

PREDICTION THE THEORETICAL INTERIOR BALLISTIC PROPERTIES OF SOLID PROPELLANT ROCKET MOTORS

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Abstract

Process for prediction the interior ballistic properties of solid propellant rocket motors is based on identification and quantitative estimation of idealized performances deviations. Solid propellants combustion and expansion of combustion gases within a rocket motor and nozzle represent a complex problem, which includes influences of chemical reactions, erosive burning, transport phenomena etc.

The computer program TCPSP (Thermo-Chemical Properties Solid Propellant), which ensures calculation the equilibrium contents of combustion gases, transport properties of combustion gases and theoretical performances of rocket motors with specified propellant grains, has been developed.

Comparative analyses of results from the TCPSP computer code with referring codes Ophelie and CEA have been carried out. A very good agreement has obtained.

Key words: *rocket motors, solid propellant, combustion chamber, nozzle, combustion, expansion, combustion products, thermodynamic properties, transport properties, rocket performances*

1. INTRODUCTION

Theoretical model, which describes complex phenomena appearing within rocket motor, is based on several hypotheses. These are referred to conditions of combustion process taking place in rocket motor, to expansion of exhaust products through nozzle and to properties of combustion products.

Calculation of energetic performances of solid propellants is directed to determination of combustion products mixture, in conditions of energetic, phase and chemical equilibrium. This calculation includes setting and solving the equation system describing phase and chemical equilibrium.

Necessary data for calculation of energetic characteristics of solid propellants are: chemical constituents and their enthalpies of formation, thermodynamic properties of prospective combustion products within a wide temperature diapason and parameters of inter-molecular potentials for all compounds within corresponding temperature diapason. Basic sources for these data are data bases and publications [1, 2, 3, 12]. Calculation, based on the model as above specified, should:

- provide optimization a solid propellant composition relating to energetic properties, and
- provide necessary data for design of rocket motor.

2. COMPUTATIONAL MODEL FOR CALCULATION THE THEORETICAL PROPERTIES OF SOLID ROCKET PROPELLANTS

2.1 Assumptions

A basic assumption, which was also used in different models [10,14,4,16,9,13,7], is that solid propellant combustion and expansion of exhaust combustion products represent two separate processes located in the combustion chamber and in the nozzle.

Combustion and expansion through the nozzle have an adiabatic character and they occur as steady-state processes. Combustion gaseous mixture is homogeneous across any cross-section of the combustion chamber and the nozzle normal to the nozzle axis.

The gaseous combustion products mixture behaves as a mixture of perfect gases, which is not soluble into condensed phases, so that such a mixture obey the perfect gas law [10,14,4,16,9,13,7]. Condensed-phase particles within the combustion products mixture are small so that their total volume is negligible when compared to the gases volume. Combustion products mixture is homogeneous, and condensed-phase particles are in thermal and kinetic equilibrium with gaseous phase.

Nonisentropic and irreversible process occur within the combustion chamber. Flow through the nozzle is considered as steady-state and adiabatic, which gives it an isentropic character. Velocity of gases at inlet nozzle area is neglected when compared to one which is obtained throughout the nozzle. During expansion throughout the nozzle, composition of combustion products, can be considered as:

- Gaseous mixture, generated by the burning of solid propellant, stays „frozen“– „frozen“ equilibrium expansion, or
- Gaseous mixture stays in chemical equilibrium, which depends on local pressure and temperature in any moment of expansion – “shifting” equilibrium expansion.

Parameters of the real process are among values obtained by calculations under both above conditions.

2.2 Combustion products mixture under conditions of „shifting“ equilibrium

Calculation of combustion product constituents represents an essence of procedure for prediction the solid propellant properties.

Regarding the assumption in which the total thermodynamic equilibrium is „frozen“, contents of the combustion product mixture will be calculated at „shifting“ equilibrium conditions. For calculation of „shifting“ equilibrium combustion products mixture, a method of minimum Gibbs energy is used in this paper.

Generally, combustion products of solid propellants generate a mixture consisting of multi-phase constituents, although in most cases there are usually two phases. The basic condition for equilibrium state of mixture at constant pressure and temperature is [15]:

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

where; G –Gibbs free energy.

