogen obtained by the conversion of methane and other gaseous hydrocarbons. The solubility of nitrogen, oxygen, and water in liquid
hydrogen is very low. With an extremely low hydrogen temperature oxygen, nitrogen, and water are in a solid state, usually fall out as a precipitate, and are removed. Therefore, liquid hydrogen is obtained with an extremely low quantity of admixtures.

At room temperature hydrogen consist of a mixture of approximately 25% para hydrogen and approximately 75% ortho hydrogen which is in equilibrium. At the boiling temperature of liquid hydrogen the equilibrium content of ortho hydrogen is about 0.2% and the content of the para modification is approximately 99.8%.

In this Reference Book it is accepted that there are no admixtures of other substances in liquid hydrogen and the content of the para modification can be greater than the equilibrium. The coefficients of the extrapolation formulas $A_4$, $B_4$, $C_4$, $D_4$, $L_4$ in the calculations of compounds with liquid hydrogen pertain to extrapolation for oxidizer content.

Kerosene. Kerosenes are obtained from petroleum and are a mixture of various hydrocarbons of several homologous series; present in them is a small quantity of heteroorganic compounds which contain nitrogen, sulfur, and oxygen. The content of individual hydrocarbons depends on the method of obtaining the kerosene and the oil deposit. The hydrocarbon content of individual homologous series except for aromatic hydrocarbons is usually not standardized or is standardized indirectly (for example, the content of unsaturated hydrocarbons is limited by the iodine or bromine number). The fractional composition of kerosene is regulated, i.e., the temperatures up to which a given portion of the kerosene is distilled.

Table 2.2 presents the physical-chemical properties of Soviet kerosenes which are employed for rocket motors. In accordance with the indicated GOST's these kerosenes should contain no mechanical admixtures, insoluble resins, hydrogen sulfide, water, water soluble acids, and bases.

Kerosenes contain a small amount of oxygen and nitrogen and a small quantity of sulfur; therefore, they are not considered in
calculations for the Reference Book. It is accepted that at a temperature of 250°C the density of the kerosene equals 0.830 g/cm³; the lowest heat of combustion is 10,300 kcal/kg; the carbon content equals 85.9% by weight and the hydrogen content - 14.1% (conventional chemical formula CH₁.₉₅₆, C/H ratio = 0.5113).

In order to have the opportunity to extrapolate the results of the calculations for kerosenes of various composition, a substance with a conventional chemical composition, an addition of 1% of which changes the C/H ratio by 1%, is taken as the basic admixture. The enthalpy of this conventional substance is taken as equal to the enthalpy of kerosene. The derivatives for the composition of the fuel which are presented in the tables of the reference book are derivatives for the change in the C/H ratio in the fuel expressed in fractions.

Table 2.2. Physical-chemical properties of some kerosenes.

<table>
<thead>
<tr>
<th>Физико-химические показатели</th>
<th>(2) ГОСТ 10 2027-62</th>
<th>(3) ГОСТ 12 304-66</th>
<th>МРТУ-28-1</th>
<th>244-86</th>
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<tbody>
<tr>
<td>(1) Плотность при 20°C, g/cm³, не ниже</td>
<td>0.800</td>
<td>0.775</td>
<td>0.755</td>
<td>0.840</td>
</tr>
<tr>
<td>(2) Кислотность, мг KOH/100 мл горючего, не более</td>
<td>0.7</td>
<td>0.7</td>
<td>0.7</td>
<td>0.5</td>
</tr>
<tr>
<td>(3) Иодное число, г йода/100 г горючего, не более</td>
<td>2.0</td>
<td>3.5</td>
<td>3.5</td>
<td>1.0</td>
</tr>
<tr>
<td>(4) Содержание ароматических углеводородов, %, не более</td>
<td>20</td>
<td>22</td>
<td>22</td>
<td>10</td>
</tr>
<tr>
<td>(5) Содержание функциональных смол, мг/100 мл горючего, не более</td>
<td>6</td>
<td>5</td>
<td>5</td>
<td>6</td>
</tr>
<tr>
<td>(6) Содержание серы, %, не более, в том числе меркаптановой, не более</td>
<td>0.10</td>
<td>0.25</td>
<td>0.25</td>
<td>0.05</td>
</tr>
<tr>
<td>(7) Зольность, %, не более</td>
<td>0.003</td>
<td>0.001</td>
<td>0.003</td>
<td>0.003</td>
</tr>
<tr>
<td>(8) Темпера смеси изоляционная, ккал/кг, не менее</td>
<td>10 300</td>
<td>10 300</td>
<td>10 300</td>
<td>10 300</td>
</tr>
</tbody>
</table>

KEY: (1) Physical-chemical indices; (2) All-Union State Standard; (3) Density at 20°C, g/cm³, no lower than; (4) Acidity, mg KOH/100 ml of fuel, no more than; (5) Iodine number, g iodine/100 g of fuel, no more than; (6) Content of aromatic hydrocarbons, %, no more than; (7) Content of actual resins, mg/100 ml of fuel, no more than; (8) Sulfur content %, no more than, including mercaptan, no more than; (9) Ash content, %, no more than; (10) Lowest heat of combustion, kcal/kg, no more than.

Asymmetrical dimethylhydrazine (CH₃)₂NNH₂. The basic admixtures when obtaining asymmetrical dimethylhydrazine (NDMG) are water, dimethylamine (CH₃)₂NH, and methylene dimethylhydrazine (CH₃)₂NCH₂. Some quantity of these substances can also be formed with the oxidation of 13.
NDMG with oxygen of the air. The remaining admixtures are present in small quantity and are not considered in this Reference Book.

Table 2.3. The effect of the content of (CH₃)₂NH and (CH₃)₂NNCH₂ on the characteristics of combustion products.

<table>
<thead>
<tr>
<th>№</th>
<th>Состав горючего</th>
<th>Tᵥ, K</th>
<th>a₀, м/сек</th>
<th>Jₜ, м/сек</th>
<th>P</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>98.5% (CH₃)₂NNH + 0.5% (CH₃)₂NH + +1% (CH₃)₂NNCH₂</td>
<td>3672</td>
<td>1800</td>
<td>3176</td>
<td>3330</td>
</tr>
<tr>
<td>2</td>
<td>96.5% (CH₃)₂NNH + 1.5% (CH₃)₂NH + +3% (CH₃)₂NNCH₂</td>
<td>3674</td>
<td>1799</td>
<td>3175</td>
<td>3329</td>
</tr>
<tr>
<td>3</td>
<td>97% (CH₃)₂NNH + 1% (CH₃)₂NH + +2% (CH₃)₂NNCH₂</td>
<td>3673</td>
<td>1800</td>
<td>3176</td>
<td>3330</td>
</tr>
</tbody>
</table>

KEY: (1) Composition of fuel; (2) m/s.

Special thermodynamic calculations were conducted in order to determine the effect of changes in the content of dimethylamine and methylene dimethylhydrazine in asymmetrical dimethylhydrazine on the basic characteristics of combustion products.

Table 2.4. Synthetic liquid ammonia.

<table>
<thead>
<tr>
<th>Наименование показателей</th>
<th>(a) Нормы</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1-й сот.</td>
</tr>
<tr>
<td>(1) Содержание аммиака в %, не менее</td>
<td>99.9</td>
</tr>
<tr>
<td>(2) Содержание влаги в %, не более</td>
<td>0.1</td>
</tr>
<tr>
<td>(3) Содержание масла в мг/л, не более</td>
<td>10.0</td>
</tr>
<tr>
<td>(4) Содержание железа в мг/л, не более</td>
<td>2.0</td>
</tr>
</tbody>
</table>

KEY: (1) Name of indices; (2) Norms; (3) 1st grade; (4) 2nd grade; (5) Ammonia content in %, not less than; (6) Moisture content in %, not less than; (7) Oil content in mg/l, no more than; (8) Iron content in mg/l, no more than; (9) Not standardized.

As an example, Table 2.3 presents the results of these calculations for a fuel compound of O₂ + NDMG with pCO = 10 MN/m² and a₀ = 1.0.
Table 2.5. Chemical composition of fuel compounds taken in calculations.

<table>
<thead>
<tr>
<th>Типливая композиция (1)</th>
<th>(O_2 + H_2)</th>
<th>(O_2 + \text{kerosene} \Delta)</th>
<th>(O_2 + (CH_3)_2NNH_2)</th>
<th>(O_2 + NH_4)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Исходный состав (2)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Присадка (3)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Содержание присадки по весу до (4)</td>
<td>0,008</td>
<td>0,008</td>
<td>0,008</td>
<td>0,008</td>
</tr>
<tr>
<td>Коэффициенты экстраполяционных формул (5)</td>
<td>(A_1, B_1, C_1, D_1)</td>
<td>(A_2, B_2, C_2, D_2)</td>
<td>(A_3, B_3, C_3, D_3, L_3)</td>
<td>(A_4, B_4, C_4, D_4)</td>
</tr>
<tr>
<td>Горючее (6)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Содержание горючего по весу (7)</td>
<td>100% (H_2)</td>
<td>(C-85.9%)</td>
<td>(H-14.1%)</td>
<td>100% (NH_3)</td>
</tr>
<tr>
<td>Присадка (3)</td>
<td></td>
<td>(CH_2=CH_2\text{H}_2\text{O})</td>
<td>(H_2\text{O})</td>
<td>(H_2\text{O})</td>
</tr>
<tr>
<td>Содержание присадки по весу до (4)</td>
<td>-</td>
<td>(+0,06)</td>
<td>0,005</td>
<td>0,004</td>
</tr>
<tr>
<td>Коэффициенты экстраполяционных формул (5)</td>
<td>-</td>
<td>(A_1, B_1, C_1, D_1)</td>
<td>(A_2, B_2, C_2, D_2)</td>
<td>(A_3, B_3, C_3, D_3, L_3)</td>
</tr>
</tbody>
</table>

KEY: (1) Fuel composition; (2) Kerosene; (3) Oxidizer; (4) Initial composition; (5) Admixture; (6) Admixture content by weight up to; (7) Coefficients of extrapolation formulas; (8) Fuel; (9) Initial composition in % by weight.

As is evident, with an average content of dimethylamine and methylene dimethylhydrazine in the NDMG the deviation of the specific impulse in a vacuum does not exceed 1 m/s of the value with minimum or maximum taken content of \((CH_3)_2NH\) and \((CH_3)_2NNCH_2\). Proceeding from this, asymmetrical dimethylhydrazine with mean weight fractions of dimethylamine and methylene dimethylhydrazine have been taken as the basic composition in the Reference Book.

Water has been taken as the basic admixture for NDMG.

Liquid ammonia \(NH_3\). The composition is standardized in accordance with GOST 6221-62, "Synthetic liquid ammonia." Liquid ammonia is produced in two varieties depending on the physical-chemical indices. Its composition is presented in Table 2.4.
The basic admixture for liquid ammonia, in which regard in comparatively small quantity, is water. Other admixtures are present in even lesser quantity and are not considered in the calculations.

2.1.3. Fuel Compounds

In summing up the result, to substantiate the fuel components which are adopted in the calculation and the admixtures which are considered we present a generalizing Table 2.5. For each of the fuel compounds examined in Volume II Table 2.5 presents the initial chemical composition of the fuel components (all calculation tables and graphs correspond to it). The admixtures in the fuel and oxidizer which are considered and the ranges of their possible variation are indicated. In these ranges, the effect of the admixtures can be estimated by extrapolation methods with the aid of the derivatives $A_4, B_4, C_4, D_4, L_4, A_5, B_5, C_5, D_5, L_5$, which are presented in the Tables.

2.2. Enthalpy of Fuel Components

The parameters of the combustion products of fuels in calculations were determined using the thermodynamic properties of combustion product components presented in the Reference Book [49]. Therefore, similar to the Reference Book [49], it is accepted that the enthalpies of the elements in the standard state at a temperature of 293.15°C are equal to zero. In accordance with this condition, the enthalpy of any substance at temperature $T$ equals

$$I^o = \Delta H^o_{293.15} + (H^o_T - H^o_{293.15}), \quad (2.1)$$

where the heat of formation $\Delta H^o_{293.15}$ is equal to the change in enthalpy with the transition of the substance's component elements to the substance being considered.

The following standard states of chemical elements have been accepted: oxygen, hydrogen, and nitrogen - diatomic gases; argon - monatomic gas; carbon - graphites. The same standard states of elements are adopted in reference books [45-48, 50, 79, 88] and works [14, 21, 31, 74].
It is also accepted that high-boiling fuel components have a temperature of 298.15\(^0\)K and low boiling - boiling temperature.

The heats of formation, heat of mixing, boiling temperature, and heats of evaporation of the majority of individual substances which form the fuel components and which are necessary for determining enthalpy are taken from Reference Books [45-48]. These Reference Books present the most reliable and systematized values of the heat constants of inorganic substances. These constants were selected on the basis of a thorough analysis of virtually all published data (in the first edition, up to the middle of 1963; in the second - up to the end of 1964; in the third - up to March 1967; and in the fourth - to the end of 1968).

In the Reference Books [45-48, 88] and other works which were used the heats of formation are given with a temperature of 298.15\(^0\)K. It is known that the heat of formation at a temperature of 293.15 is determined from the heat of formation with a temperature of 298.15 from the equation

\[
\Delta H_{293.15}^\circ = \Delta H_{298.15}^\circ + (H_{293.15}^\circ - H_{298.15}^\circ) - \\
\Sigma (H_{293.15}^\circ - H_{298.15}^\circ).
\]

(2.2)

Here \((H_{293.15}^\circ - H_{298.15}^\circ)\) and \(\Sigma (H_{293.15}^\circ - H_{298.15}^\circ)\) - the changes in enthalpy from a temperature of 298.15\(^0\)K to a temperature of 293.15\(^0\)K respectively of the given substance and the elements which form it in standard states.

Substituting expression (2.2) into equation (2.1) we find

\[
H_o^\circ = \Delta H_{298.15}^\circ + \Sigma (H_{293.15}^\circ - H_{298.15}^\circ) + \\
+ (H_o^\circ - H_{298.15}^\circ).
\]

(2.3)

The values of the differences in the enthalpies \((H_{293.15}^\circ - H_{298.15}^\circ)\) for the elements are presented in Reference Book [49].
2.2.1. Heats of Formation of Individual Substances which go into the Fuel Components

Table 2.6 presents the accepted heats of formation $\Delta H^0_{f298.15}$ of individual substances from elements taken in the standard state. The aggregate state of a substance to which the accepted heat of formation pertains is indicated. The reference to the bibliographic source on whose recommendation the heat of formation was selected is given.

**Table 2.6. Accepted heats of formation of individual substances.**

<table>
<thead>
<tr>
<th>Название индивидуального вещества (1)</th>
<th>Химическая формула (2)</th>
<th>Агрегатное состояние (3)</th>
<th>Теплота образования $\Delta H^0_{f298.15}$, kcal/моль</th>
<th>Литература (6)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Кислород (1)</td>
<td>$O_2$</td>
<td>газ</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>Азот (2)</td>
<td>$N_2$</td>
<td>газ</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>Водород (3)</td>
<td>$H_2$</td>
<td>газ</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>Аргон (4)</td>
<td>$Ar$</td>
<td>газ</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>Диаметилгидразин ненасыщенный (5)</td>
<td>$(CH_2)NNH_2$</td>
<td>жидк.</td>
<td>$11.9 \pm 0.4$</td>
<td>48</td>
</tr>
<tr>
<td>Вода (6)</td>
<td>$H_2O$</td>
<td>жидк.</td>
<td>$-18.3 \pm 0.0096$</td>
<td>45</td>
</tr>
<tr>
<td>Диметиламин (7)</td>
<td>$(CH_2)NNH$</td>
<td>жидк.</td>
<td>$-10.8 \pm 0.1$</td>
<td>47</td>
</tr>
<tr>
<td>Метильноаминолетилгидразин (8)</td>
<td>$(CH_2)NNCH_2$</td>
<td>жидк.</td>
<td>$28.6$</td>
<td>31</td>
</tr>
<tr>
<td>Вода (9)</td>
<td>$H_2O$</td>
<td>газ</td>
<td>$-57.796 \pm 0.01$</td>
<td>48</td>
</tr>
<tr>
<td>Оксис углерода (10)</td>
<td>$CO_2$</td>
<td>газ</td>
<td>$-34.082 \pm 0.011$</td>
<td>47</td>
</tr>
<tr>
<td>Окис углерода (10)</td>
<td>$CO$</td>
<td>газ</td>
<td>$-36.418 \pm 0.031$</td>
<td>47</td>
</tr>
<tr>
<td>Аммиак (11)</td>
<td>$NH_3$</td>
<td>газ</td>
<td>$-11.04 \pm 0.07$</td>
<td>46</td>
</tr>
</tbody>
</table>

KEY: (1) Name of individual substance; (2) Chemical formula; (3) Aggregate state; (4) Heat of formation $\Delta H^0_{f298.15}$, kcal/mole; (5) Bibliography; (6) Oxygen; (7) Nitrogen; (8) Hydrogen; (9) Argon; (10) Asymmetrical dimethylhydrazine; (11) Water; (12) Dimethylamine; (13) Methylene dimethylhydrazine; (14) Water; (15) Carbon dioxide; (16) Carbon monoxide; (17) Ammonia; (18) Gas; (19) Liquid.

