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RESEARCH ARTICLE

The Generalized Tensor Model for Numerical Investigation of Combustion and Flow Processes in Liquid Rocket Engine Chamber

Sıvı Roket Motoru Odasında Yanmave Akış Süreçlerinin Sayısal Araştırılması için Genelleştirilmiş Tensör Modeli

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Abstract

Combustion and flow thermogasdynamics is one of the most sophisticated computational stages in liquid rocket engine (LRE) design. A considerable amount of different methodologies used to conduct the thermogasdynamic analysis of the combustion and flow process and obtain the accurate estimates of the parameters of the LRE chamber is known. However, the development of a generalized mathematical model that would have a capability of being applied for any unique combustion case by, hence, yielding reliable results and, nevertheless, be efficient in any application still remains to be an issue. The following paper considers the development of a generalized tensor model the application of which for any desired propellant configuration yields unique results. In addition considered the application of the mentioned model at significant nozzle sections. Moreover the current paper, also, considers an approach based on the specific area in order to compute the parameters at the nozzle throat. The uniqueness of this methodology stems from the fact that the findings appear to be more accurate than those acquired using conventional methods. The paper accurately summarizes the application of the generalized tensor model based on an example problem which involves the combustion of liquid methane with liquid oxygen.

Keywords: Liquid Rocket Engine, Combustion and Flow Processes, Generalized Tensor Model

Özet

Yanma ve akış termogazdinamiği sıvı roket motoru (SRM) tasarımındaki en karmaşık hesaplama aşamalarından biridir. Şu anda yanma ve akış sürecinin termogazdinamik çözümlemesini (analizini) yürütmek ve SRM odasının parametrelerinin (değişkenlerinin) doğru değerlerini elde etmek için kullanılan önemli miktarda farklı metodolojiler bilinmektedir. Bununla birlikte, herhangi bir benzersiz yanma durumu için uygulanma kabiliyetine sahip olacak, dolayısıyla güvenilir sonuçlar veren ve yine de herhangi bir uygulamada etkili olabilecek genelleştirilmiş bir matematiksel modelin geliştirilmesi hâlâ bir sorun olmaya devam etmektedir. Aşağıdaki makale, herhangi bir yakıt konfigürasyonu için uygulamanın benzersiz sonuçlar verdiği genelleştirilmiş bir tensör modelinin geliştirilmesini ele almaktadır. Ayrıca söz konusu modelin önemli lüle (nozul) bölümlerinde uygulanması düşünülmüştür. Bunun yanında, mevcut makale, lüle boğazının değişkenlerini hesaplamak için özel enine kesite dayalı bir yaklaşımı ele almaktadır. Bu metodolojinin benzersizliği, sonuçların geleneksel yöntemler kullanılarak elde edilenlerden daha doğru görünmesine dayanmaktadır. Makale, sıvı metanın sıvı oksijen ile yanmasını içeren örnek bir probleme dayanılarak genelleştirilmiş tensör modelinin uygulamasını doğru bir şekilde özetlemektedir.

Anahtar Kelimeler: Sıvı Roket Motoru, Yanma ve Akış Süreçleri, Genelleştirilmiş Tensör Modeli

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1. INTRODUCTION

The thermogasdynamic analysis (TGDA) of the combustion process is a topic of major interest in liquid rocket engine (LRE) design [1-6]. An immense amount of different methodologies and thermodynamic approaches used to conduct the analysis of the combustion process in LRE has been developed until now [7-12]. However, an accurate study of these methodologies reveals the fact that various mathematical models have been developed for various computation conditions (temperature and pressure in combustion chamber-T_c, P_c; oxidizer excess ratio α) which are shown in literature [9],[10],[13-15]:

1) $400 \le T_c \le 1500K$, $\alpha < 1$ and $\alpha > 1$,

2) $1500 \le T_c \le 2000K$, $\alpha < 1$ and $\alpha > 1$,

3) $2000 \le T_c \le 3000K$, $\alpha < 1$ and $\alpha > 1$,

4) $T_c > 3000K$, $\alpha < 1$and $\alpha > 1$.

For each case above a specific composition of combustion products is considered. However, these studies do not show the features of the calculation cases $\alpha >> 1$, $T_c < 1500K$, $P_c > 50MPa$ and $0.01 < \alpha << 0.1$, $T_c > 3000K$, $P_c > 50MPa$ [16].