Gibbs free energy for two-phase system is equal to sum of energies of particular phases, which are assumed to be homogeneous:

$$G = \sum_{i=1}^{NG} n_i \left(\mu_i^0 + RT \ln \frac{n_i}{n} + RT \ln P \right) + \sum_{i=NG+1}^{NS} \tilde{n}_i \left(\mu_i^0 + RT \ln \frac{\tilde{n}_i}{\tilde{n}} \right), \quad (2)$$

where, NG – number of gaseous combustion products, NS – total number of combustion products, n_i - number of mols, μ_i^0 - chemical potential at the standard conditions, P – pressure referred to the standard pressure (pressure of $p_0 = 0.10132472$ MPa is chosen as the standard state) [15]. Sign \sim is referred to condensed phase.

During calculation of the composition such a two-phase system in conditions of chemical equilibrium, besides the condition (1), conditions of mass balance for all chemical elements, consisting in combustion products, must be fulfilled:

$$\sum_{i=1}^{NG} a_{ij} n_i + \sum_{i=NG+1}^{NS} a_{ij} \tilde{n}_i - a_{0j} = 0, \quad \text{for } j = 1, 2, \dots, l \quad (3)$$

where: a_{ij} – stoichiometric coefficients of components, or number of atoms j consisted in component i , a_{0j} – total number of atoms of the element j consisted in combustion products, and l – number of elements consisted in combustion products.

In order to be calculated composition of combustion products mixture, conditions of mols balance for particular phases, must be also fulfilled.

$$\sum_{i=1}^{NG} n_i - n = 0 \quad \text{and} \quad \sum_{i=NG+1}^{NS} \tilde{n}_i - \tilde{n} = 0 \quad (4)$$

Procedure

It can be seen from equations (1) to (4) that a system of $NS + l + 2$ non-linear equations should be solved in order to be predicted composition of combustion products. Number of equations for calculation of combustion products can be decreased to $l + 2$ if a geometric programming is used [15]. Let the function v be defined as:

$$v = e^{-\frac{G}{RT}} \quad (5)$$

and after substitution of the equation (2) for Gibbs energy

$$v = \prod_{i=1}^{NS} \left(\frac{c_i}{n_i} \right)^{n_i} n^n \tilde{n}^{\tilde{n}} \quad (6)$$

where:

$$c_i = \frac{e^{-\mu_i^0/RT}}{p} \quad \text{and} \quad \tilde{c}_i = e^{-\tilde{\mu}_i^0/RT} \quad (7)$$

Minimum of Gibbs free energy with limitations (3) and (4) can be presented through maximum of the function v , which is defined by the equation (6) under same limitations.

Using theory of geometric programming [15], it can be seen that function v , with limitations (3) and (4), represents a bipartite function, whose direct criterion function has a following form:

$$g_0 = \prod_{j=1}^l t_j^{a_{0j}} \quad (8)$$

where: t – independent variable of the criterion function. Then, limitations (3) and (4) are reduced to two limitations:

$$g_1 = \sum_{i=1}^{NG} c_i \prod_{j=1}^l t_j^{a_{0j}} = 1 \quad \text{and} \quad g_2 = \sum_{i=NG+1}^{NS} \tilde{c}_i \prod_{j=1}^l t_j^{a_{0j}} = 1 \quad (9)$$

Maximum of the function v with limitations (3) and (4) corresponds to minimum of the function g_0 with limitations (9). Assignment of minimum of the function g_0 with given limitations leads to assignment of mathematical minimum of function

$$f = g_0 + \lambda_1 g_1 + \lambda_2 g_2, \quad (10)$$

where λ_1 and λ_2 – Lagrange's multipliers.

In accordance with above considerations, problem of assignment of minimum of Gibbs free energy with limitations (3) and (4) is reduced to assignment of minimum of the function (10) with $l + 2$ variables.