The heat of formation of methylene dimethylhydrazine was estimated by V. P. Kolesov and M. P. Kozina [31]. Here, the heat of formation of gaseous methylene dimethylhydrazine was found from the corresponding group contributions which were taken on the recommendation of the article by Benson et al [57] ($\Delta H^0_{f298.15} = 36.6$ kcal/mole) while the heat of evaporation was estimated from the recommendation by Klager [68] ($\Delta H^0_{v298.15} = 8$ kcal/mole).

As mentioned earlier, the accepted value of the lowest heat of combustion of kerosene equals 10,300 kcal/kg.
2.2.2. Heat of Mixing of Individual Substances when Forming Fuel Components

Heats of mixing of nonreacting gaseous substances in the ideal state equal zero.

The heat of mixing of liquid nitrogen and oxygen is extremely low and it is disregarded. Heats of solution of water, dimethylamine, and methylene dimethylhydrazine in asymmetrical dimethylhydrazine are unknown; however, it can be assumed that they are not great. The heat of solution of an extremely small quantity of water in liquid ammonia is unknown and is not considered in the Reference Book; however, it may have a noticeable value. Heats of solution of hydrocarbons with the formation of kerosene are low; they are considered in the experimental value of the heat of combustion.

2.2.3. Boiling Temperature and Heat of Evaporation of Low Boiling Fuel Components

Table 2.7 presents the boiling temperatures at which the pressure of saturated vapor is equal to 1 atm and the heats of evaporation which correspond to them for low-boiling individual substances which are part of the fuel components. The boiling temperatures of liquid hydrogen and oxygen are taken from a report [54] which presents some refined data in comparison with Reference Book [54].

In the Reference Book, when determining the enthalpy of solutions of a small quantity of nitrogen (≪1% by weight) in liquid oxygen it is accepted that the solutions have a boiling temperature of liquid oxygen of 90.188 K although the boiling temperature of liquid nitrogen is substantially lower. The error in enthalpy which is caused by this assumption is low and it can be disregarded. For example, in the case of 0.8%* by weight of the nitrogen solution this error equals ~3 cal/mole, i.e., less than the error in determining the heat of evaporation of liquid oxygen.

*The maximum possible amount of nitrogen in liquid technical oxygen in accordance with GOST 6331-68.
Table 2.7. Some physical properties of low-boiling individual substances.

<table>
<thead>
<tr>
<th>Химическая формула (1)</th>
<th>Температура кипения (2)</th>
<th>Тройчатое изменение в состоянии кипения (3)</th>
<th>Назначение виталий в состоянии жидкого пара (4)</th>
<th>Литература</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$T_{кип}, K$</td>
<td>$\Delta H_f, \text{кал/моль}$ (5)</td>
<td>$\Delta U_f, \text{кал/моль}$ (6)</td>
<td></td>
</tr>
<tr>
<td>$O_2$, норм (7)</td>
<td>90.188±0.010</td>
<td>1.632±0.004</td>
<td>625</td>
<td>45</td>
</tr>
<tr>
<td>$H_2$, норм (7)</td>
<td>20.397±0.010</td>
<td>0.216±0.0008</td>
<td>54, 84</td>
<td>45</td>
</tr>
<tr>
<td>$H_2$, пара (7)</td>
<td>20.29±0.01</td>
<td>0.216±0.0008</td>
<td>101</td>
<td>45</td>
</tr>
<tr>
<td>$NH_3$</td>
<td>239.73±0.04</td>
<td>5.570±0.005</td>
<td>1913</td>
<td>45</td>
</tr>
<tr>
<td>$N_2$</td>
<td>90.188±0</td>
<td>1.21 (4)</td>
<td>6284</td>
<td>45</td>
</tr>
</tbody>
</table>

KEY: (1) Chemical formula; (2) Boiling temperature; (3) Bibliography; (4) Heat of evaporation at $T_{кип}$; (5) kcal/mole; (6) Change in enthalpy in the state of an ideal gas; (7) Normal; (8) Equilibrium.

1) Normal hydrogen is a mixture of 25% para hydrogen and 75% ortho hydrogen.

2) Changes in enthalpy are presented for the case where at boiling temperatures and 298.50K hydrogen is normal, and at a temperature of 00K-para hydrogen.

3) Equilibrium at 20.40K hydrogen contains 99.8% para hydrogen and 0.2% ortho hydrogen.

4) These parameters are presented with a nitrogen temperature of 90.1880K.

Let us estimate the enthalpy error being considered in the case of 0.8% by weight of a nitrogen solution.

It is known that the partial pressure of the vapor of some substance above an ideal liquid solution is equal to the pressure of the saturated vapor above a pure substance (at a given temperature) multiplied by the molar fraction of this substance in the liquid phase. Here, it is assumed that the vapor is a mixture of ideal gases. Consequently, the pressure of the saturated vapor above a 0.8% by weight nitrogen solution in liquid oxygen at a temperature of 90.1880K approximately equals

$$P_v = P_{S,O_2}n_{O_2} + P_{S,N_2}n_{N_2} = 1.0238 \text{ atm.} \quad (a)$$

Here $P_{S,O_2} = 1 \text{ atm}$ and $P_{S,N_2} = 3.160 \text{ atm}$ - the pressure of saturated vapors respectively above liquid oxygen and nitrogen, with $90.1880K$, $n_{O_2} = 0.9909$, and $n_{N_2} = 9.13 \cdot 10^{-3}$ - the molar fraction in the solution of oxygen and nitrogen respectively.
The approximate amount of reduction in the temperature of the solution necessary to obtain a pressure of saturated vapor above the solution \(p_S = 1\) atm is found using the Clapeyron-Clausius equation

\[
\frac{\Delta p}{\Delta T} = \frac{\rho \Delta H_D}{R T^2},
\]

where \(\Delta p\) - the given amount of reduction in the pressure of the saturated vapor.

Substituting in equation (a), which is written through finite differences, the values of \(\Delta p\) for oxygen and nitrogen from equation (b) we find

\[
\Delta p_s = (p_{s,0} n_{o} \Delta H_{o,0} + p_{s,1} n_{n} \Delta H_{n,1}) \frac{\Delta T}{R T^2}.
\]

From equation (c) it follows that to obtain the pressure of a saturated vapor above a solution with \(p_S = 1\) atm it is necessary to reduce the solution's temperature by the amount \(\Delta T = 0.23^\circ\) in comparison with a temperature of \(90.188^\circ\)K. Here, the change in the solution's enthalpy equals

\[
\Delta I = -\Delta(\Delta H) + c_p\Delta T =
- (c_{pH} - c_m) \Delta T + c_p \Delta T = c_m \Delta T.
\]

where \(c_{pH}\) and \(c_m\) - the specific heats of the vapor and liquid at constant pressure respectively.

The value of \(\Delta I = -2.9\) cal/mole is equal to the unknown error.

2.2.4. Preheating Heat of Vapors of Low-Boiling Components

The heats of preheating of vapors of low-boiling individual substances in the state of an ideal gas from boiling temperature to \(298.15^\circ\) are found from the expression

\[
H_{T=298.15}^0 - H_{T=0}^0 = (H_{T=298.15}^0 - H_0^0) -
- (H_{T=298.15}^0 - H_0^0).
\]

Here \((H_{T=298.15}^0 - H_0^0)\) and \((H_{T=0}^0 - H_0^0)\) - the changes in enthalpy of a substance in the state of an ideal gas from 0\(^\circ\)K respectively to the boiling temperature or 298.15\(^\circ\)K.
The values of changes in enthalpy \((\Delta H^0_{\text{Fus}} - H^0_0)\) and \((\Delta H^0_{\text{Fus,15}} - H^0_0)\) are presented in Table 2.7 with references to the literature from which they are taken.

The values of the change in enthalpy \((\Delta H^0_{\text{Fus}} - H^0_0)\) are presented in the report [54] obtained for \(O_2\) - by interpolation of Woolley's data [90], for \(N_2\) (normal and equilibrium) - by direct addition in accordance with the levels of energy of molecular hydrogen and for \(NH_3\) - by the interpolation of Haar's data [63].

2.3. Density of Fuel Components

Table 2.8 presents the densities of individual substances which are the basic component parts (content \(>96-99\%\)) of the corresponding fuel components and of components which are mixtures of substances (kerosene). Also presented is the density of liquid hydrogen with a content of 75\% ortho hydrogen (normal hydrogen). The density values presented are given with references to the literature from which they were taken.

In performing precise calculations, for example, when calculating the volumes of fuel tanks or the mass flow rates of fuel components by volumes (especially with the experimental determination of the specific impulse) use should be made of experimental values of the density of fuel components of a given chemical composition.

Table 2.8. Density of fuel components.

<table>
<thead>
<tr>
<th>Substance</th>
<th>Density, g/cm(^3)</th>
<th>Literature</th>
</tr>
</thead>
<tbody>
<tr>
<td>(O_2)</td>
<td>1.135</td>
<td>(1, 17)</td>
</tr>
<tr>
<td>Kerosene</td>
<td>0.830</td>
<td>(2, 5, 18)</td>
</tr>
<tr>
<td>((\text{CH}_3)_2\text{NNH}_2)</td>
<td>0.786</td>
<td>(33, 44)</td>
</tr>
<tr>
<td>(N_2)  (norm.)(^#)</td>
<td>0.0709</td>
<td>(44)</td>
</tr>
<tr>
<td>(N_2)  (para)(^#)</td>
<td>0.0708</td>
<td>(44)</td>
</tr>
<tr>
<td>(NH_3)</td>
<td>0.082</td>
<td>(17)</td>
</tr>
</tbody>
</table>

\#Mixture 25\% para hydrogen and 75\% ortho hydrogen.
Table 2.8 presents the densities of substances in the liquid state. The densities of high-boiling substances are given at a temperature of 250°C and of low boiling - at boiling temperature.

The density of kerosene depends on the content of individual hydrocarbons in it; the table presents an arbitrarily accepted value.

2.4. Thermodynamic Properties of Individual Substances

2.4.1. Individual substances which are being considered

The components of the combustion products of fuel compounds which are presented in Volume II of the Reference Book include individual substances which are formed from atoms of oxygen, hydrogen, carbon, and nitrogen.

The components of combustion products are presented in Table 2.9. Their list was prepared on the basis of recommendations in Reference Book [49] and with consideration of the data obtained for the third edition of the Reference Book [49] under preparation. When performing the calculations, only the gaseous state of these substances is considered.

Table 2.9. Components of combustion products.

<table>
<thead>
<tr>
<th></th>
<th>H₂O</th>
<th>NH</th>
<th>CO, CO⁺</th>
<th>H₂CO</th>
</tr>
</thead>
<tbody>
<tr>
<td>O, O⁺, O⁻</td>
<td>H₂O₂</td>
<td>NH₂</td>
<td>CO₂</td>
<td>CN</td>
</tr>
<tr>
<td>O₂, O⁺⁺</td>
<td>N₂, N⁺⁺</td>
<td>NH₂</td>
<td>C₂O₂</td>
<td>HCN</td>
</tr>
<tr>
<td>O₃</td>
<td>N₂, N₄⁺⁺</td>
<td>N₄H₄</td>
<td>CH</td>
<td>C₄H</td>
</tr>
<tr>
<td>H, H⁺, H⁻</td>
<td>N₂</td>
<td>HNO</td>
<td>CH₄</td>
<td>C₄H₄</td>
</tr>
<tr>
<td>H₂</td>
<td>NO, NO⁺⁺</td>
<td>C, C⁺⁺, C⁺⁺</td>
<td>CH₄</td>
<td>C₄H₄</td>
</tr>
<tr>
<td>OH, OH⁺⁺, OH⁻</td>
<td>NO₂</td>
<td>C₄</td>
<td>CH₄</td>
<td>C₄N₄</td>
</tr>
<tr>
<td>H₂O₂</td>
<td>N₂O</td>
<td>C₄</td>
<td>HCO</td>
<td></td>
</tr>
</tbody>
</table>
Monotomic carbon C is considered not only in the gaseous but also in the condensed state.

2.4.2. Thermodynamic properties of individual substances

The thermodynamic properties (enthalpy, change in enthalpy, entropy, $\log K_p$) of individual substances are presented in tabular form in Reference Book [49] and the thermoconstants of substances - in the Reference Book [45-48]. For use in calculations, the tabular values of enthalpy $h^0$ are approximated by polynomials of the seventh (gaseous substances) and third (condensed substances) orders. The remaining thermodynamic properties of individual substances are determined from known relationships of thermodynamics with the use of the values $h^0$.

The coefficients of approximating polynomials are presented in Volume I of the Reference Book. In preparing the first volume changes in the thermoconstants of gaseous substances were considered in accordance with the data of the Reference Book [45-48] and the zero of polynomials $A_1$ and $A_3$ were corrected accordingly.

2.5. Transfer Properties of Individual Substances

The transfer properties - coefficients of viscosity $\eta$ and thermoconductivity $\lambda$ of individual substances and mixtures of individual substances are determined in considerable measure by the integrals of collisions $\omega_{ij}$. For the calculation of integrals $\omega_{ij}$, model potentials are used in the Reference Book. The types of potentials used in studies and the method for determining their parameters are examined in detail in Volume I of the Reference Book. For convenience in using this volume of the Reference Book, Table 2.10 provides a brief list of these methods.

For all the individual substances which are considered in the calculations, the Lennard-Jones potential is taken as the model of interaction (12-6):
\[ \varphi(r) = 4\pi \frac{\alpha}{r} \left( \frac{\sigma}{r} \right)^{\nu} - \left( \frac{\alpha}{r} \right)^{\nu} \]  

(2.5)

where \( r \) - the intermolecular distance at which \( \varphi(r) = 0 \); \( \varphi \) - the depth of the potential well.

Table 2.10. Methods for determining the parameters of potentials.