Since among optimal values of independent variables of the direct criterion and the bipartite function exists a mutual relation, molar constituents are as follows:

$$\delta_i = c_i \prod_{j=1}^l t_j^{a_{ij}} \quad \text{and} \quad \tilde{\delta}_i = \tilde{c}_i \prod_{j=1}^l t_j^{a_{ij}} \quad (11)$$

Each of two equations of chemical elements balance (3) might be used for assignment of condensed phase constituents. Taking into consideration following:

$$n_i = \delta_i n \quad \text{and} \quad \tilde{n}_i = \tilde{\delta}_i \tilde{n} \quad (12)$$

from the balance each of two chemical elements one gets:

$$n \sum_{i=1}^{NG} a_{ij1} \delta_i + \tilde{n} \sum_{i=NG+1}^{NS} a_{ij1} \tilde{\delta}_i - a_{0j1} = 0 \quad \text{and} \quad n \sum_{i=1}^{NG} a_{ij2} \delta_i + \tilde{n} \sum_{i=NG+1}^{NS} a_{ij2} \tilde{\delta}_i - a_{0j2} = 0 \quad (13)$$

Minimum of the direct criterion function with corresponding limitations, equations (3) and (4), is assigned by application of the Newton-Raphson method. As criterion for assignment of values for independent variables at minimum of the direct criterion function, the following condition is used:

$$\left| \frac{v - g_0}{c} \right| \leq 10^{-16} \quad (14)$$

Initial values of Lagrange multipliers $\lambda_1 = -2,45$ and $\lambda_2 = -0,0003$ are taken on the basis of number of iterations, which are needed for determination of minimum of the direct criterion function g_0 [15].

Convergence and its rate depend on selection of the initial values for all independent variables of direct criterion function g_0 . Initial values for all independent variables of direct criterion function g_0 in the equation (8) are same and equal to $10^{-5,5}$. These values are used for calculation of gaseous combustion products, for all initial temperatures and selected pressure at each cross-sectional area of rocket motor. A possible case that there is no convergence, when combustion products mixture which has condensed phase products is being calculated. In such a case, calculated data for gaseous phase of each independent variable, should be used as initial values of condensed phase.

Thermodynamic properties of combustion products are assigned by known relations for properties of ideal-gas mixture [10,15,18]:

- molar mass

$$M = \frac{n \sum_{i=1}^{NG} \delta_i M_i + \tilde{n} \sum_{i=NG+1}^{NS} \tilde{\delta}_i \tilde{M}_i}{n} \quad \text{and} \quad M_w = \frac{n \sum_{i=1}^{NG} \delta_i M_i + \tilde{n} \sum_{i=NG+1}^{NS} \tilde{\delta}_i \tilde{M}_i}{n + \tilde{n}} \quad (15)$$

- enthalpy

$$h = \frac{n \sum_{i=1}^{NG} H_i \delta_i + \tilde{n} \sum_{i=NG+1}^{NS} \tilde{H}_i \tilde{\delta}_i}{M(n + \tilde{n})}; \quad (16)$$

- entropy

$$s = \frac{n \left(\sum_{i=1}^{NG} S_i \delta_i - R \sum_{i=1}^{NG} \delta_i \ln \delta_i - R \ln P \right) + \tilde{n} \left(\sum_{i=NG+1}^{NS} \tilde{S}_i \tilde{\delta}_i - R \sum_{i=NG+1}^{NS} \tilde{\delta}_i \ln \tilde{\delta}_i \right)}{M(n + \tilde{n})}; \quad (17)$$

- specific heat at constant pressure

- no reacting mixture

$$c_{p_f} = \frac{n \sum_{i=1}^{NG} C_{p_i} \delta_i + \tilde{n} \sum_{i=NG+1}^{NS} \tilde{C}_{p_i} \tilde{\delta}_i}{M(n + \tilde{n})} \quad (18)$$

- reacting mixture

$$c_p = \frac{1}{M} \left(\frac{\partial h}{\partial T} \right)_p \quad (19)$$

Gas constant and density of gaseous phase are assigned in the same way as for ideal gas:

$$R_g = \frac{R}{M}, \quad (20)$$

$$\rho = \frac{P}{R_g T}. \quad (21)$$

The ratio of specific heats and speed of sound for no reacting mixture are assigned by relations ^[15]:

$$\gamma_f = \left(1 - \frac{R_g}{c_{p_f}} \right)^{-1}, \quad (22)$$

$$a_f = \sqrt{\gamma R_g T}, \quad (23)$$

and for reacting mixture:

$$\gamma = \left\{ 1 - \frac{R_g \left[1 - \frac{T}{M} \left(\frac{\partial M}{\partial T} \right)_p \right]^2}{c_p \left[1 + \frac{P}{M} \left(\frac{\partial M}{\partial P} \right)_T \right]} \right\}^{-1}, \quad (24)$$

$$a = \sqrt{\frac{\gamma R_g T}{1 + \frac{P}{M} \left(\frac{\partial M}{\partial P} \right)_T}}. \quad (25)$$

Partial derivations from equations (19), (24) and (25) are assigned by numerical procedure with increments $\Delta T = 0,01$ K and $\Delta P = 0,1$ Pa.