<table>
<thead>
<tr>
<th>No.</th>
<th>Methods for determining parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.</td>
<td>Approximation of initial potential</td>
</tr>
<tr>
<td></td>
<td><strong>Experimental</strong></td>
</tr>
<tr>
<td>2.</td>
<td>Use of transfer properties</td>
</tr>
<tr>
<td>3.</td>
<td>Use of ( p-v-T ) properties</td>
</tr>
<tr>
<td>4.</td>
<td>Use of properties of crystal with ( 0^\circ )K</td>
</tr>
<tr>
<td>5.</td>
<td>Rydberg-Klein-Riesz method</td>
</tr>
<tr>
<td>6.</td>
<td>Method of scattering on gas targets</td>
</tr>
<tr>
<td>7.</td>
<td>Use of data on vibrational relaxation</td>
</tr>
<tr>
<td></td>
<td><strong>Calculation-theoretical</strong></td>
</tr>
<tr>
<td>8.</td>
<td>Quantum-mechanical calculation</td>
</tr>
<tr>
<td>9.</td>
<td>Use of the Thomas-Fermi-Dirac model of the atom</td>
</tr>
<tr>
<td>10.</td>
<td>Semiempirical method of valence bonds</td>
</tr>
<tr>
<td>11.</td>
<td>Calculation of dispersion energy</td>
</tr>
<tr>
<td></td>
<td><strong>Indirect</strong></td>
</tr>
<tr>
<td>12.</td>
<td>Employment of similarity theory</td>
</tr>
<tr>
<td>13.</td>
<td>Method of equivalent solid spheres</td>
</tr>
<tr>
<td>14.</td>
<td>Use of parameters in the critical point</td>
</tr>
<tr>
<td>15.</td>
<td>Use of parameters in the boiling point</td>
</tr>
<tr>
<td>16.</td>
<td>Use of parameters in the melting point</td>
</tr>
<tr>
<td></td>
<td><strong>Empirical</strong></td>
</tr>
<tr>
<td>17.</td>
<td>( \sigma_A = 0.75\sigma_A + 0.45 )</td>
</tr>
<tr>
<td>18.</td>
<td>( \sigma_A = 0.413 + (0.171 + 0.54\sigma_A)^{1/2} )</td>
</tr>
<tr>
<td>19.</td>
<td>( \sigma_A = \frac{4}{3} \sigma_A - 0.6; \sigma_{AB} = \frac{4}{3}(r_A + r_B) + 1.8 )</td>
</tr>
<tr>
<td>20.</td>
<td>( \sigma_{AB} = (1.84\sigma_A^2 + 5.13r_{AB} + 3.24)^{1/2} )</td>
</tr>
<tr>
<td>21.</td>
<td>( \sigma_{ABC} = \frac{5}{12}(\sigma_A + \sigma_B + \sigma_C) - 0.55 )</td>
</tr>
<tr>
<td>22.</td>
<td>( \sigma_{AB} = (\sigma_A + \sigma_B)^{1/2}; \sigma_{AB} = \frac{1}{3}(\sigma_A + \sigma_B) )</td>
</tr>
<tr>
<td>23.</td>
<td>Linear relationships</td>
</tr>
<tr>
<td>24.</td>
<td>Estimate in accordance with the distance between atoms in molecule</td>
</tr>
<tr>
<td>25.</td>
<td>( \sigma_{ij} = \frac{1}{3} \left( \frac{1}{\sqrt{\sigma_{ij}^{\pi}^{\alpha}}} + \frac{1}{\sqrt{\sigma_{ij}^{\pi}^{\beta}}} \right) )</td>
</tr>
</tbody>
</table>
For a number of individual substances, especially if their temperature is high (~2000-3000°K), the use of the Lennard-Jones potential is not preferable. In such cases, the "true" and more substantiated potential was approximated by potential (12-6) from the condition of acceptable conformance of the collision integrals $\tilde{J}^{12-6}$ and $\tilde{J}^{12-6}$ of potential (12-6) and the "true" potential. Such an approximation is not strictly a method for determining the parameters of the potentials; this method is presented conventionally in Table 2.10.

A list of individual substances (components of combustion products) which are considered when determining the equilibrium composition is presented above in Table 2.9. Depending on the possible content in the combustion products, it is expedient to combine these substances into two groups (Table 2.11 and Table 2.12 respectively). Individual substances whose molar fraction $x_q$ may be more than 0.01-0.05 and atomic substances are separated into the first group; substances with a lesser content in combustion products are combined in the second. Such an arbitrary division was accomplished on the basis of the results of thermodynamic calculations which are available, for example, [2, 10-12], and from the results presented in this volume.

The parameters of the Lennard-Jones potential for individual substances of the first group are presented in Table 2.11. For the majority of substances we determine (estimate) the parameters $\sigma$ and $\varepsilon/k$ again. In those cases where parameters $\sigma$ and $\varepsilon/k$ are taken from published data, reference to the source (in the brackets) is given in the table directly along side the value of the parameter. The table also indicates the method for determining the parameters of the potential in accordance with the numbering of Table 2.10; given in the corresponding column is the reference to the literature from which the necessary initial values were taken for the employment of the method (for example, $\tilde{J}^{12-6}$, $T_{kp}$, $q_{kp}$, $p_{kp}$, etc.).

We determined the parameters of the potentials for atomic oxygen, hydrogen, and nitrogen and molecules of oxygen, hydrogen, nitrogen, water, carbon dioxide, carbon monoxide, and nitric oxide as a result of the approximation of collision integrals $\tilde{J}^{12-6}$ and $\tilde{J}^{12-6}$. The
collision integrals were obtained by Ye. V. Samuylov and associates in [40, 41] with the involvement of various methods and potentials depending on the nature of the substances and the intermolecular distances. The data from [40] are used in the Reference Book.

Table 2.11. Parameters of the Lennard-Jones potential for individual substances.

<table>
<thead>
<tr>
<th>Substance</th>
<th>( \sigma, \text{Å} )</th>
<th>( \epsilon/k_B, \text{K} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>O</td>
<td>2,631</td>
<td>295.6</td>
</tr>
<tr>
<td>H</td>
<td>2,120</td>
<td>505.4</td>
</tr>
<tr>
<td>N</td>
<td>2,496</td>
<td>419.0</td>
</tr>
<tr>
<td>C</td>
<td>3,098</td>
<td>52.0</td>
</tr>
<tr>
<td>O_2</td>
<td>3,347</td>
<td>150.8</td>
</tr>
<tr>
<td>H_2</td>
<td>2,934</td>
<td>34.1</td>
</tr>
<tr>
<td>OH</td>
<td>3,846 [28]</td>
<td>180.8 [28]</td>
</tr>
<tr>
<td>H_2O</td>
<td>2,526</td>
<td>846.7</td>
</tr>
<tr>
<td>N_2</td>
<td>3,120</td>
<td>332.6</td>
</tr>
<tr>
<td>NO</td>
<td>3,669</td>
<td>75.5</td>
</tr>
<tr>
<td>NO_2</td>
<td>3,765 [61]</td>
<td>210.0 [61]</td>
</tr>
<tr>
<td>NH_3</td>
<td>3,016 [29]</td>
<td>311.2 [29]</td>
</tr>
<tr>
<td>CO</td>
<td>2,942</td>
<td>477.8</td>
</tr>
<tr>
<td>CO_2</td>
<td>3,900</td>
<td>210.5</td>
</tr>
</tbody>
</table>

KEY: (1) Substance; (2) Value; (3) Method; (4) Literature.
Table 2.12. Parameters of Lennard-Jones potential for individual substances.

<table>
<thead>
<tr>
<th>Substance</th>
<th>r, Å</th>
<th>Method</th>
<th>α</th>
<th>Method</th>
<th>α/μ, °K</th>
</tr>
</thead>
<tbody>
<tr>
<td>O₂</td>
<td>4,010</td>
<td>2</td>
<td>49</td>
<td></td>
<td>2</td>
</tr>
<tr>
<td>H₂</td>
<td>168,1</td>
<td>14</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>H₂O₂</td>
<td>289,3 [86]</td>
<td>2</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>N₂</td>
<td>247,0</td>
<td>23</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>N₂O</td>
<td>232,4 [86]</td>
<td>2</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>NH</td>
<td>306,0</td>
<td>20</td>
<td>49</td>
<td></td>
<td>22</td>
</tr>
<tr>
<td>NH₂</td>
<td>308,6</td>
<td>23</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>N₂H₄</td>
<td>320,4</td>
<td>14</td>
<td>49</td>
<td></td>
<td>14, 49</td>
</tr>
<tr>
<td>HNO</td>
<td>171,4</td>
<td>14</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C₈</td>
<td>1505,0</td>
<td>20</td>
<td>49</td>
<td></td>
<td>22</td>
</tr>
<tr>
<td>C₃</td>
<td>1958,0</td>
<td>23</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>CO₂</td>
<td>330,4</td>
<td>14</td>
<td></td>
<td>18</td>
<td>64</td>
</tr>
<tr>
<td>CH</td>
<td>640,0</td>
<td>20</td>
<td>49</td>
<td></td>
<td>22</td>
</tr>
<tr>
<td>CH₂</td>
<td>476,0</td>
<td>23</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>CH₄</td>
<td>312,0</td>
<td>23</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>HCO</td>
<td>187,4</td>
<td>14</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>H₂CO</td>
<td>312,0</td>
<td>14</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>CN</td>
<td>707,0</td>
<td>20</td>
<td>49</td>
<td></td>
<td>22</td>
</tr>
<tr>
<td>HCN</td>
<td>569,1 [86]</td>
<td>2</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C₅H</td>
<td>176,8</td>
<td>14</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C₅H₂</td>
<td>231,8 [86]</td>
<td>2</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C₅H₄</td>
<td>209,0 [30]</td>
<td>2, 3</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C₅N₂</td>
<td>348,6 [86]</td>
<td>2</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

KEY: (1) Substance; (2) Value; (3) Method; (4) Literature.
An estimate of the errors in the approximation of the collision integrals $\sigma^{Q1,1+}$ and $\sigma^{Q1,2+}$ by the Lennard-Jones potential is presented in Table 2.13 where, depending on temperature, the moduli of relative deviations in percents $\xi^{Q1,1}$ and $\xi^{Q2,2}$ (the numerator and denominator respectively) are presented in the form of a fraction:

\[ \xi^{Q1,1} = \frac{\sigma^{Q1,1+} - (\sigma^{Q1,1+})_{n, a}}{\sigma^{Q1,1+}}, \]

(2.6)

\[ \xi^{Q2,2} = \frac{\sigma^{Q2,2+} - (\sigma^{Q2,2+})_{n, a}}{\sigma^{Q2,2+}}, \]

(2.7)

where $(\sigma^{Q1,1+})_{n, a}$ - the collision integral calculated using the Lennard-Jones potential.

### Table 2.13. Errors in approximating collision integrals.

<table>
<thead>
<tr>
<th>Взаимодействие</th>
<th>Метод определения</th>
<th>T-600 К</th>
<th>1000</th>
<th>1400</th>
<th>1800</th>
<th>2200</th>
<th>2600</th>
<th>3000</th>
<th>3400</th>
<th>3800</th>
<th>4200</th>
</tr>
</thead>
<tbody>
<tr>
<td>O—O</td>
<td>10</td>
<td>—</td>
<td>—</td>
<td>2/5</td>
<td>0/3</td>
<td>2/2</td>
<td>3/0</td>
<td>5/1</td>
<td>6/2</td>
<td>7/3</td>
<td></td>
</tr>
<tr>
<td>H—H</td>
<td>10</td>
<td>—</td>
<td>—</td>
<td>4/8</td>
<td>2/6</td>
<td>0/4</td>
<td>2/2</td>
<td>5/0</td>
<td>7/2</td>
<td>9/5</td>
<td></td>
</tr>
<tr>
<td>N—N</td>
<td>10</td>
<td>—</td>
<td>—</td>
<td>0/6</td>
<td>1/5</td>
<td>3/3</td>
<td>5/1</td>
<td>7/1</td>
<td>8/2</td>
<td>9/3</td>
<td></td>
</tr>
<tr>
<td>O₂—O₂</td>
<td>2, 6, 7, 10</td>
<td>0/1</td>
<td>2/3</td>
<td>2/3</td>
<td>2/3</td>
<td>1/3</td>
<td>0/3</td>
<td>2/2</td>
<td>3/1</td>
<td>5/0</td>
<td>7/1</td>
</tr>
<tr>
<td>H₂—H₂</td>
<td>2, 6, 10</td>
<td>0/3</td>
<td>3/9</td>
<td>2/10</td>
<td>1/9</td>
<td>4/8</td>
<td>7/6</td>
<td>9/4</td>
<td>12/3</td>
<td>13/1</td>
<td>17/1</td>
</tr>
<tr>
<td>N₂—N₂</td>
<td>2, 6, 7, 10</td>
<td>3/3</td>
<td>6/9</td>
<td>5/9</td>
<td>2/8</td>
<td>1/6</td>
<td>4/5</td>
<td>6/3</td>
<td>8/2</td>
<td>10/0</td>
<td>12/1</td>
</tr>
<tr>
<td>H₂O—H₂O</td>
<td>2</td>
<td>1/0</td>
<td>1/1</td>
<td>1/2</td>
<td>1/1</td>
<td>1/1</td>
<td>1/1</td>
<td>1/1</td>
<td>1/1</td>
<td>1/1</td>
<td></td>
</tr>
<tr>
<td>CO—CO</td>
<td>2, 6, 7</td>
<td>1/0</td>
<td>7/9</td>
<td>8/10</td>
<td>6/9</td>
<td>3/6</td>
<td>1/3</td>
<td>5/1</td>
<td>9/5</td>
<td>14/9</td>
<td>18/12</td>
</tr>
<tr>
<td>CO₂—CO₂</td>
<td>2, 6</td>
<td>0/0</td>
<td>0/0</td>
<td>0/0</td>
<td>0/0</td>
<td>0/0</td>
<td>0/0</td>
<td>0/0</td>
<td>0/0</td>
<td>0/0</td>
<td></td>
</tr>
<tr>
<td>NO—NO</td>
<td>2, 6, 10</td>
<td>0/0</td>
<td>0/0</td>
<td>0/0</td>
<td>0/0</td>
<td>0/0</td>
<td>0/1</td>
<td>0/1</td>
<td>1/1</td>
<td>1/1</td>
<td>2/1</td>
</tr>
</tbody>
</table>

**KEY:** (1) Interaction; (2) Method of determining.
The column "Method of determining \( \sigma^{\text{rel}} \)" in Table 2.13 indicates the methods on the basis of which the collision integrals (numbering of the methods corresponds to Table 2.12) are calculated in [40, 41]. For atomic substances, the results are given only with \( T \geq 1800^\circ \text{K} \) since with a lower temperature the content of these substances in the combustion products is insignificant.

In determining the parameters \( \tau \) and \( \varepsilon/k \) for the remaining individual substances of the first group, use was made of the experimental data on the viscosity coefficient and the virial coefficients (Ar, NO\(_2\), NH\(_3\), CH\(_4\)) and semi-emperical, indirect, and empirical methods (OH, C).

The parameters of the potentials for individual substances of the second group (see Table 2.12) were determined primarily by indirect and empirical methods. The selection of these methods was conditioned by the absence of direct experimental data on the equilibrium (virial coefficients) and nonequilibrium (collision integrals, \( \gamma \), \( \lambda \), \( D \)) properties for these substances. For molecules H\(_2\)O\(_2\), HNO, C\(_3\)O\(_2\), HCO, H\(_2\)CO, the conventional critical constants were first estimated by empirical methods of work [78].

It should be noted that the probable error in calculations of transfer properties here will be comparatively low since the content of the individual substances listed above in the combustion products is low.

It is customary to estimate the constant potentials in the case of the interaction of unlike molecules of combustion products by empirical rules of combination

\[
\begin{align*}
\sigma_{ij} &= \frac{1}{2} (\sigma_i + \sigma_j) \\
\varepsilon_{ij} &= \sqrt{\varepsilon_i \varepsilon_j}.
\end{align*}
\] (2.8)

Some of the results from such an estimate are presented in Volume I of the Reference Book, and we obtained more detailed results using collision integrals \( \sigma^{\text{rel}} \) from [40].
Table 2.14. Errors in the approximation of potential constants.

<table>
<thead>
<tr>
<th>Interaction</th>
<th>Method Approximation</th>
<th>200 K</th>
<th>1000 K</th>
<th>1500 K</th>
<th>2000 K</th>
<th>2500 K</th>
<th>3000 K</th>
<th>3500 K</th>
<th>4000 K</th>
<th>4500 K</th>
<th>5000 K</th>
</tr>
</thead>
<tbody>
<tr>
<td>O—N₂</td>
<td>6, 10</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>O—O₂</td>
<td>6, 10</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>O—NO</td>
<td>10</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>O—H₂</td>
<td>22 (10)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>O—N</td>
<td>10</td>
<td></td>
<td></td>
<td></td>
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Table 2.14 continued.

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<th>1600</th>
<th>1900</th>
<th>2200</th>
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<th>3000</th>
<th>3400</th>
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<td>39/2</td>
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</tbody>
</table>

KEY: (1) Interaction; (2) Method of determining.

Depending on temperature, Table 2.14 gives the moduli of relative errors in percents

\[ \delta Q_{1,3} = \frac{\sigma Q_{1,3}^* - (\sigma Q_{1,3}^*)^{hub}}{\sigma Q_{1,3}^*} \]  

\[ \delta Q_{2,3} = \frac{\sigma Q_{2,3}^* - (\sigma Q_{2,3}^*)^{hub}}{\sigma Q_{2,3}^*} \]

where the values of \( \sigma Q_{1,3}^* \) are taken from [40] and integrals \( (\sigma Q_{1,3}^*)^{hub} \) are determined using the rules of combination. The table also indicates the methods which were employed in [40] when calculating integrals \( \sigma Q_{1,3}^* \) for the case of the interaction of molecules i-j.

Several methods for determining the potential parameters can be recommended for a number of interactions of molecules i-j. In such cases, in [40] the final values of the parameters were determined as a result of averaging. For some interactions, used as initial data for averaging were the rules for combining in combination with the results from measurements of viscosity, with the use of the semi-empirical method, and with the use of measurements of the time of vibrational relaxation and the semi-empirical method (in Table 2.14 designated 22 (2), 2 (10), and 22 (7, 10) respectively).

As is evident from Table 2.14, the errors in the rules of combining are comparative small; in the majority of cases they do not exceed the errors of the experimental data for the intermolecular interaction under high-temperature conditions. Similar data for the
interactions H-O, H-OH, O-OH are presented in Blank's work [16].

Rotational relaxation was considered for a number of individual substances when calculating the coefficient of thermal conductivity. The numbers of the collisions $z_{\text{rot}}$ necessary for the exchange of rotational energy were accepted in the Reference Book on the basis of experimental data. The dependence of $z_{\text{rot}}$ on temperature was considered by an approximate formula of the type (see Volume I, Chapter VIII):

$$z_{\text{rot}} = z_{\text{rot}}^\infty \left[1 + 2.784 \sqrt{\frac{kT}{\varepsilon}} + 5.609 \frac{kT}{\varepsilon} \right]^{-1},$$

(2.11)

where $\varepsilon/k$ - the parameter of the Lennard-Jones potential.

Literature presents data on $z_{\text{rot}}$ at a temperature $\sim 300^\circ K$. On the basis of these data, from formula (2.11) we estimated the values of $z_{\text{rot}}$, and subsequently for the calculations of $z_{\text{rot}}(T)$ formula (2.11) was used. Table 2.15 presents the numbers $z_{\text{rot}}^\infty$ and $z_{\text{rot}}$ with $T = 300^\circ K$ with the corresponding references to the literature. It is appropriate to note that for the combustion products of the fuels examined in Volume II of the Reference Book, the effect of rotational relaxation is relatively low (see Volume I, Chapter VIII). For the majority of cases, the contribution of rotational energy to the coefficient of thermal conductivity can be considered on the basis of the diffusion mechanism of transfer.

<table>
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<tr>
<th>Substance</th>
<th>$z_{\text{rot}}^\infty$</th>
<th>$z_{\text{rot}}$</th>
<th>Literature</th>
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<td>$N_2$</td>
<td>60.0</td>
<td>6.0</td>
<td>72.73</td>
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<tr>
<td>$O_2$</td>
<td>40.8</td>
<td>7.0</td>
<td>72.71</td>
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<tr>
<td>$CO_2$</td>
<td>36.4</td>
<td>5.0</td>
<td>81</td>
</tr>
<tr>
<td>$H_2$</td>
<td>2210.0</td>
<td>250.0</td>
<td>81</td>
</tr>
<tr>
<td>$CH_4$</td>
<td>53.8</td>
<td>9.4</td>
<td>73</td>
</tr>
<tr>
<td>$C_2H_4$</td>
<td>119.6</td>
<td>2.4</td>
<td>73</td>
</tr>
</tbody>
</table>

KEY: (1) Substance; (2) Literature.
2.6. Constants of Rates of Chemical Reactions

The following system of determining reactions was selected on the recommendations of Academician V. N. Kondrat'ev and in accordance with the data of [32, 36, 52, 65, 75, 80] for the fuels which contain atoms of oxygen, carbon, hydrogen, and nitrogen in their composition and are examined in Volume II of the Reference Book:

\[
\begin{align*}
\text{CO} + \text{O} + \text{M} & \rightarrow \text{CO}_2 + \text{M}, \\
\text{H} + \text{H} + \text{M} & \rightarrow \text{H}_2 + \text{M}, \\
\text{O} + \text{O} + \text{M} & \rightarrow \text{O}_2 + \text{M}, \\
\text{OH} + \text{H} + \text{M} & \rightarrow \text{H}_2\text{O} + \text{M}, \\
\text{H} + \text{O} + \text{M} & \rightarrow \text{OH} + \text{M}, \\
\text{N} + \text{N} + \text{M} & \rightarrow \text{N}_2 + \text{M}, \\
\text{OH} + \text{CO} & \rightarrow \text{CO}_2 + \text{H}, \\
\text{OH} + \text{H}_2 & \rightarrow \text{H}_2\text{O} + \text{H}, \\
\text{OH} + \text{OH} & \rightarrow \text{H}_2\text{O} + \text{O}, \\
\text{H}_2 + \text{O} & \rightarrow \text{OH} + \text{H}, \\
\text{O}_2 + \text{H} & \rightarrow \text{OH} + \text{O}, \\
\text{N}_2 + \text{O} & \rightarrow \text{NO} + \text{NO}, \\
\text{NO} + \text{N} & \rightarrow \text{N}_2 + \text{O}, \\
\text{NO} + \text{O} & \rightarrow \text{O}_2 + \text{N}, \\
\text{N} + \text{O} + \text{M} & \rightarrow \text{NO} + \text{M}. 
\end{align*}
\]

The constants of the rates of indicated reactions are presented in Table 2.16. Their values are taken primarily in accordance with the materials of Reference Book [32] and also from the data in [36, 51, 52, 65, 75].

As is known, the rate of reactions which take place with triple collisions depends on the type of catalytic particle M. This question has hardly been studied for the complex mixtures being examined. In this connection, the equations of chemical kinetics for such reactions were written without consideration of the type of catalytic particle although in the selection of a specific constant of the rate of reaction in accordance with the data in Reference Book [32] the dependence of this constant on the type of catalytic particles (with the presence of the corresponding data in the Reference Book) was considered. The rate constant here was selected for such M particles whose concentration is maximum in the combustion products.
Table 2.16. Constants of the rate of direct reactions.

<table>
<thead>
<tr>
<th>Реакция</th>
<th>Константа скорости</th>
<th>Равновесие</th>
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</thead>
<tbody>
<tr>
<td>CO + O + M → CO₂ + M</td>
<td>(3.5 \times 10^{14} \exp \left[- \frac{2.1 \times 10^{-3}}{R_T T} \right])</td>
<td>(\text{см}^3/(\text{моль})^2\text{сек})</td>
</tr>
<tr>
<td>H + H + M → H₂ + M</td>
<td>(1.4 \times 10^{15} \ T^{-1.4})</td>
<td>(\text{см}^3/(\text{моль})^2\text{сек})</td>
</tr>
<tr>
<td>O + O + M → O₂ + M</td>
<td>(3.5 \times 10^{11} \ T^{-0.87})</td>
<td>(\text{см}^3/(\text{моль})^2\text{сек})</td>
</tr>
<tr>
<td>OH + H + M → H₂O + M</td>
<td>(1.2 \times 10^{14} \ T^{-1})</td>
<td>(\text{см}^3/(\text{моль})^2\text{сек})</td>
</tr>
<tr>
<td>H + O + M → OH + M</td>
<td>(3.3 \times 10^{11} \ T^{-0.8})</td>
<td>(\text{см}^3/(\text{моль})^2\text{сек})</td>
</tr>
<tr>
<td>N + N + M → N₂ + M</td>
<td>(2.7 \times 10^{15} \ T^{-0.3})</td>
<td>(\text{см}^3/(\text{моль})^2\text{сек})</td>
</tr>
<tr>
<td>OH + CO → CO₂ + H</td>
<td>(2.5 \times 10^{15} \exp \left[- \frac{5.1 \times 10^{-1}}{R_T T} \right])</td>
<td>(\text{см}^3/(\text{моль})^2\text{сек})</td>
</tr>
<tr>
<td>OH + H₂ → H₂O + H</td>
<td>(1.1 \times 10^{16} \exp \left[- \frac{8.6 \times 10^{-1}}{R_T T} \right])</td>
<td>(\text{см}^3/(\text{моль})^2\text{сек})</td>
</tr>
<tr>
<td>OH + OH → H₂O + O₂</td>
<td>(10^{19} \exp \left[- \frac{1.2 \times 10^{1}}{R_T T} \right])</td>
<td>(\text{см}^3/(\text{моль})^2\text{сек})</td>
</tr>
<tr>
<td>H₂ + O → OH + H</td>
<td>(1.3 \times 10^{19} \exp \left[- \frac{9.86 \times 10^{1}}{R_T T} \right])</td>
<td>(\text{см}^3/(\text{моль})^2\text{сек})</td>
</tr>
<tr>
<td>O₂ + H → OH + O</td>
<td>(2.2 \times 10^{19} \exp \left[- \frac{16.5 \times 10^{1}}{R_T T} \right])</td>
<td>(\text{см}^3/(\text{моль})^2\text{сек})</td>
</tr>
<tr>
<td>N₂ + O → NO + NO</td>
<td>(5.2 \times 10^{15} \exp \left[- \frac{0.107}{R_T T} \right])</td>
<td>(\text{см}^3/(\text{моль})^2\text{сек})</td>
</tr>
<tr>
<td>NO + N → N₂ + O</td>
<td>(3.0 \times 10^{16} \exp \left[- \frac{0.2 \times 10^{-2}}{R_T T} \right])</td>
<td>(\text{см}^3/(\text{моль})^2\text{сек})</td>
</tr>
<tr>
<td>NO + O → O₂ + N</td>
<td>(1.1 \times 10^{16} \exp \left[- \frac{7.1 \times 10^{1}}{R_T T} \right])</td>
<td>(\text{см}^3/(\text{моль})^2\text{сек})</td>
</tr>
<tr>
<td>N + O + M → NO + M</td>
<td>(3.3 \times 10^{11})</td>
<td>(\text{см}^3/(\text{моль})^2\text{сек})</td>
</tr>
</tbody>
</table>

KEY: (1) Reaction; (2) Rate constant; (3) Dimension; (4) \text{см}^6/(\text{моль})^2\text{s}; (5) \text{см}^3/\text{моль s}.

In the accomplishment of the calculations it is accepted that the rate constants of a direct and reverse reaction are connected through the equilibrium constants. The latter are taken from data in Reference Book [49].

Calculation of the nonequilibrium flow in the nozzle was conducted in a linear approximation with a given pressure distribution along the length of the nozzle or along the line of current [27]. This pressure
distribution was determined in the following manner. The value of the mean index of isoentropy of expansion $n$ was calculated for each fuel from the results of the thermodynamic calculation of equilibrium isoentropy expansion. The value of the latter was used for the calculation (by the characteristic method) of pressure distribution along the axis of axisymmetrical nozzles with an angle point and with a uniform flow in the exit section of the nozzle. The pressure distribution which was obtained in this manner was then used in calculations of a unidimensional nonequilibrium flow.

The method for calculating chemically nonequilibrium flows is described in detail in Volume I of the Reference Book. The results for this volume of the Reference Book were obtained on the BESM-4, M-20, and BESM-3M computers in accordance with a special program prepared by V. F. Kolmogorov.

The calculation of a nonequilibrium flow was accomplished from the section in the subsonic part of the nozzle in which the pressure is $p = (0.9-0.95)p_{co}$. From the inlet section of the nozzle and before this section the expansion process is presumed to be equilibrium. Losses in specific impulse $\xi_N$ caused by the nonequilibrium course of the chemical reaction are determined as the difference of the specific impulse of the equilibrium and nonequilibrium flows (with identical values of $\bar{F}$) referred to the specific impulse of the equilibrium flow.

The accuracy of the data obtained was monitored by integral checks for impulse and subdivision of the step. The total error in determining losses of specific impulse $\xi_N$ which arises in connection with the unidimensional approximation, imprecision of the knowledge of constants for the rates of reactions, and errors in numerical integration were estimated at 15-25% of the value of the loss coefficient $\xi_N$.

As shown in Volume I of the Reference Book, losses in specific impulse $\xi_N$ as a result of the nonequilibrium course of chemical reactions depend on the geometry of the nozzle (diameter of the critical section $d_N$ and the relative radius $\bar{r} = r/r^*$), the type of fuel used, the excess oxidant ratio $\alpha_{ok}$, and the stagnation pressure
at the inlet to the nozzle \( P_{co} \). In this connection, this volume of the Reference Book presents for a fixed family of nozzles (in the case being examined, this is a family of shortened nozzles which, with full length, have a uniform and parallel axis of flow in the exit section) results for the following range of change in the parameters:
excess oxidant ratio \( \alpha_{ok} = 0.2 (0.4) - 1.2 (1.4) \) with a change step of 0.2; diameter of critical section \( d_\ast = 5, 10, 20, 50, 150, 250 \text{ mm} \);
relative radius \( \tau = 1-15 \); stagnation pressure at inlet to nozzle \( P_{co} = 0.5, 1, 2, 5, 15, 25 \text{ MN/m}^2 \).
CHAPTER III

ACCURACY OF THE CALCULATION RESULTS

3.1. Effective Changes in the Initial Data on Fuel

The data necessary for the thermodynamic calculation about fuel are the enthalpy and chemical composition of its components. If the interconnection between changes in these data $\Delta x_i$ is absent, the error in the parameters of the combustion products which arises as the result of changes in the data which are accepted is estimated from the formula:

$$|\Delta \varphi| = \sum \left| \frac{\partial \varphi}{\partial x_i} \right| \Delta x_i,$$

where $\varphi$ - the parameter of combustion products.

Because of the large volume of information in this volume of the Reference Book, it was not possible to present the errors of each tabular value. However, for the basic properties of combustion products: $T_{CO}$, $\beta$, $I_s$, $F$, $z$ - the tables of the Reference Book provide the derivatives $(\partial \varphi/\partial x_i)$, which permit estimating the effect of the discrepancies in the initial data.

The derivatives of the parameters for enthalpy are determined with the use of the differential relationships of thermodynamics which are examined in detail in the first volume of the Reference Book.
The derivatives of the parameters of combustion products \( T_{co}, \beta, I_{S}, F, z \) for the chemical composition of the fuel components are determined numerically in the Reference Book by varying the given weight fraction of the admixture in the component. This varying is conducted in such a way as to ensure the necessary accuracy of linear interpolation for extrapolation for the case of the real admixture content in the fuel components. Examined below is a method for selecting the weight fraction of admixture \( g \) from the range \( 0 < g \leq g_{\text{max}} \) for the numerical determination of the derivatives.

Let a change in any parameter depending on the content (for example weight fraction) of the admixture in the fuel component be described by the function \( y = f(x) \).

With small quantities of admixture the function \( y = f(x) \) can be described with sufficient accuracy by a second-order curve, for example, by the parabola

\[
y_i = ax + bx^2.
\] (3.1)

In the Reference Book, the linear approximation of the function \( y = f(x) \) is taken, i.e.,

\[
y \approx y_i = kx.
\] (3.2)

It is necessary to select point \( x_1 \) in such a way that with the approximation of the parabola \( y_1 \) with a straight line which passes through point \( y = 0 \) and \( y = y_1(x_1) \) the greatest error in the range \( 0 - x_{\text{max}} \) is minimum.

From the condition for the intersection of curves at point \( x = x_1 \) we find the value of \( k \):

\[
k = a + bx_1.
\] (3.3)

Now the error in the linear approximation can be calculated from the formula:
\[ \Delta y = y_1 - y_2 = bx(x - x_1). \]  

(3.4)

It can be shown that the value of \(x_2\) which corresponds to the extremum of the function \(\Delta y\) in the range \(0 \leq x \leq x_1\) is equal to \(1/2 \cdot x_1\).

Thus, the least maximum error of linear approximation arises in the case

\[ |\Delta y(x)_{\text{max}}| = |\Delta y_\left(\frac{x_1}{2}\right)|. \]  

(3.5)

From this condition we obtain that the value of \(x_1\) does not depend on the parameters of a parabola and equals \(\sim 0.83 \cdot x_{\text{max}}\).

With consideration of this, when determining the derivatives for each fuel component the weight fraction of the admixture was designated from the range \(0 \leq g \leq g_{\text{max}}\). The estimate of the accuracy of extrapolation or interpolation when using the derivatives found in this manner was conducted by special thermodynamic calculations. Several illustrating results of these calculations are presented in Tables 3.1-3.4. The following designations are adopted in the Tables: 

- \(g_{\text{max}}\) - the maximum weight fraction of the admixture in the component (%),
- \(\Delta_1\) - the absolute change in the parameter with a change in the admixture content from \(g = 0\) to \(g = g_{\text{max}}\) \((T_{\text{CO}}^0K, \beta, I_s'\text{ m/s})\),
- \(\Delta_2\) - the maximum absolute error in determining \(\Delta_1\) when using the derivatives \((T_{\text{CO}}^0K, \beta, I_s'\text{ m/s})\).

The values of \(\Delta_1\) are found from the results of thermodynamic calculation with \(g = 0\) and \(g = g_{\text{max}}\).