Properties of components are calculated by means of reduced thermodynamic potential, which is determined by the following relation:

$$\Phi^0 = \varphi \ln(10^{-4} T) + \sum_{\alpha=-2}^3 \varphi_{\alpha} (10^{-4} T)^{\alpha} \quad (26)$$

and relation

$$\mu = \Delta_f H - T\Phi^0, \quad (27)$$

where $\Delta_f H$ – enthalpy of formation at temperature of 298,15 K

Data for coefficients φ in the equation (26), enthalpy of formation and molar mass of particular components were taken from Ref. [1,2,3]. Relations for calculation thermodynamic properties by means of thermodynamic potentials and their values for particular components are given in ref. [18].

2.3 Relations for calculation of transport properties

Transport properties of combustion products mixture are assigned only for gaseous phase. They are calculated by means of following relations:

- Kinematic viscosity of the mixture ^[6]:

$$\eta_g = \sum_i \frac{\eta_i \delta_i}{\sum_j \Phi_{ij} \delta_j}, \quad (28)$$

Where:

$$\Phi_{ij} = \frac{1}{\sqrt{8}} \frac{\left[1 + \sqrt{\frac{\eta_i}{\eta_j}} \sqrt{\frac{M_j}{M_i}} \right]^2}{\sqrt{1 + \frac{M_i}{M_j}}}, \quad (29)$$

- Kinematic viscosity of a component ^[4]:

$$\eta = 2,7627 \cdot 10^{-6} \frac{\sqrt{MT}}{\sigma^2 \Omega_*^{2,2}} \quad (30)$$

- Reduced integral of crash

$$\Omega_*^{l,s} = \sum_{i=0}^5 d_i (\ln T^*)^i, \quad (31)$$

- σ – diameter of the effective cross-section of crash [10^{-10} m], $T^* = T \frac{k}{\varepsilon}$, k – Boltzman constant, and ε – maximal energy of attraction between two molecules.

- Thermal conductivity coefficient for combustion products mixture of reacting gases^[15,10,4]:

$$\lambda = \lambda_{fr} + \lambda_{rr}, \quad (32)$$

were:

- thermal conductivity coefficient of no reacting gases mixture ^[6,15,4]:

$$\lambda_{fr} = \lambda' + \lambda'' \quad (33)$$

- thermal conductivity coefficient of one-atom gases mixture

$$\lambda' = \sum_i \frac{\delta_i \lambda'_i}{\sum_j \psi_{ij} \delta_j} \quad (34)$$

- thermal conductivity coefficient of the one-atom gas ^[6,15,4]:

$$\lambda'_i = \frac{15}{4} \frac{R}{M_i} \eta_i, \quad (35)$$

$$\psi_{ij} = \left[1 + 2,41 \frac{(M_i - M_j)(M_i - 0,142M_j)}{(M_i + M_j)^2} \right] \times \frac{\left[1 + \left(\frac{\lambda_i}{\lambda_j} \right)^{1/2} \left(\frac{M_j}{M_i} \right)^{1/4} \right]^2}{2\sqrt{2} \left(1 + \frac{M_i}{M_j} \right)^{1/2}}. \quad (36)$$

- share of the thermal conductivity coefficient caused by energy transfer of atom interior degrees of freedom.

$$\lambda'' = \sum_i \frac{(\lambda_i - \lambda'_i) \delta_i}{\sum_j \delta_j \frac{D_{ii}}{D_{ij}}} \quad (37)$$

- thermal conductivity coefficient of multi-atom gas ^[6,15]:

$$\frac{\lambda_i M_i}{\eta_i c_{vi}} = \frac{\rho_i D_i}{\eta_i} + \frac{3}{2} \frac{R}{c_{vi}} \left(\frac{5}{2} - \frac{\rho_i D_i}{\eta_i} \right) \quad (38)$$