For the fuel compounds being examined in this volume, the derivatives for the chemical composition of components permit a determination of the change in parameters in the ranges of change of weight fractions of admixtures taken with the same accuracy as the accuracy in presenting the parameters themselves in the tables of the Reference Book.

Variations in pressure at the inlet of the nozzle \(p_{\text{CO}}\) and the excess oxidant ratio in the ranges adopted in the Reference Book
have a weak influence on the accuracy of calculating the change in parameters.

With an increase in the degree of reduction of pressure $\xi$ the error in determining the change in relative area is usually increased. The accuracy in determining the change in specific impulse in a vacuum is virtually unchanged with a change in $\xi$.

Tables 3.1-3.4 illustrate these conclusions.

Table 3.1. Accuracy in calculating the properties of combustion products with extrapolation for the composition of components.

$q_{ok} = 1$, $p_{co} = 10$ MN/m$^2$

| \hline
<table>
<thead>
<tr>
<th>$\xi_{ok}$</th>
<th>Components (f)</th>
<th>$\xi_{max}$</th>
<th>$T_{co}^*\Delta$</th>
<th>$\Delta_t$</th>
<th>$\Delta_e$</th>
<th>$I_{co}^*\Delta$</th>
<th>$\Delta_t$</th>
<th>$\Delta_e$</th>
<th>$F_0(\xi=100)$</th>
<th>$\Delta_t$</th>
<th>$\Delta_e$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>O$_2$ N$_4$ 0.8</td>
<td>3.3 &lt;0.1</td>
<td>0.1 &lt;0.1</td>
<td>0.8 &lt;0.1</td>
<td>0.012 &lt;0.001</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>O$_3$ N$_4$ 0.5</td>
<td>4.7 &lt;0.1</td>
<td>2.4 &lt;0.1</td>
<td>4.5 &lt;0.1</td>
<td>&lt;0.4 &lt;0.001</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>H$_2$ N$_4$ 0.8</td>
<td>6.4 0.4</td>
<td>0.8 0.3</td>
<td>1.3 0.3</td>
<td>0.004 0.002</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>N$_4$ H$_2$ 0.8</td>
<td>5.7 0.4</td>
<td>0.7 0.1</td>
<td>1.8 0.1</td>
<td>0.008 0.003</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

KEY: (1) Components; (2) Admixtures; (3) m/s; (4) m/s; (5) Kerosene; (6) Change.

When conducting calculations with the use of derivatives, it is necessary to keep the following in mind. The derivatives for the content of admixtures in the fuel components are calculated with a constant relationship of the fuel components $k_1$ which is presented in the table. Thus, the thermodynamic parameters which are calculated by extrapolation for components which contain an admixture in the range of $0 < \xi < \xi_{max}$ correspond to the constant value $k_1$ and to the value $q_{ok}$ which varies depending on the weight fraction of the


admixture \( g \). The value of \( \alpha_{ok} \) should be determined in such cases from formulas (1.8) and (1.10) of Volume I of the Reference Book after the composition of the fuel components, i.e., the weight fractions of the admixtures, has been selected.

Table 3.2. Accuracy of calculation of properties of combustion products with extrapolation for composition of components \( \alpha_{ok} = 1, P_{co} = 10 \) MN/m².

<table>
<thead>
<tr>
<th>Компоненты (1)</th>
<th>Примеси (2)</th>
<th>( \alpha_{max} ), %</th>
<th>( P_{co} ), MN/m²</th>
<th>( T_{298}, ) °K</th>
<th>( v, ) м/сек (3)</th>
<th>( \rho_{2}, ) м/сек (5)</th>
<th>( \varphi )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \delta )</td>
<td>( \delta )</td>
<td>0,8</td>
<td>0,1</td>
<td>0,5</td>
<td>0,9</td>
<td>0,2</td>
<td>0,002</td>
</tr>
<tr>
<td>Kerosene</td>
<td>Изменение C/H (( \delta ))</td>
<td>±6</td>
<td>0,5</td>
<td>0,1</td>
<td>0,9</td>
<td>0,2</td>
<td>0,006</td>
</tr>
<tr>
<td>( \delta )</td>
<td>( \delta )</td>
<td>0,8</td>
<td>10</td>
<td>0,9</td>
<td>0,1</td>
<td>1,4</td>
<td>0,002</td>
</tr>
<tr>
<td>Kerosene</td>
<td>Изменение C/H (( \delta ))</td>
<td>±6</td>
<td>0,4</td>
<td>0,1</td>
<td>1,4</td>
<td>0,2</td>
<td>0,007</td>
</tr>
<tr>
<td>( \delta )</td>
<td>( \delta )</td>
<td>0,8</td>
<td>50</td>
<td>0,9</td>
<td>0,1</td>
<td>1,8</td>
<td>0,002</td>
</tr>
<tr>
<td>Kerosene</td>
<td>Изменение C/H (( \delta ))</td>
<td>±6</td>
<td>&lt;0,1</td>
<td>0,2</td>
<td>1,1</td>
<td>0,2</td>
<td>0,008</td>
</tr>
</tbody>
</table>

| KEY: (1) Components; (2) Admixtures; (3) m/s; (4) Kerosene; (5) Change. |

Table 3.3. Accuracy of calculation of properties of combustion products with extrapolation for composition of components \( \alpha_{ok} = 1.0; \varepsilon = 100. \)

<table>
<thead>
<tr>
<th>Компоненты (1)</th>
<th>Примеси (2)</th>
<th>( \alpha_{max} ), %</th>
<th>( P_{co} ), MN/m²</th>
<th>( T_{298}, ) °K</th>
<th>( v, ) м/сек (3)</th>
<th>( \rho_{2}, ) м/сек (5)</th>
<th>( \varphi )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \delta )</td>
<td>( \delta )</td>
<td>0,8</td>
<td>1,0</td>
<td>0,5</td>
<td>0,9</td>
<td>0,2</td>
<td>0,002</td>
</tr>
<tr>
<td>Kerosene</td>
<td>Изменение C/H (( \delta ))</td>
<td>±6</td>
<td>0,5</td>
<td>0,1</td>
<td>0,9</td>
<td>0,2</td>
<td>0,002</td>
</tr>
<tr>
<td>( \delta )</td>
<td>( \delta )</td>
<td>0,8</td>
<td>10</td>
<td>0,9</td>
<td>0,1</td>
<td>1,4</td>
<td>0,002</td>
</tr>
<tr>
<td>Kerosene</td>
<td>Изменение C/H (( \delta ))</td>
<td>±6</td>
<td>0,4</td>
<td>0,1</td>
<td>1,4</td>
<td>0,2</td>
<td>0,007</td>
</tr>
<tr>
<td>( \delta )</td>
<td>( \delta )</td>
<td>0,8</td>
<td>50</td>
<td>0,9</td>
<td>0,1</td>
<td>1,8</td>
<td>0,002</td>
</tr>
<tr>
<td>Kerosene</td>
<td>Изменение C/H (( \delta ))</td>
<td>±6</td>
<td>&lt;0,1</td>
<td>0,2</td>
<td>1,1</td>
<td>0,2</td>
<td>0,008</td>
</tr>
</tbody>
</table>

| KEY: (1) Components; (2) Admixtures; (3) m/s; (4) Kerosene; (5) Change. |
Table 3.4. Accuracy of calculation of properties of combustion products with extrapolation for composition of components $P_{CO} = 10$ MH/m$^2$, $\xi = 100$.

<table>
<thead>
<tr>
<th>Компоненты (1)</th>
<th>Признак (2)</th>
<th>$E_{max.}$ (3)</th>
<th>$a_{ok}$</th>
<th>$T_{CO}K$</th>
<th>$A_{m/s$ (4)</th>
<th>$t_{c}^0$ (5)</th>
<th>$a$</th>
<th>$\gamma$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$O_2$</td>
<td>$N_2$</td>
<td>0.8</td>
<td>0.4</td>
<td>32.7</td>
<td>&lt;0.1</td>
<td>10.7</td>
<td>&lt;0.1</td>
<td>12.6</td>
</tr>
<tr>
<td>1.0</td>
<td>6.6</td>
<td>0.6</td>
<td>0.9</td>
<td>0.1</td>
<td>1.4</td>
<td>0.2</td>
<td>0.002</td>
<td>0.001</td>
</tr>
<tr>
<td>1.2</td>
<td>5.4</td>
<td>0.6</td>
<td>0.9</td>
<td>0.2</td>
<td>0.8</td>
<td>0.2</td>
<td>0.010</td>
<td>0.002</td>
</tr>
<tr>
<td>$\text{Керосин}$</td>
<td></td>
<td>±6</td>
<td>0.4</td>
<td>19.0</td>
<td>1.2</td>
<td>8.7</td>
<td>0.8</td>
<td>17.2</td>
</tr>
<tr>
<td>1.0</td>
<td>0.4</td>
<td>0.1</td>
<td>11.4</td>
<td>1.0</td>
<td>20.9</td>
<td>1.8</td>
<td>0.007</td>
<td>0.002</td>
</tr>
<tr>
<td>1.2</td>
<td>3.2</td>
<td>0.2</td>
<td>10.5</td>
<td>1.1</td>
<td>19.7</td>
<td>1.8</td>
<td>0.006</td>
<td>0.002</td>
</tr>
</tbody>
</table>

KEY: (1) Components; (2) Admixtures; (3) m/s; (4) Kerosene; (5) Change.

3.2. The Effect of Errors in Thermodynamic Properties of Individual Substances

Sources of errors in calculated values of properties of combustion products were examined in the first volume of the Reference Book. In particular, the absence of methods which permit making a substantiated evaluation of the error in calculations which arises as a result of errors in the thermodynamic properties of individual substances in the literature was noted. In preparing this volume of the Reference Book, a special method was worked out which permits estimating the errors [5].

With a constant elementary chemical composition of fuel any parameter of the combustion products, we will designate it additionally by $\varphi$, can be represented by the function of enthalpy $i$ and entropy $s$ of the mixture. The latter, in turn, are determined by the elementary chemical composition, pressure of the combustion products, thermodynamic properties (by enthalpy $i_0^q$ and entropy $s_0^q$ of the individual substances), and the enthalpy of the fuel. Consequently, the error $\Delta \varphi$ which arises...
due to the errors in the thermodynamic properties of individual substances can be expressed by $\Delta H^0_q$ and $\Delta S^0_q$ in the final analysis.

The following expressions which describe the enthalpy and entropy of the q-th substance in the gaseous state are known:

\[
I_q^0 = \Delta H^0_q + (H^0_1 - H^0_0)_q - (H^0_2 - H^0_0)_q,
\]

\[
(H^0_1 - H^0_0)_q = R_0 T^2 \left( \frac{\partial \ln Q_q}{\partial T} \right)_p,
\]

\[
S^0_q = R_0 \ln \frac{Q_q}{Q_0} + R_0 T \left( \frac{\partial \ln Q_q}{\partial T} \right)_p,
\]

where $Q_q$ - the statistical sum for the states of the molecules.

As is evident, the errors $\Delta H^0_q$ and $\Delta S^0_q$ are determined by the errors of a number of values, for example, $\Delta H_{1000}$, $R_0 \ln Q/N$ and so forth which are arbitrarily designated further as $\omega_{qk}$ ($k = 1, 2, 3, \ldots n$).

Consequently, the error of any parameter $\Phi$ with small errors $\omega_{qk}$ is a linear functional relative to $\Delta \omega_{qk}$:

\[
\Delta \Phi = \sum_q \sum_k \left( \frac{\partial \Phi}{\partial \omega_{qk}} \right)_{\text{co}, \text{pc}, \text{co}} \Delta \omega_{qk}. \tag{3.9}
\]

To calculate $\Delta \Phi$ in the general case it is necessary to solve the problem of linear programming since interconnections exist for certain $\omega_{qk}$.

Of greatest practical interest is the estimate of errors in the calculation of specific impulse in a vacuum $I_s$ and also of the flow-rate complex $\beta$, temperature $T_{co}$, and molecular weight $\mathcal{M}_{co}$. In particular, differentiating the well-known expression for specific impulse $I_s$, we can write with $\text{co}_{co}$, $\text{pc}_{co}$, $p = \text{const}$ (the subscript "k" is omitted here and subsequently):

\[
\left( \frac{\partial I_s}{\partial \omega} \right)_{\text{co}_{co}, \text{pc}_{co}, p} = \frac{1}{m} \left( \frac{\partial I_s}{\partial \omega} \right)_{\text{co}_{co}, \text{pc}_{co}, p} \times (3.10)
\]

\[
\times [\rho_p - 1 - \rho_{co} (\partial \rho / \partial \omega_{co})_{\text{co}_{co}, \text{pc}_{co}, p}]
\]
where \( f \) - the specific area of the nozzle's exit section.

We present the entropy of the combustion products at the inlet to the nozzle \( S_{co} \) and in the exit section of the nozzle \( S \) in the form of the functions

\[
s_{co} = S_{co}(p_{co}, l_{co}, w_{eco}), \\
S = S(p, \varphi, \omega),
\]

(3.11)

where \( \varphi \) - any parameter of combustion products in the nozzle, for example, \( T, \rho, l_{co}, \mu \), and so forth.

Equating the total differentials of the functions (3.11) for the isoentropic process of expansion (\( s = \text{const} \)) with \( i_{co}, p_{co}, p = \text{const} \), we obtain

\[
\left( \frac{\partial p}{\partial w_{eco}} \right)_{i_{co}, p_{co}, p} = \left[ \left( \frac{\partial p}{\partial w_{eco}} \right)_{p_{co}, i_{co}} - \left( \frac{\partial p}{\partial \varphi} \right)_{p, \omega} \right] \left( \frac{\partial \varphi}{\partial w_{eco}} \right)_{i_{co}}
\]

(3.12)

where the given relationship

\[
t_{\varphi} = \frac{\partial w_{eco}}{\partial p_{eco}} = \frac{\Delta w_{eco}}{\partial p_{eco}}.
\]

Expression (3.12) can be reduced to a more rational form using the equality

\[
\left( \frac{\partial p}{\partial \varphi} \right)_{p, \omega} \left( \frac{\partial \varphi}{\partial l_{eco}} \right)_{s, p} \left( \frac{\partial l_{eco}}{\partial \varphi} \right)_{p, \omega} = -1.
\]

(3.14)

As a result, we obtain

\[
\left( \frac{\partial p}{\partial w_{eco}} \right)_{i_{co}, p_{co}, p} = \left( \frac{\partial p}{\partial w_{eco}} \right)_{p_{co}, i_{co}} \left( \frac{\partial \varphi}{\partial \varphi} \right)_{\omega} + \left( \frac{\partial \varphi}{\partial \varphi} \right)_{p, \omega} \cdot t_{\varphi}.
\]

(3.15)
Equation (3.15) coincides with equation (11.39) obtained in Volume I of this Reference Book and which describes the change in the thermodynamic function $\phi$ with a change in content of the chemical element $b_{T_1}$ in the fuel. This agreement is caused by the circumstance that in both cases the thermodynamic function $\phi$ is a function of the type $\phi = \phi(\alpha, \beta, \xi)$, where $\alpha$ and $\beta$ are any two other thermodynamic functions and $\xi$ is the content of the chemical element in the fuel, the error in calculating the function or any parameter of a nonthermodynamic character, which determines the function $\phi$.

The derivatives $\left(\frac{\partial \phi}{\partial \xi}\right)_p$ are determined using known thermodynamic relationships presented, for example, [6]. To determine the derivatives $\left(\frac{\partial s_{res}}{\partial \omega_{res}}\right)_{p, T} = \frac{\partial f}{\partial \omega}$ it is expedient to obtain additional relationships which permit finding derivatives as a result of a differentiation with $p, T = \text{const}$. These relationships substantially simplify the computing scheme of the calculation.

Any parameter of the combustion products $\psi$ can be represented by the functions

$$\begin{align*}
\psi &= \psi(p, T, \omega) \\
\psi &= \psi(p, \psi, \omega)
\end{align*}$$

where $\psi$ - is some thermodynamic function, for example, enthalpy or entropy.

Equating the total differentials of the functions $\phi$ expressed through both systems of arguments, with $p, \psi = \text{const}$ we obtain:

$$\left(\frac{\partial \phi}{\partial \omega}\right)_{p, \psi} = \left(\frac{\partial \phi}{\partial \omega}\right)_{p, T} + \left(\frac{\partial \phi}{\partial \omega}\right)_{T, p}$$

To determine the derivative $\left(\frac{\partial T}{\partial \omega}\right)_{p, \psi}$ we write the total differential of the function $\phi = \phi(p, T, \omega)$: With $p, \psi = \text{const}$, we have:

$$\left(\frac{\partial T}{\partial \omega}\right)_{p, \psi} = -\frac{\left(\frac{\partial \phi}{\partial \omega}\right)_{p, \psi}}{\left(\frac{\partial \phi}{\partial T}\right)_{p}}$$
Substituting this result into equality (3.17), we finally obtain

$$
\left( \frac{\partial \psi}{\partial \omega} \right)_{p, T} = \left( \frac{\partial \psi}{\partial \omega} \right)_{p, r} - \left( \frac{\partial \psi}{\partial \omega} \right)_{p, T} \left( \frac{\partial \psi}{\partial \omega} \right)_{p, r}.
$$

(3.19)

For derivatives which enter into the formula for \((\partial \psi/\partial \omega)_{p, T}/(\partial \psi/\partial \omega)_{p, r}\), on the basis of (3.15) with consideration of the differential relationships of thermodynamics we can write: for enthalpy \(i\) (with \(\psi = s\)):

$$
\left( \frac{\partial i}{\partial \omega} \right)_{p, s} = \left( \frac{\partial i}{\partial \omega} \right)_{p, r} - T \left( \frac{\partial s}{\partial \omega} \right)_{p, r};
$$

(3.20)

for density of combustion products \(\rho = \mu_{MT}/RT\) (with \(\psi = s\)):

$$
\left( \frac{\partial \rho}{\partial \omega} \right)_{p, s} = \rho \left[ \left( \frac{\partial \ln \mu_{MT}}{\partial \omega} \right)_{p, r} + \frac{a_{e} T}{\epsilon_{p}} \left( \frac{\partial s}{\partial \omega} \right)_{p, r} \right];
$$

(3.21)

for entropy \(S_{co}\) (with \(\psi = ic_{co}\)):

$$
\left( \frac{\partial S_{co}}{\partial \omega} \right)_{p, c_{co}} = \left( \frac{\partial S_{co}}{\partial \omega} \right)_{p, c_{co}, T_{co}} - \frac{1}{T_{co}} \left( \frac{\partial i_{co}}{\partial \omega} \right)_{p, c_{co}, T_{co}}.
$$

(3.22)

Here \(MT\) - the number of moles of fuel which ensures the equality \(p = \Sigma nq\) (see Volume I, Chapter V).

As is evident, the determination of derivatives \((\partial \psi/\partial \omega)_{p, c_{co}, T_{co}}\) in the final analysis is reduced to the calculation of derivatives \((\partial \psi/\partial \omega)_{p, r}\) \((\psi = i, s)\) in the corresponding sections of the nozzle. Derivatives \((\partial \psi/\partial \omega)_{p, r}\) are determined as a result of differentiation of expressions for specific enthalpy and entropy. In particular, for homogeneous combustion products we obtain:

$$
\left( \frac{\partial i}{\partial \omega} \right)_{p, r} = \frac{\sum n_{\psi} \zeta_{n} \left( \frac{\partial \ln \mu_{n}}{\partial \omega} \right)_{p, r} + n_{\psi} \left( \frac{\partial i_{n}^{0}}{\partial \omega} \right)_{p, r}}{\mu_{T} \cdot M_{T}} - i \left( \frac{\partial \ln M_{T}}{\partial \omega} \right)_{p, r},
$$

(3.23)

$$
\left( \frac{\partial S}{\partial \omega} \right)_{p, r} = \frac{\sum n_{\psi} \left( \frac{\partial \ln \mu_{n}}{\partial \omega} \right)_{p, r} \left[ S_{n}^{0} - R_{n} (1 + \ln \mu_{n}) \right] + n_{\psi} \left( \frac{\partial S_{n}^{0}}{\partial \omega} \right)_{p, r}}{\mu_{T} M_{T}} - s \left( \frac{\partial \ln M_{T}}{\partial \omega} \right)_{p, r},
$$

(3.24)

47
where \( n \) - the subscript of any component of the combustion products, 
\( q \) - the subscript of the component of the combustion products, the 
effect of whose errors in the thermodynamic functions is being studied.

To determine the partial derivatives \((\partial \ln n_i/\partial \omega_q)_{p,T}\) and \((\partial \ln M_i/\partial \omega_q)_{p,T}\)
we differentiate the system of equations for thermodynamic equilibrium 
with respect to \( \omega_q \) with \( p, T = \text{const.} \) As a result, we obtain 
closed systems of equations for the calculation of derivatives:

\[
\left(\frac{\partial \ln n_i}{\partial \omega_q}\right)_{p,T} - \sum_j a_{ij} \left(\frac{\partial \ln n_j}{\partial \omega_q}\right)_{p,T} = \delta_{iq} R_j + \delta_{ij} R_i, \tag{3.25}
\]

\[
\sum_j a_{ij} n_j \left(\frac{\partial \ln n_j}{\partial \omega_q}\right)_{p,T} + n_i \left(\frac{\partial \ln n_i}{\partial \omega_q}\right)_{p,T} -
- B_i \left(\frac{\partial \ln M_i}{\partial \omega_q}\right)_{p,T} = 0, \tag{3.26}
\]

\[
\sum n_i \left(\frac{\partial \ln n_i}{\partial \omega_q}\right)_{p,T} = 0, \tag{3.27}
\]

where \( B_i = \sum a_{ij} n_j + n_i, \) \( i \) - the subscript of atomic substance, \( j \) - the subscript of molecular substance, \( a_{ij} \) - the stoichiometric coefficient of the dissociation reaction to the atoms, \( \delta_{iq}, \delta_{ij} \) - the Kronecker symbols. The values of \( R_i, R_j \) and also the derivatives \((\partial S_i/\partial \omega_q)_{p,T}\), 
\((\partial M_i/\partial \omega_q)_{p,T}\) are obtained respectively by differentiation of the expression 
for the equilibrium constant and formulas (3.6) - (3.8).

A similar approach can be used to determine errors of parameters 
in the combustion chamber. Writing the total differential of the 
function \( i = i(p, \varphi, \omega_q) \) with \( p = p_0 = \text{const} \) and \( i = i_{CO} = \text{const} \), we obtain:

\[
\left(\frac{\partial \varphi}{\partial \omega_q}\right)_{p,T} = -\left(\frac{\partial i}{\partial \omega_q}\right)_{p,T} \left(\frac{\partial \varphi}{\partial i}\right)_p. \tag{3.28}
\]

An expression of the type (3.19) is valid for the derivative 
\((\partial \omega_q/\partial \omega_q)_{p,T}\), consequently,
For the stagnation temperature at the inlet to the nozzle ($\varphi = T_{co}$) and molecular weight ($\varphi = \mu_{co}$) expression (3.29) takes the form:

\[ \left( \frac{\partial T_{co}}{\partial \omega_{eco}} \right)_{\mu_{co}, T_{co}, \varphi} = -\frac{1}{c_{p}} \left( \frac{\partial \mu_{co}}{\partial \omega_{eco}} \right)_{\mu_{co}, T_{co}, \varphi} \]  

(3.30)

\[ \left( \frac{\partial \mu_{co}}{\partial \omega_{eco}} \right)_{\mu_{co}, T_{co}, \varphi} = \mu_{co} \left( \frac{\partial (T_{co} \ln Q_{co})}{\partial \omega_{eco}} \right) \]  

(3.31)

where $\left( \frac{\partial \mu_{co}}{\partial \omega_{eco}} \right)_{\mu_{co}, T_{co}, \varphi}$ is calculated from a formula of the type (3.23).

The arguments $\omega_{q,k}$ should be selected on the basis of an analysis of known expressions for the thermodynamic properties of individual substances, for example, (3.6)-(3.8). The errors $\Delta \omega_{q,k}$ can be selected on the basis of published data. In particular, for such arguments of $\omega_{q,k}$ as $\Delta H_{f,co}$, $R_{0} \ln Q_{co}$, heat of fusion (polymorphic transformations) and others, systematic data are presented in Reference Books [45-49]. For some values, for example, $R_{0} \left( \frac{\partial \ln Q_{co}}{\partial \varphi} \right)_{\mu}$, reliable data are absent. Information on the interconnection among $\omega_{q,k}$ both for the given substance ($k = 1, 2, 3 \ldots n$) as well as among $\omega_{q,k}$ for various substances ($q = 1, 2, 3, \ldots l$) is also extremely limited.

3.3. The Effect of Errors in the Thermophysical Properties of Individual Substances

As is known, the procedure for determining the transfer properties - coefficients of viscosity, heat conductivity, and diffusion - is based on the following mandatory conditions.

1. Information on the composition of the combustion products is necessary.
This information is provided by methods presented in Volume I of the Reference Book.

2. A kinetic theory which is applicable for the combustion products systems being examined must be developed.

We cannot fail to note that despite the considerable theoretical studies, a rigid kinetic theory is virtually absent for actual combustion products systems (nonspherical molecules, the presence of internal degrees of freedom and excited molecules, dense gases). Consequently, the basic source of information on transfer properties is the molecular-kinetic theory of monoatomic rarefied gases which is also used in the Reference Book. Here, an estimate of the corresponding corrections for actual special features of combustion products systems is necessary.

The first volume of the Reference Book provides an estimate of the effect of density and internal degrees of freedom. It was adjudged expedient not to consider the effect of density and to consider the effect of internal degrees of freedom (except for several individual substances) on the basis of the diffusion transfer mechanism. This leads to the corresponding errors in transfer coefficients which, as shown in Volume I of the Reference Book, do not exceed several percent. Also insignificant is the error which arises as a result of the use of excited molecules and atoms of the same interaction potentials as for molecules and atoms in the basic state.

3. Quantitative information on the intermolecular interaction which, at the present time, it is customary to give in the form of an empirical function (potential) of interaction \( \phi(r) \) is necessary. For the temperature region of 2000-4000 K, which is most characteristic for combustion products of chemical fuels, the parameters of the potential in the majority of cases cannot be found using direct experimental data. Virtually the only way is the extrapolation of low-temperature data \((T \leq 1000 K)\) on the properties of transfer to the region of high temperatures or the extrapolation of high-temperature experimental data \((T \sim 5000 K)\) on the scattering of molecular beams.
to the region of low temperature with subsequent matching of the extrapolation results with each other.

It should be noted, however, that such an approach is possible now only for a narrow range of individual substances, primarily components of carbon fuel combustion products. Only an empirical estimate of the parameters of the potential is possible for the remaining components of combustion products, especially of those containing atoms of metal, as a result of the absence of experimental data.

The method of matching experimental data on properties of the transfer and scatter of molecular beams in the work of Samuylov and Tsitelauri [41] was used to determine the section of collisions \( \sigma^{Q^{*}} \) for the interactions \( O_2 - O_2, H_2 - H_2, N_2 - N_2, CO - CO, \) and \( CO_2 - CO_2. \) In this volume of the Reference Book this method is realized as a result of the approximation of the sections of collisions \( \sigma^{Q^{*}} \) by the Lennard-Jones potential (the approximation error is characterized above in Table 2.13).

It is of interest to estimate the errors of the transfer coefficients for the substances mentioned above and several others in comparison with the experimental data and which were calculated in the Reference Book. Presented as an example in Tables 3.5 and 3.6 are the results of such an estimate for the coefficients of viscosity \( \eta \) and heat conductivity \( \lambda \) in the form of errors:

\[
\delta \eta = \frac{\eta - \eta_{\text{expt}}}{\eta_{\text{expt}}} \cdot 100\%.
\]
\[
\delta \lambda = \frac{\lambda - \lambda_{\text{expt}}}{\lambda_{\text{expt}}} \cdot 100\%.
\]

The values of \( \eta_{\text{expt}}, \lambda_{\text{expt}} \) are taken from the data in Reference Book [17, 18]. As is evident from the tables, the error of the coefficients \( \eta \) and \( \lambda \) is permissible in the case where these coefficients are used in calculations of the processes of heat- and mass exchange in engines which use chemical fuel.
For higher temperatures \((T \sim 3000-4000^\circ K)\) the errors in the transfer coefficients of the individual substances mentioned above as well as of atoms and free radicals of \(O,\ H,\ N,\) and \(OH,\) and molecules of \(NO\) comprise approximately 30\% \((-20\% - \) the error in the method for scattering molecular beams and the semi-empirical method of valance bonds for \(OH,\sim 10\% - \) the error in the approximation of \(G_221^*\) by the Lennard-Jones potential).

It is not possible to provide a reliable estimate of the errors in calculating the properties of the transfer of mixtures because of the practical absence of experimental data for combustion products of the fuels examined in the Reference Book. The following approximate relationship was taken to estimate the errors in the viscosity coefficient in the Reference Book (Volume I, Chapter XIV):

\[
\delta\eta = \frac{1}{\mu} \sum \frac{C_\eta}{\eta} \delta\eta_n. \tag{3.32}
\]

Table 3.5. Error in the viscosity coefficient of several gaseous substances.

<table>
<thead>
<tr>
<th></th>
<th>(H_2)</th>
<th>(H_2O)</th>
<th>CO</th>
<th>CO(_2)</th>
<th>CH(_4)</th>
<th>N(_2)</th>
<th>NH(_3)</th>
<th>O(_3)</th>
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<tr>
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<td>1.5</td>
<td>373</td>
<td>7.8</td>
<td>373</td>
<td>15.4</td>
<td>500</td>
<td>1.1</td>
<td>373</td>
</tr>
<tr>
<td>473</td>
<td>0.9</td>
<td>473</td>
<td>1.3</td>
<td>473</td>
<td>9.3</td>
<td>700</td>
<td>0.9</td>
<td>473</td>
</tr>
<tr>
<td>573</td>
<td>0.2</td>
<td>573</td>
<td>1.6</td>
<td>573</td>
<td>3.7</td>
<td>900</td>
<td>0.7</td>
<td>573</td>
</tr>
<tr>
<td>673</td>
<td>0.3</td>
<td>673</td>
<td>3.8</td>
<td>673</td>
<td>0.5</td>
<td>1100</td>
<td>0.1</td>
<td>673</td>
</tr>
<tr>
<td>773</td>
<td>0.6</td>
<td>773</td>
<td>4.8</td>
<td>773</td>
<td>3.6</td>
<td>1300</td>
<td>0.2</td>
<td>773</td>
</tr>
<tr>
<td>873</td>
<td>0.8</td>
<td>873</td>
<td>6.0</td>
<td>873</td>
<td>6.5</td>
<td>1500</td>
<td>0.6</td>
<td>873</td>
</tr>
<tr>
<td>973</td>
<td>2.1</td>
<td>973</td>
<td>7.3</td>
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<td>—</td>
<td>1073</td>
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<td>1.7</td>
<td>1073</td>
</tr>
<tr>
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<td>—</td>
<td>—</td>
<td>1173</td>
<td>10.6</td>
<td>2000</td>
<td>1.9</td>
<td>1173</td>
</tr>
<tr>
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<td>2.3</td>
<td>—</td>
<td>—</td>
<td>1273</td>
<td>11.5</td>
<td>2500</td>
<td>3.5</td>
<td>1273</td>
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52
Table 3.6. Error in the coefficient of heat conductivity of gaseous substances.