- self-diffusion and binary-diffusion coefficients, D, D_{ii} and D_{ij} in the equations (37) and (38) are assigned by the relation ^[4]:

$$D_{ij} = 0,2628 \cdot 10^{-6} \frac{T \sqrt{T(M_i + M_j) / 2M_i M_j}}{p \sigma_{ij}^2 \Omega_{*ij}^{1,1}}, \quad (39)$$

- share of the thermal conductivity originated due to chemical reactions within the mixture ^[4,15,13]:

$$\lambda_{re} = -\frac{1}{RT^2} \begin{vmatrix} A_{11} & A_{12} & \dots & \Delta H_1 \\ A_{12} & A_{22} & \dots & \Delta H_2 \\ \vdots & & & \\ A_{1\nu} & A_{2\nu} & \dots & \Delta H_\nu \\ \Delta H_1 & \Delta H_2 & \dots & 0 \end{vmatrix} \quad (40)$$

- heat effect of independent reaction at temperature of the mixture is

$$\Delta H_j = \sum a_{ij} (H_i - H_j), \quad j=1, 2, \dots, \nu \quad (41)$$

- elements of determinants in the equation (40) are assigned by means of relations:

$$A_{ij} = \sum_{k=1}^{NG-1} \sum_{l=k+1}^{NG} \frac{(a_{ik}\delta_k - a_{il}\delta_l)(a_{jk}\delta_l - a_{jl}\delta_k)}{\delta_k\delta_l D_{kl}}. \quad (42)$$

Stoichiometric coefficients in independent reactions, are components of a vector of basic coefficients from homogeneous system of linear equations, representing balance of mass of elements [15].

2.4 Theoretical rocket performances

Besides the cited assumptions, calculation of theoretical performances of rocket motors is based on assumption of the Infinite-area combustion chamber (IAC) model [10].

For calculation of theoretical performances of a rocket motor, following simplified equations are used [10]:

1. Equation of continuity:

$$\rho_2 A_2 u_2 = \rho_1 A_1 u_1 \quad (43)$$

2. Equation of momentum:

$$P_2 + \rho_2 u_2^2 = P_1 + \rho_1 u_1^2 \quad (44)$$

3. Equation of energy:

$$h_2 + \frac{u_2^2}{2} = h_1 + \frac{u_1^2}{2} \quad (45)$$

Equation (43) describes condition of constant mass flow rate \dot{m} , given by the following relation:

$$\dot{m} = \rho A u \quad (46)$$

where: A – referent nozzle cross-sectional area (throat or exit area), u – gas stream velocity.

If the combustion chamber is marked by subscript c , and the exit area by subscript e , then relation for gas stream velocity can be obtained from equation of energy (45) [10,13]:

$$u_e = \sqrt{2(h_c - h_e)} \quad (47)$$

where: h – enthalpy at given cross-sectional area, expressed in J/kg, u – gas stream velocity, expressed in m/s.

Rocket motor thrust for one-dimensional and steady-state flow can be defined by the relation:

$$F = \dot{m} u_e + (P_e - P_a) A_e \quad (48)$$

where, P_a – external (atmospheric) pressure.

Specific impulse is defined as the ratio of thrust to mass flow rate:

$$I_{sp} = \frac{F}{\dot{m}} = u_e + \frac{(P_e - P_a) A_e}{\dot{m}}. \quad (49)$$

Mach number is defined as the ratio of the flow velocity to the local sonic velocity:

$$M = \frac{u}{a} \quad (50)$$

The flow velocity is given by the relation (47), and the sonic velocity is given by relations (23) or (25).

Characteristic velocity, marked as C^* , is defined as

$$C^* = \frac{P_c A_t}{\dot{m}} \quad (51)$$

where subscript t is referred to the nozzle throat region.

Using the equation of continuity (43) one gets the relation for ratio of the nozzle exit cross-sectional area to the nozzle throat cross-sectional area:

$$\frac{A_e}{A_t} = \frac{\rho_t u_t}{\rho_e u_e} \quad (52)$$

The thrust coefficient is defined by:

$$C_F = \frac{I_{sp}}{C^*}. \quad (53)$$

2.5 Characteristics of the combustion process

Determination of characteristics of the combustion process is based on assumptions in which the combustion chamber pressure and the propellant enthalpy of formation are considered as constants. Input data for the procedure are composition and enthalpy of formation of the propellant.

According to hypothesis referring to the combustion process, basic equation of energy conservation at the combustion chamber ($p_c = const$) is given by:

$$h_c - h_{f_{pm}} = 0 \quad (54)$$

where: h_c – enthalpy of combustion products in the combustion chamber, $h_{f_{pm}}$ – enthalpy of formation of the solid propellant.

The combustion temperature is assigned from the following relation by means of Newton method:

$$\Delta T = -\left(h_i - h_{f_{pm}}\right) / \left(\frac{\partial h}{\partial T}\right)_p = -\frac{h_i - h_{f_{pm}}}{c_p}. \quad (55)$$

Temperature for each further iteration is:

$$T^{(r+1)} = T^{(r)} + \Delta T^{(r+1)} \quad (56)$$

where, r – number of iterations.

Iteration procedure is repeated until condition $\Delta T \leq 0,01$ being satisfied.

2.6 Expansion characteristics in the nozzle

The basic equation for assignment of characteristics of gas expansion in the nozzle is the equation of isentropic process:

$$s - s_c = 0 \quad (57)$$

where: s_c – entropy of combustion products in the combustion chamber, s – entropy of combustion products at a cross-sectional area of the nozzle.

For both „frozen“ and „shifting“ equilibrium conditions, three cases are considered as follows [10,4,9,13]:

- expansion to given pressure at the nozzle exit,
- expansion to given Mach number,
- expansion to given expansion ratio (ratio of cross-sectional area at the nozzle exit to the throat area).

For the expansion up to given pressure:

$$\left(\frac{\partial s}{\partial \ln T} \right)_p \Delta \ln T = -\delta_s, \quad (58)$$

where: $\delta_s = S - S_c$ and

$$\Delta \ln T = -\delta_s / \left(\frac{\partial s}{\partial \ln T} \right)_p = -\frac{\delta_s}{c_p} \quad (59)$$

Iteration procedure is repeated until the condition $|\Delta \ln T| < 0,1 \cdot 10^{-4}$ being satisfied.

For the expansion up to given Mach number, the equations (59), (47), (23) or (25), are solved simultaneously, until the following condition being satisfied:

$$\left| \frac{u_t^2 - a_t^2}{u_t^2} \right| \leq 0,4 \cdot 10^{-4}. \quad (60)$$

Pressure at the nozzle throat, is obtained by the following relation:

$$P_t = P_c \left(\frac{2}{\gamma + 1} \right)^{\frac{\gamma}{\gamma - 1}} \quad (61)$$

For the expansion up to given expansion ratio A_t/A_e , relation (59) is solved, until the condition $|\Delta \ln T| < 0,1 \cdot 10^{-4}$ being satisfied.

Initial pressure estimation at the nozzle exit is predicted on the basis of the following empirical relation [10]:

$$\ln \frac{P_c}{P_e} = \gamma + 1,4 \ln \frac{A_e}{A_t} \quad \text{za} \quad \left(\frac{A_e}{A_t} \geq 2 \right) \quad (62)$$

where, value of γ is taken from the previous cross-sectional nozzle area. For further iterations, pressure is calculated from the equation of state.

In case of expansion at „frozen“ equilibrium conditions, combustion products mixture is considered as non-reacting, while an expanding gas mixture at „shifting“ conditions is chemically reacting mixture.

3. VERIFICATION OF THE MODEL FOR CALCULATION OF THEORETICAL PERFORMANCES OF ROCKET MOTORS

On the basis of the presented mathematical model, the computer code *TCPSP* (*Thermo-Chemical Properties Solid Propellant*) has been developed. This program enables calculation of the combustion products composition at chemical equilibrium, transport properties of gaseous combustion products and theoretical performances of rocket motors. This model describes procedures for obtaining theoretical performances of rocket motors for both cases of expansion, at “frozen” equilibrium and “shifting” equilibrium conditions.