<table>
<thead>
<tr>
<th>$\text{H}_2$</th>
<th>$\text{H}_2\text{O}$</th>
<th>$\text{CO}_2$</th>
<th>$\text{CH}_4$</th>
<th>$\text{N}_2$</th>
<th>$\text{NH}_3$</th>
<th>$\text{O}_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Delta \lambda_k$</td>
<td>$\Delta \lambda_{H_2}$</td>
<td>$\Delta \lambda_{H_2O}$</td>
<td>$\Delta \lambda_{CO_2}$</td>
<td>$\Delta \lambda_{CH_4}$</td>
<td>$\Delta \lambda_{N_2}$</td>
<td>$\Delta \lambda_{NH_3}$</td>
</tr>
<tr>
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<td>2.0</td>
<td>393</td>
<td>9.6</td>
<td>400</td>
<td>4.1</td>
<td>373</td>
</tr>
<tr>
<td>600</td>
<td>1.5</td>
<td>443</td>
<td>11.5</td>
<td>500</td>
<td>0.6</td>
<td>393</td>
</tr>
<tr>
<td>800</td>
<td>3.0</td>
<td>493</td>
<td>12.8</td>
<td>600</td>
<td>2.0</td>
<td>433</td>
</tr>
<tr>
<td>1000</td>
<td>3.8</td>
<td>543</td>
<td>13.4</td>
<td>700</td>
<td>2.5</td>
<td>493</td>
</tr>
<tr>
<td>1200</td>
<td>5.7</td>
<td>593</td>
<td>13.6</td>
<td>800</td>
<td>2.7</td>
<td>533</td>
</tr>
<tr>
<td>1400</td>
<td>7.6</td>
<td>—</td>
<td>—</td>
<td>900</td>
<td>2.6</td>
<td>573</td>
</tr>
<tr>
<td>1600</td>
<td>9.6</td>
<td>—</td>
<td>—</td>
<td>1000</td>
<td>2.5</td>
<td>623</td>
</tr>
<tr>
<td>1800</td>
<td>11.5</td>
<td>—</td>
<td>—</td>
<td>1100</td>
<td>2.2</td>
<td>673</td>
</tr>
<tr>
<td>2000</td>
<td>12.2</td>
<td>—</td>
<td>—</td>
<td>1200</td>
<td>1.5</td>
<td>—</td>
</tr>
<tr>
<td>—</td>
<td>—</td>
<td>—</td>
<td>—</td>
<td>1300</td>
<td>1.8</td>
<td>—</td>
</tr>
<tr>
<td>—</td>
<td>—</td>
<td>—</td>
<td>—</td>
<td>1400</td>
<td>1.8</td>
<td>—</td>
</tr>
</tbody>
</table>

For the fuel compounds being examined in this volume, the basic components of the combustion products are $\text{H}_2$, $\text{O}_2$, $\text{H}_2\text{O}$, $\text{CO}$, $\text{CO}_2$, $\text{N}_2$, $\text{OH}$, $\text{H}$, $\text{O}$; the molar fraction of $\text{O}$, $\text{H}$, and $\text{OH}$ for the majority of values of $\alpha_{\text{ok}}$, $p_{\text{so}}$, and $\varepsilon$ is no more than 10%. Consequently, the basic error in calculating the viscosity coefficient of a mixture is introduced by the errors in $\delta_{\eta_{H_2}}$, $\delta_{\eta_{O_2}}$, $\delta_{\eta_{H_2O}}$, $\delta_{\eta_{CO}}$, $\delta_{\eta_{CO_2}}$, and $\delta_{\eta_{N_2}}$. Considering the approximate nature of relation (3.32), it is expedient to take the values of $\delta_{\eta_{H_2}}$ for these substances as identical, as approximately 20-30%. Thus, the possible error in the viscosity coefficient of the combustion products in the tables of the Reference Book is 20-30%; the error in the coefficient of heat conductivity is estimated as

$$\delta_{\lambda} = (1.0 - 1.2)\delta_{\eta}.$$  \hspace{1cm} (3.33)

3.4. Extrapolation Accuracy

The tables in the Reference Book present derivatives which, with a constant elementary chemical composition of the fuel, permit the extrapolation of stagnation temperature on the inlet to the nozzle $T_{co}$.
the flow-rate complex $\beta$, the specific impulse in a vacuum $I_0^\prime$, and the relative area (the geometric degree of expansion) of the nozzle $\tilde{F}$. These values can be extrapolated in accordance with the pressure in the combustion chamber $p_{CO}$, according to the degree of the nozzle's expansion, according to pressure $\varepsilon$, and according to the fuel's enthalpy $it$. The data in Volume I of the Reference Book can be used to calculate the derivatives which are necessary for extrapolation in accordance with the geometric degree of expansion $\tilde{F}$ and to determine the coefficients of interpolation polynomials.

The expansion of the function of several independent variables into a Taylor series is used for extrapolation. The accuracy of the extrapolation depends on the type of fuel, the accepted form of functional dependence of parameters on $p_{CO}$, $it$, or $\varepsilon$, the number of terms considered in the series, and the amount of change in the argument with extrapolation. The latter is determined by the intervals of values $p_{CO}$ and $\varepsilon$. The logarithmic form of expansion into a series and linear extrapolation are recommended on the basis of the studies which have been conducted (see Volume I, Chapter XI).

As numerous calculations have shown, the accuracy of extrapolation for all fuels is determined primarily by the values $\kappa_{0k}$, $p_{CO}$, and $\varepsilon$ in the vicinity of which the extrapolation is accomplished. Extrapolation for fuel enthalpy with $p_{CO}$, $\varepsilon = \text{const}$ in all cases of interest to us (for example, even with a change in the aggregate state of the fuel components) provides acceptable accuracy (see Volume I, Chapter XV).

3.4.1. Estimate of extrapolation errors

As a result of the variety of fuels which are presented in the Reference Book and the broad range of changes in parameters $\kappa_{0k}$, $p_{CO}$, and $\varepsilon$, it is not possible to provide an estimate of the errors in extrapolating values for each fuel and for each value of $\kappa_{0k}$, $p_{CO}$, $t_{eq}$. When necessary, to determine possible errors in extrapolation for a selected tabular interval $\ln p_{co}^{(1)} - \ln p_{co}^{(2)}$ or $\ln s^{(1)} - \ln s^{(n)}$ the error in extrapolation can be estimated from the value of the second term in the Taylor expansion which is discarded.
temperature $T_{co}$

$$
\delta T_{co}^\% = \frac{1}{2} 10^{-1} \frac{A^{(1)} - A^{(2)}}{\ln \frac{\rho_{co}^{(1)}}{\rho_{co}^{(2)}}} \left[ \ln \frac{\rho_{co}^{(1)}}{\rho_{co}^{(2)}} \right]^2;
$$

(3.34)

flow-rate complex $\beta$

$$
\delta \beta^\% = \frac{1}{2} 10^{-1} \frac{B^{(1)} - B^{(2)}}{\ln \frac{\rho_{co}^{(1)}}{\rho_{co}^{(2)}}} \left[ \ln \frac{\rho_{co}^{(1)}}{\rho_{co}^{(2)}} \right]^2;
$$

(3.35)

specific impulse in a vacuum $I_s^r$ with $p_{co} = \text{const}$

$$
\delta I_s^r\% = \frac{1}{2} 10^{-1} \frac{C_s^{(1)} - C_s^{(2)}}{\ln \frac{\rho_{co}^{(1)}}{\rho_{co}^{(2)}}} \left[ \ln \frac{\rho_{co}^{(1)}}{\rho_{co}^{(2)}} \right]^2;
$$

(3.36)

generalized geometric degree of expansion of nozzle $F$

$$
\delta F^\% = \frac{1}{2} 10^{-1} \frac{D_F^{(1)} - D_F^{(2)}}{\ln \frac{\rho_{co}^{(1)}}{\rho_{co}^{(2)}}} \left[ \ln \frac{\rho_{co}^{(1)}}{\rho_{co}^{(2)}} \right]^2.
$$

(3.37)

In expressions (3.34) and (3.37) the superscripts "1" and "2" designate the amounts of the values on the boundary of the selected interval, without superscripts - in the middle of the interval, and coefficients $A, B, C, D$ - the corresponding partial derivatives which are presented in the tables of the Reference Book.

To estimate possible errors in extrapolation, we can also recommend third-power interpolation polynomials whose coefficients are determined from the value of the function and its first derivative with $p_{co}^{(1)}$ and $p_{co}^{(2)}$ or $s^{(1)}$ and $s^{(2)}$. A method for determining coefficients is given in the first volume of Reference Book [5]. Another possible method for estimating is calculation of errors in the middle of the interval $p_{co}^{(1)} - p_{co}^{(2)}$ or $s^{(1)} - s^{(2)}$ in accordance with values $\delta T_{co}, \delta \beta, \delta I_s^r, \delta F$ on the boundaries of the interval. For example, using tabular data with $p_{co}^{(1)}$ or $s^{(1)}$, we can determine from extrapolation formulas the parameters with $p_{co}^{(2)}$ or $s^{(2)}$ and find the errors $\delta T_{co}, \delta \beta, \delta I_s^r, \delta F$ by comparison with

55
tabular data with \( p_{\text{CO}} \) or \( \varepsilon \). The error in the middle of the indicated intervals \( p_{\text{CO}} \) or \( \varepsilon \) is approximately 0.25 of the amounts of the values \( f \) found.

An impression about the possible errors in extrapolation is provided by the materials in Chapter XV of the Reference Book's first volume as well as by the data in [2].

3.4.2. Regions of greatest extrapolation errors. Some recommendations

Temperature in the combustion chamber \( T_{\text{CO}} \). The maximum errors in extrapolation for \( p_{\text{CO}} \) should be expected in the region of values of the excess oxidant ratio which corresponds to the greatest rate of change in the composition of the combustion products. Usually this occurs with \( (T_{\text{CO}})_{\text{max}} \). Since the position of the maximum of the function \( T_{\text{CO}} = f(\alpha_{\text{OK}}) \) usually depends very weakly on the temperature in the combustion chamber, it is sufficient to provide an estimate of possible extrapolation errors with one value of \( p_{\text{CO}} \). The degree of dissociation is decreased with an increase in pressure in the combustion chamber; therefore the rate of change of the function \( T_{\text{CO}} = f(p_{\text{CO}}) \) is somewhat greater in the region of low pressures in the combustion chamber than in the region of high pressures. Consequently, large extrapolation errors are possible with low pressures \( p_{\text{CO}} \).

Flow-rate complex \( \beta \). Just as in the case of temperature \( T_{\text{CO}} \), the greatest errors should be expected in the region of the excess oxidant ratio which corresponds to the maximum \( \beta \). The rate of change in the function \( \beta = f(p_{\text{CO}}) \) is determined by the rate of change in the combustion products composition depending on \( p_{\text{CO}} \). With an increase in pressure the degree of dissociation decreases and the effect of \( p_{\text{CO}} \) is weakened. Therefore, with comparatively low pressures \( (p_{\text{CO}} \approx 10 \text{ MN/m}^2 \) or less) a higher extrapolation accuracy is given by an expansion of the type \( \ln \beta = f(\ln p_{\text{CO}}) \), and with high \( -\beta = f(p_{\text{CO}}) \).

The step of pressure change \( p_{\text{CO}} \) adopted in the Reference Book permits us to extrapolate \( \beta \) in accordance with \( p_{\text{CO}} \) with high accuracy (see Volume I, Chapter XV). The employment of one or another form of expansion is dictated by convenience in performing the calculations.
Specific pulse in a vacuum $I_s$. The greatest errors in extrapolating $I_s$ in accordance with $p_{co}$ and $\varepsilon$ should be expected with values of $\varepsilon_{ok}$ which correspond to the maximum $I_s$. These values of $\varepsilon_{ok}$ usually correspond to the greatest deviation of the relation $I_s(\varepsilon)$, $p_{co} = \text{const}$ and $I_s(p_{co}) = \text{const}$ from linear values as a result of the joint influence of dissociation and recombination.

A numerical analysis shows that the greatest values of the derivatives $(dI_s/dp_{co})$ with $\varepsilon = \text{const}$ is observed in the case of low values of $p_{co}$ and $\varepsilon$. With values of pressure $p_{co}$ selected in the Reference Book the relative changes in $I_s$ depending on $p_{co}$ between any adjacent values, i.e., $I_s(\varepsilon, p_{co})$, usually do not exceed 1%. Consequently, in this case the extrapolation error in the middle of the interval, as a rule, does not exceed 0.25%.

A change in the degree of expansion for pressure $\varepsilon$ can be caused by a change in $p_{co}$ or $p_a$ as well as of both parameters simultaneous. It should be noted that in the case of $\varepsilon = \text{const}$ the value of $I_s$ depends comparatively weakly on the value of $p_{co}$. With a simultaneous change in $p_{co}$ and $p_a$, the extrapolation of $I_s$ can be accomplished for two parameters: for $p_{co}$ with $p_a = \text{const}$ and for $\varepsilon$ or $(p_a)$ with $p_{co} = 0$ = const.

Calculations and their analysis show that the greatest errors in extrapolation should be expected with low values of $\varepsilon$ and $p_{co}$. However, the interval in pressure values $p_{co}$ and $\varepsilon$ adopted in the Reference Book permits avoiding large errors in certain measure: with $p_{co} < 2$ MN/m$^2$ the interval of change $\varepsilon \sim 2.5$ and with $p_{co} > 2$ MH/m$^2$ this interval is $\sim 6$.

A comparison of the results of thermodynamic calculations in accordance with extrapolation formulas shows that with the use of the first derivatives alone with a 2.5-fold change in $\varepsilon$ the error in extrapolation in accordance with $\varepsilon$ does not exceed 1%. For example, for the fuel $O_2 + NH_3$ in the case of initial parameters $p_{co}^0 = 2$ MN/m$^2$, $\varepsilon^0 = 5$ with extrapolation to the limit of the interval $p_{co} = 2$ MN/m$^2$, 57
With extrapolation to the middle of the interval the extrapolation error is substantially reduced.

The geometric degree of expansion of the nozzle $F$. With a constant degree of pressure reduction in the nozzle $\delta$ relative changes of adjacent values of $F$ depending on $p_{co}$ in the tables of the Reference Book are comparatively low and comprise 1-2%. Under these conditions, employment of only the first two derivatives in formulas with extrapolation in accordance with pressure $p_{co}$ with $\delta = \text{const}$ provides acceptable accuracy.

Calculations and their analysis show that with extrapolation in accordance with $\delta$ with $p_{co} = \text{const}$ the greatest errors should be expected in the region of low $p_{co}$ and low $\delta$. The accuracy in extrapolation of $F$ in accordance with $\delta$ with the use of only the first derivatives is lowest in comparison with the extrapolation of other parameters; here, a large error should be expected with extrapolation from high $\delta$ in the direction of low.

Above we examined the most unfavorable cases of extrapolation where we should expect the greatest errors. Basically, these are the extreme points of parameters $p_{co}$ and $\delta$ in the tables of the Reference Book. With mean values of the parameters the accuracy of extrapolation with the use of the first derivatives is rather high for the use of extrapolation results in practical calculations.

When necessary, extrapolation accuracy can be increased by using second finite differences.

3.5. Accuracy of Graphic Representation

The graphic representation of functions in semilogarithmic and logarithmic coordinates is used in the Reference Book.

Inaccuracies in the construction of graphs lead to errors in the values being represented on them. An estimate of such errors with the construction of graphs in the indicated coordinates is offered below.
Let the function \( y = f(\log x) \) be represented graphically in semi-logarithmic coordinates on a graph with height \( H \). The scale of the function \( y \)

\[
M_y = \frac{y_{\text{max}} - y_{\text{min}}}{H}
\]  

(3.38)

is constant and the same for any point on the graph. An inaccuracy in constructing \( \Delta y \) entails an error \( \Delta y \) of the function

\[
\Delta y = M_y \Delta y.
\]

(3.39)

The maximum relative error with \( \Delta y = \text{const} \) equals

\[
\delta y_{\text{max}} = \frac{\Delta y}{y_{\text{min}}}.
\]

(3.40)

When presenting a function in decimal logarithmic coordinates \( \log y = f(\log x) \) the scale of logarithmic values will be

\[
M_y = \frac{1}{l},
\]

where \( l \) - the length of a segment \( (\log 10 - \log 1) \) on the graph.

Inaccuracy in the construction of the graph \( \Delta \log y \) causes the error

\[
\Delta \log y = (\Delta \log y) M_y.
\]

(3.42)

Consequently, the error \( \Delta y \) of the function \( y \) is

\[
\Delta y = y [10^{(\Delta \log y) M_y} - 1].
\]

(3.43)

From expression (3.43) with a constant error \( \Delta \log y \) it follows that

\[
\delta y = \frac{\Delta y}{y} = 10^{(\Delta \log y) M_y} - 1 = \text{const},
\]

(3.44)

where \( \delta y \) - the relative error.
As an example, we estimate the errors in the functions $T_C$, $I_s$, $\beta$ and $\log F$ for the case $H \equiv 160$ mm, $\lambda = 50$-80 mm.

In constructing the graphs, one can "err" by approximately 0.5-1.0 mm, i.e., $\Delta y, \Delta \log y \approx 1$ mm. In the region of values $T_C = 3000^\circ K - 1000^\circ K$ and $I_s = 4000-2000$ m/s according to expressions (3.39)-(3.40) we obtain

$$M_r \approx 12.8^\circ K/mm, \Delta T = 12.8^\circ K,$$

$$\delta T_{max} = 1.2\%; M_{\delta} \approx 12.8 \frac{m/s}{mm}, \Delta \delta = 12.8 \text{ m/s;}$$

$$\delta \delta_{max} = 0.6\%.$$

In the region of values of $\log F = \log 1000-\log 1$ the results are presented in Table 3.7.