The computer program *TCPSP* enables calculation of theoretical performances of rocket motors with propellants consisting of the following chemical elements: *Al, C, Ca, H, K, Mg, N, Na, O, P, S, Si, Ti, F, Fe, Cl, Pb*. The data-base consisting of 100 propellant ingredients based on available data published by MARTIN MARIETA^[8] and STANAG 4400^[5] has been established. This program is capable to predict properties of combustion products mixture with 156 gaseous and 39 phase-condensed ingredients. The data bases, which consist of propellant ingredients and combustion products, can be upgraded by new ingredients.

A comparative analysis of results obtained by the *TCPSP* program with results from French computer code *Ophelia*, version 3, for a composite solid propellant BUTALANE 82/4^[13] and with American computer code *CEA* (Chemical Equilibrium with Applications) for a composite solid propellant with the following composition: ammonium perchlorate, CHOS-Binder, Al, MgO, H₂O (with percentage contents of 72.06/18.58/9/0.2/0.16)^[11].

Besides, a detailed comparative analysis of several double base rocket propellants has been performed, and an analysis of some theoretical performances of DB propellants NGR-A and NGR-B compared to experimental results, has been considered particularly.

By analyzing the values of molar parts of combustion products for composite propellants, a small deviation of results obtained by *TCPSP* program compared to results obtained by programs *Ophelia* and *CEA* for all variants of calculation, has been noted. Maximum deviations of calculated results for combustion products mixture, obtained by *TCPSP* program^[18] are:

- compared to results from *Ophelia* V3 about 1,2 %,
- compared to results from *CEA* about 1,5 %.

A good agreement of calculated thermodynamic properties of combustion products mixtures with results from the program *Ophelia* V3 (Fig. 1 and 2), for both cases of expansion, has been obtained. Maximum deviation of results obtained by *TCPSP* program compared to those from *Ophelia* V3 is 4.5 % (pressure at nozzle exit for $A_e/A_t=30$).

A good agreement of thermodynamic properties of combustion products mixture in the combustion chamber, calculated by *TCPSP* compared to those from *CEA* code has also been obtained (Table 1).

The program *TCPSP* gives a good accuracy of prediction for combustion products viscosity and thermal conduction coefficient in the combustion chamber and at the nozzle throat when compared to results from *Ophelia* V3 program. Maximum deviations of 7.5% to 10.5% have appeared only at thermal conductivity coefficient prediction, at the nozzle exit and for the expansion ratio of $A_e/A_t=30$.

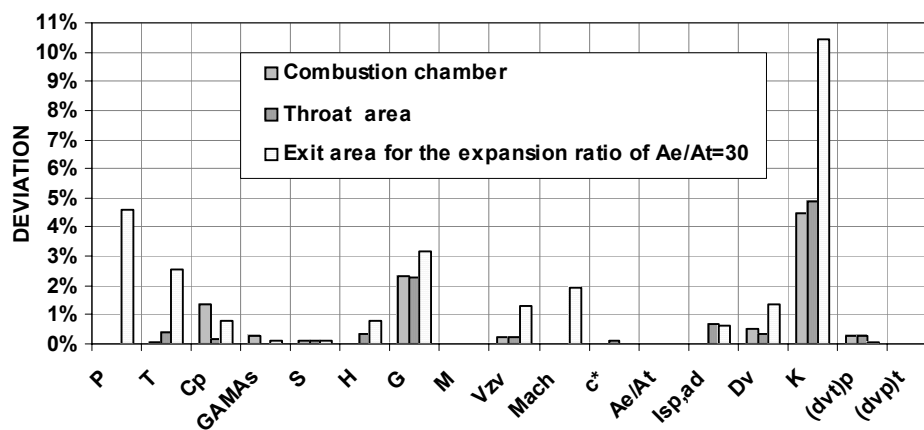


Fig. 1. Comparative analysis of some properties for solid propellant BUTALANE 82/4 in case of „shifting“ equilibrium expansion when compared to results from Ophelia version 3