### Table 3.7. Estimate of errors in the construction of the relation $\log F = f(\log \delta)$

<table>
<thead>
<tr>
<th>$\ell$, mm</th>
<th>20</th>
<th>80</th>
</tr>
</thead>
<tbody>
<tr>
<td>$M_{1F}\delta$</td>
<td>0.02</td>
<td>0.0125</td>
</tr>
<tr>
<td>$\delta F$, %</td>
<td>2.3</td>
<td>1.9</td>
</tr>
<tr>
<td>$\Delta F$, $F = 10$</td>
<td>0.23</td>
<td>0.19</td>
</tr>
<tr>
<td>$\Delta F$, $F = 100$</td>
<td>2.3</td>
<td>1.9</td>
</tr>
<tr>
<td>$\Delta F$, $F = 1000$</td>
<td>23</td>
<td>19</td>
</tr>
</tbody>
</table>

When determining a function from its graph, the values of the quantities are obtained with an error which depend on an erroneous determination of both $\ell$ of the coordinates of the graph of the function. In this case, the errors in determining the values exceed the errors in constructing the graph of the function.
CHAPTER IV

BRIEF DESCRIPTION OF TABLES AND GRAPHS

A detailed description of the tables and graphs and instructions are presented in Chapter XIII, Volume I. Presented below is a brief description of the tables and graphs which are necessary for convenience in using each volume separately.

4.1. Tables

The columns of the table (from left to right) present the following information.

First column - conventional designations of the values being presented.

Second column - values pertaining to conditions at the inlet to the nozzle (stagnation pressure $p_{co}$).

Third column - values pertaining to conditions in the critical section of the nozzle (pressure $p_{s}=p_{co}/\varepsilon$).

Fourth and subsequent columns - values pertaining to sections in the supersonic portion of the nozzle (pressure in the section corresponds to the current stage of expansion $\varepsilon$ and comprises $p = p_{co}/\varepsilon$).

The lines of the table (from top to bottom) present the following information.
The first line contains some information on the fuel and combustion products, and namely:

$\lambda_{ok}$ - excess oxidant ratio;

$k_1$ - coefficient of the fuel component ratio, kg oxidizer/kg fuel;

$\rho_T$ - the mean fuel density, g/cm$^3$;

$i_T$ - specific enthalpy of the fuel, kJ/kg;

$s$ - specific enthalpy of the combustion products which is constant on the section from the inlet to the nozzle to the exit section, kJ/kg deg.

The group of lines under the heading "General Values" contains the following data:

$\varepsilon = \frac{p_{co}}{p}$ - the degree of nozzle expansion with pressure;

$p$ - pressure, kN/m$^2$;

$T$ - temperature, $^\circ$K;

$\mu$ - mean molecular weight, kg/mole;

$a, M$ - speed of sound in equilibrium-reacting mixture ($a$), m/s, in the second column; Mach number ($M$) for the values $\varepsilon > \varepsilon$;

$n$ - the mean index of isoentropy of expansion in the interval from $p_{co}$ to $p = \frac{p_{co}}{6}$;

$w$ - the speed of flow, m/s;

$\beta, \eta$ - the flow-rate complex $\beta$, m/s, for values $\varepsilon > \varepsilon$: specific impulse in a vacuum $\eta$, m/s, for values $\varepsilon > \varepsilon$;

$P = \frac{P_{co}}{P}$ - the geometric degree of expansion of the nozzle (relative area);

$c_{pf}$ - specific "frozen" specific heat of combustion products at constant pressure, kJ/kg deg;

$c_p$ - equilibrium specific heat of combustion products at constant pressure, kJ/kg deg;

$\eta \cdot 10^4$ - coefficient of dynamic viscosity of gas phase of mixture, N s/m$^2$;

$\lambda_Y$ - the coefficient of "frozen" specific heat of the gas phase of combustion products, W/m deg;

$\lambda$ - coefficient of equilibrium heat conductivity of the combustion products gas phase, W/m deg;

$\frac{\rho}{\rho_o}$ - the ratio of the equilibrium specific heats with constant pressure and constant volume;
\( a_p \times T \) - the product of the isobaric expansion coefficient times temperature;

\( \gamma_r \times p \) - the product of the isothermal contraction coefficient times pressure;

\( z \) - the total fraction by weight of substances in a condensed state.

In the group of lines under the heating "coefficients of extrapolation formulas" the following partial derivatives are presented.

\[ A_1 = \left( \frac{\partial \ln T_{co}}{\partial \ln \rho_{co}} \right)_{T_1} \cdot 10^4 \] - in the second column;

\[ B_1 = \left( \frac{\partial \ln R}{\partial \ln \rho_{co}} \right)_{T_1} \cdot 10^3 \] - in the third column;

\[ C_1 = \left( \frac{\partial \ln I^a}{\partial \ln \rho_{co}} \right)_{T_1} \cdot 10^3 \] - in the fourth and subsequent columns;

\[ D_1 = \left( \frac{\partial \ln P}{\partial \ln \rho_{co}} \right)_{T_1} \cdot 10^3 \] - in the fourth and subsequent columns;

\[ A_2 = \left( \frac{\partial \ln T_{co}}{\partial \ln \rho_{co}} \right)_{p_{co},} \cdot 10^3 \] - in the second column;

\[ C_2 = \left( \frac{\partial \ln I^a}{\partial \ln \rho_{co}} \right)_{p_{co},} \cdot 10^3 \] - in the fourth and subsequent columns;

\[ B_2 = \left( \frac{\partial \ln R}{\partial \ln \rho_{co}} \right)_{p_{co},} \cdot 10^3 \] - in the third column;

\[ D_2 = \left( \frac{\partial \ln P}{\partial \ln \rho_{co}} \right)_{p_{co},} \cdot 10^3 \] - in the fourth and subsequent columns;

\[ A_3 = \left( \frac{\partial T_{co}}{\partial \rho_{co}} \right)_{p_{co}} \] - in the second column;

\[ C_3 = \left( \frac{\partial I^a}{\partial \rho_{co}} \right)_{p_{co},} \] - in the fourth and subsequent columns;

\[ B_3 = \left( \frac{\partial R}{\partial \rho_{co}} \right)_{p_{co}} \] - in the third column;

\[ D_3 = \left( \frac{\partial P}{\partial \rho_{co}} \right)_{p_{co},} \] - in the fourth and subsequent columns;
\[ L_1 = \frac{\delta_1}{\delta_1 \rho_{co}} \] - in the second column;
\[ L_1 = \frac{\delta_{1o}}{\delta_{1o} \rho_{co}} \] - in the third column;
\[ C_1 = \frac{d_1}{d_{1o}} \rho_{co} \] - in the fourth and subsequent columns;
\[ B_2 = \frac{\mu_2}{\mu_{2o}} \rho_{co} \] - in the fourth and subsequent columns;
\[ D_2 = \frac{\mu_{2o}}{\mu_{2o}} \rho_{co} \] - in the fourth and subsequent columns;
\[ L_2 = \frac{\delta_{2o}}{\delta_{2o} \rho_{co}} \] .

The group of lines under the heading "equilibrium composition" presents the molar fractions of gaseous individual substances (designated by the symbols of chemical compounds and atoms) and the fractions by weight of individual substances in the condensed state (chemical symbols have the additional sign*). The zero of whole numbers and the decimal point have been omitted in writing decimal fractions.

4.2. Graphs

The following standard graphs are presented for each of the fuel compounds examined in the volume:
1) \( \gamma = f(\alpha_{ok}, \rho_{co}) \) and \( \rho_{co} = f(\alpha_{ok}) \).
2) \( \beta = f(\alpha_{ok}, \rho_{co}) \).
3) \( T_{co} = f(\alpha_{ok}, \rho_{co}) \) and \( \alpha = f(\alpha_{ok}) \).

Since, in addition to the scale \( \alpha_{ok} \) there are the scales \( k_1 \) and \( k_2 \), other ties are also illustrated, for example, \( T_{co} = f(k_1, \rho_{co}) \) and so forth.
4) \( \bar{F} = f(\epsilon, \alpha_{ok}, \rho_{co}) \).

Since the dependence of the relative area \( \bar{F} \) on pressure \( \rho_{co} \) is weak, each line with \( \alpha_{ok} = \text{const} \) is approximately valid for the pressure interval indicated in the graph.
The results of the calculation of losses in specific impulse in a vacuum \((\zeta_n, \varphi)\), which are caused by chemical disequilibrium of the flow in the nozzle are presented in the form of graphical relationships for three fuel compounds \((O_2 + H_2, \text{kerosene, and asymmetrical dimethyl-hydrazine})\). This information is limited to only three fuels in connection with the great labor intensity in the calculation of non-equilibrium flows and, primarily, in connection with the absence of much data on the mechanism and constants of the reaction rates in a gas phase.

The results of calculations of chemically nonequilibrium flows are presented in the form of graphical dependences of the coefficient of loss in specific impulse \(\zeta_n\) on the relative radius \(\bar{r}\) for a series of fixed values \(\varphi_0, \rho_0, d_*\).

Six figures are presented on each page for the given value of excess oxidant ratio \(\varphi_0\). Each figure on a page corresponds to one selected value of stagnation pressure at the input to the nozzle \(P_{CO}\) whose value in \(\text{MN/m}^2\) is indicated on the graph, and the series of values of \(d_*\) is \(\text{mm}\).

To find \(\zeta_n\) with values of \(\varphi_0, P_{CO}\), and \(d_*\) which are not presented on the figures, graphical interpolation should be conducted. Here, it is expedient to construct additional graphs of the type:

a) \(\zeta_n = f(\varphi_0, \bar{r}, P_{CO}, d_*)\)

b) \(\zeta_n = f\left(\frac{280 \text{ MN}}{d_*}\right)\) with \(\bar{r}, P_{CO}\) and \(\varphi_0\) = const,

c) \(\zeta_n = f\left(\frac{25 \text{ MH/m}^2}{P_{CO}}\right)\) with \(\bar{r}, d_*\) and \(\varphi_0\) = const,

considering the natural condition that with \(d_*, P_{CO} \to \infty, \zeta_n \to 0\).

1) In this regard, also see Figs. 18.20 and 18.21 in the first volume of the Reference Book.
CHAPTER V.

TABLES AND GRAPHS OF CALCULATION RESULTS

FUEL - OXYGEN + HYDROGEN (O₂ + H₂)
<table>
<thead>
<tr>
<th>CHEMICAL FORMULA</th>
<th>OXIDIZER</th>
<th>FUEL</th>
</tr>
</thead>
<tbody>
<tr>
<td>ENTHALPY $\frac{\text{kJ}}{\text{kg}}$</td>
<td>$-398.3$</td>
<td>$-4353.9$</td>
</tr>
<tr>
<td>DENSITY $\frac{\text{g}}{\text{cm}^3}$</td>
<td>$1.135$</td>
<td>$0.07076$</td>
</tr>
<tr>
<td>ADMIXTURE</td>
<td>LIQUID NITROGEN $\text{N}_2$</td>
<td>NONE</td>
</tr>
</tbody>
</table>

Range of change in admixture content, by weight  

| Coefficients of extrapolation formulas | $A_0B_0C_0D_0$ | $-$ |

$e_\infty = 0.3 - 6.0$  
$ho_\infty = 0.1 - 50 \frac{\text{MN}}{\text{m}^2}$
Fig. 5.1.
Fig. 5.2.
Fig. 5.3.

70
Fig. 5.4.
Fig. 5.5.
Fig. 5.6.
Fig. 5.7. $\alpha_{on} = 0.8$
Fig. 5.8. $\lambda_{0k} = 0.8$
\[ \alpha_{\text{on}} = 1.0 \]

Fig. 5.9.
Fig. 5.10
Fig. 5.11. α_0\text{m}=1.4
FUEL - OXYGEN + KEROSENE (O₂ + KEROSENE)
\[ \omega = 0.4 - 5.0 \]
\[ P = 0.1 - 50 \text{ MN/m}^2 \]

**CHEMICAL FORMULA**

<table>
<thead>
<tr>
<th>OXIDIZER</th>
<th>FUEL</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \text{O}_2 )</td>
<td>( \text{CH}_4 )</td>
</tr>
<tr>
<td>( (C-85.9%, H-14.1%) )</td>
<td></td>
</tr>
</tbody>
</table>

**ENTHALPY** (kJ/kg)

<table>
<thead>
<tr>
<th>OXIDIZER</th>
<th>FUEL</th>
</tr>
</thead>
<tbody>
<tr>
<td>( -398.3 )</td>
<td>( -1948 )</td>
</tr>
<tr>
<td>( T = 90,188\text{K} )</td>
<td>( T = 260,18\text{K} )</td>
</tr>
</tbody>
</table>

**DENSITY** (g/cm³)

<table>
<thead>
<tr>
<th>OXIDIZER</th>
<th>FUEL</th>
</tr>
</thead>
<tbody>
<tr>
<td>( 1.135 )</td>
<td>( 0.83 )</td>
</tr>
</tbody>
</table>

**ADMIXTURE**

- **LIQUID NITROGEN, \( \text{N}_2 \)**
- Change in C/H ratio given

Range of change in admixture content, by weight

<table>
<thead>
<tr>
<th>Change in C/H by %</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.008</td>
</tr>
</tbody>
</table>

**Coefficients of extrapolation formulas**

\[ A, B, C, D, L, A, B, C, D, L \]
Fig. 5.12.
81
Fig. 5.14.
Fig. 5.18.
Fig. 5.19.

\[ \alpha_{\text{on}} = 1.0 \]
Fig. 5.20.
Fig. 5.21. $\alpha_{on}=1.4$
FUEL - OXYGEN + ASYMMETRICAL DIMETHYLHYDRAZINE \((\text{O}_2 + (\text{CH}_3)_2\text{NNH}_2)\)
\( e_{on} = 0.3 - 5.0 \)

\( P_{co} = 0.1 - 50 \ \text{MN/m}^2 \)

OXIDIZER

\( \text{O}_3 \)

97.1\% (CH\(_3\))\(_2\)NNH\(_2\) +
1.1\% (CH\(_3\))\(_2\)NH +
1.8\% (CH\(_3\))\(_2\)NNCH\(_3\)

FUEL

\( \text{H}_2 \)

ENTHALPY \( l \ \text{kJ/kg} \)

-398.3 \( T < 90,188^\circ \text{K} \)

836.5 \( T > 298,15^\circ \text{K} \)

DENSITY \( \rho \ \text{g/cm}^3 \)

1.135 \( T < 90,188^\circ \text{K} \)

0.786 \( T > 298,15^\circ \text{K} \)

ADMIXTURE

LIQUID NITROGEN \( \text{N}_2 \)

WATER \( \text{H}_2\text{O} \)

Range of change in admixture content, by weight

0.008

0.005

Coefficients of extrapolation formulas

\( A_b B_c C_d D_e L_f \)

\( A_b B_c C_d D_e L_f \)
Fig. 5.22.
Fig. 5.23.
Fig. 5.24.
Fig. 5.26.
Fig. 5.27.
\[ \alpha_m = 0.8 \]

Fig. 5.28.
Fig. 5.29.

100
Fig. 5.30.
Fig. 5.31.
FUEL - OXYGEN + AMMONIA (O₂ + NH₃)
\[ \begin{align*}
\alpha_0 &= 0.6 - 2.0 \\
\rho_\infty &= 0.2 - 50 \frac{MN}{m^2}
\end{align*} \]

<table>
<thead>
<tr>
<th>CHEMICAL FORMULA</th>
<th>OXIDIZER</th>
<th>FUEL</th>
</tr>
</thead>
<tbody>
<tr>
<td>ENTHALPY $\frac{kJ}{kg}$</td>
<td>$-398.3$</td>
<td>$-4184.8$</td>
</tr>
<tr>
<td>DENSITY $\frac{g}{cm^3}$</td>
<td>$1.135$</td>
<td>$0.6819$</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>ADMIXTURES</th>
<th>LIQUID NITROGEN $N_2$</th>
<th>WATER $H_2O$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Range of change in admixture content, by weight</td>
<td>$0.008$</td>
<td>$0.004$</td>
</tr>
</tbody>
</table>

| Coefficients of extrapolation formulas | $A_4B_6C_6D_6$ | $A_4B_6C_6D_6$ |
Fig. 5.32.
Fig. 5.33.
Fig. 5.34.
Fig. 5.35.
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