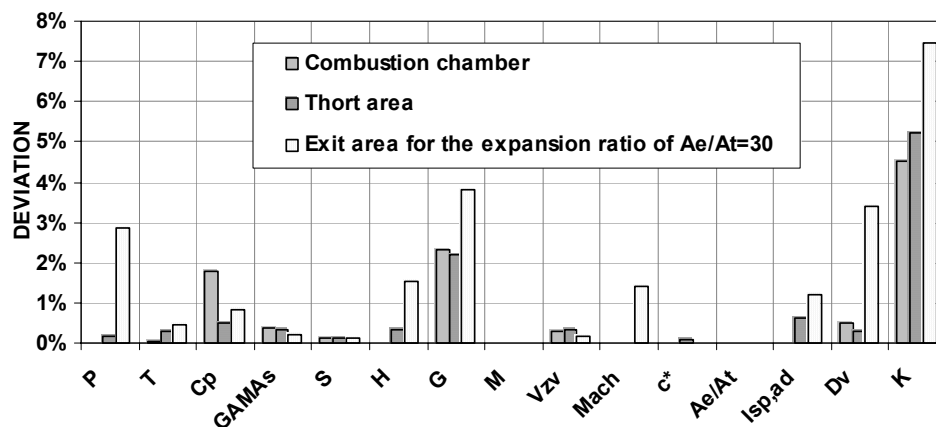


Fig. 2. Comparative analysis of some properties for solid propellant BUTALANE 82/4 in case of “frozen” equilibrium expansion when compared to results from Ophelia version 3

Table 1. Comparative analysis of some properties in the combustion chamber for the solid propellant AP/CHOS-Binder/Al/MgO/H2O

P [MPa]	3.447			1.724		
	TCPSP	CEA [11]	DEVIATION	TCPSP	CEA [11]	DEVIATION
T [K]	2716.8	2724.46	-0.28%	2700.2	2708.02	-0.29%
Cp [J/gK]	2.4185	2.40789	0.44%	2.5407	2.531738	0.35%
γ	1.1969	1.1945	0.20%	1.1926	1.189	0.30%
s [J/gK]	10.529	10.57506	-0.44%	10.788	10.82443	-0.34%
h [J/g]	-2028.3	-2028.24	0.00%	-2028.3	-2028.24	0.00%
ρ [g/m ³]	3527	3520.9	0.17%	1772	1768.1	0.22%
M (1/n)	23.112	23.136	-0.10%	23.071	23.096	-0.11%
M _w [g/mol]	22.262	22.282	-0.09%	22.225	22.246	-0.09%
a [m/s]	1080.1	1081.4	-0.12%	1075.4	1076.6	-0.11%
(dvt)p	1.0457	1.0518	-0.58%	1.069	1.0686	0.04%
(dvp)t	-1.0026	-1.00263	0.00%	-1.0035	-1.00342	0.01%

Stand tests of 128mm rocket motors with two types of DB propellants (NGR-A and NGR-B) were performed. Measured values of specific impulse of the tested rocket motors and those calculated by *TCPSP* is shown in Table 2. Deviations of the measured specific impulse compared to those calculated by *TCPSP* are: for propellant NGR-A is 7.98% and for propellant NGR-B is 9.96%. These deviations of specific impulse are in accordance with the published results given by other authors, since usual specific impulse losses are between 2% to 10 %.

Table 2. Compared results of the measured and the calculated values of specific impulse for DB solid rocket propellants NGR-A and NGR-B

Reference	I_{sp} [Ns/kg]	Type of solid propellant and rocket motor working conditions
<i>TCPSP</i>	2213.6	NGR-A, $p_c=130$ bar, $p_a=1.01325$ bar, $A_e/A_t=7.51$
Measured [17]	2050	
Deviation [%]	7.98	
<i>TCPSP</i>	2243.3	NGR-B, $p_c=130$ bar, $p_a=1.01325$ bar, $A_e/A_t=7.51$
Measured [17]	2040	
Deviation [%]	9.96	

4. CONCLUSION

The program *TCPSP* enables:

- Calculation of the chemical equilibrium composition for a multi-phase, multi-ingredient combustion products mixture, its thermodynamic and thermo-physical properties, as well as performances of the process within a rocket motor.
- Applied algorithm enables calculation of theoretical performances for double base and composite rocket propellants as well.
- Further extension of the data base:
 - includes thermo-chemical properties of different ingredients as possible constituents of wide spectrum of solid rocket propellants, and
 - coefficients of reduced thermodynamic and thermo-physical potentials for calculation of corresponding properties of possible combustion products and parameters of potentials as well.
- Very good agreement of calculated theoretical performances of rocket motors with referent programs *Ophelie* and *CEA*.

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