Therefore, a generalized model which would be unique in a sense that it would be capable of being applied for any case by, hence, yielding correct results is still absent.

The fundamentals of existing approaches for TGDA of combustion and flow processes in LRE thrust chambers were developed by S. Gordon, B.J. McBride in 1959-1994 and by V.Ye. Alemasov, A.F. Dregalin, A.P. Tishin in 1962-1989.However, the improvement of the mathematical model and numerical implementation of TGDA is still ongoing [7-10]. Currently, for TGDA of LRE such software packages as CEA (NASA, USA), Astra.4/pc, TERRA (Russia), RPA (Germany), the algorithms of which are based on matrix calculus are widely used. However, analysis of computational results yielded by these software packages show that at certain combinations of mixture ratio α and pressure P_c, the solution of the system of equations diverges. Modeling the kinetics of fuel combustion at extreme values of P_c, α or in the non-stoichiometric conditions is a complicate problem and has not been studied enough. In this case, mixture formation schemes, local aerodynamics of gases and flame have a significant impact on the final temperature of gases in the combustion zone. These conclusions are confirmed in different researches by for TGDA [17-19]. Thus this circumstance confirms the need to improve the method of numerical analysis of the combustion equilibrium.

As it is known, the effectiveness of TGDA depends on the successful application of thermochemical calculation. The thermochemical calculation allows determining the elementary composition of propellant (conditional formula), stoichiometric ratio of fuel components, actual mixture ratio, oxidizer excess coefficient and propellant enthalpy. The propellant enthalpy allows determining the temperature of the combustion products in the LRE chamber. In this case, the most important characteristic of the propellant, which determines specific impulse of the LRE, is the average molecular

weight of the combustion products. It is known that as lighter the combustion products are, the greater the specific impulse of the engine becomes. Consequently, an accurate assessment of combustion products composition determines the perfection of the LRE chamber.

However, in existing studies the problems listed below have not been solved due to their uncertainties [10, 13, 16-19]:

- final composition of combustion products,
- possibility of existence of an equilibrium state described by this mathematical model under any considered conditions in a wide range of oxidizer excess ratio α, in a wide range of temperature T_c, in a wide range of gas expansion ratio ε,
- completeness, non-redundancy and non-inconsistency of used thermochemical models for equilibrium state,
- convergence of the numerical solution of equilibrium state models for any physical calculation conditions,
- adequacy of the numerical calculation results to the known physical-chemical principles.

In this case, the main problem of thermodynamic calculation is the unknown probability distribution of the mixture ratio or different combustion products along the LRE chamber [16, 17]. The solution of these problems requires a large number of numerical experiments and evidential comparison of the results of numerical calculations with experimental data. Consequently, due to the small amount of experimental data, the numerical values of important parameters (thrust, specific impulse, pressure and temperature in various chamber sections, specific area of the nozzle throat section) of a virtual LRE are compared with the values of the same parameters obtained in tests of real engines.

Analysis of existing researches shows that the matrix form of the thermochemical model for combustion and flow processes in the LRE chamber is not effectively implemented in computational algorithms. The numerical solutions of such models are very sensitive to the initial and boundary conditions. Iterative convergence processes are poorly adapted to the extreme values of the α, T_c, P_c parameters and often lead to errors. The development of a model for the analysis of the equilibrium state and its numerical implementation for a large range of parameters α, T_c and ε values, does not allow the efficient use of computer resources due to the high array dimensions and large differences among the elements of these arrays. Therefore, it is necessary to apply the tensor mathematics for the thermodynamic calculation of the parameters of multi-component reactants mixtures in the LRE chamber. Considering the information presented above, a tensor model for the thermochemical calculation of the combustion process is considered in the next paragraphs.

2. PROBLEM FORMULATION

As noted in the previous paragraph, the numerical solution of the existing analytical models of the equilibrium state in various multidimensional subdomains of parameters α, T_c and ε often leads to erroneous results [16]. For example, the working processes

in the LRE chamber at start and shutdown stages, the internal cooling (film cooling) of the LRE chamber at these operating modes, the processes in the gas generator, as well as in the chambers for the pressurization system of fuel tanks, are characterized by large ranges of pressure and mixture ratio. Sample results of the thermochemical calculations at low mixture ratio values ($k_m = 0.5$, $\alpha = 0.125$) using CEA and RPA show large differences in chamber parameters values (Tab.1). Such differences are explained by the imperfection of the thermochemical model and the lack of efficient computational algorithms. This circumstance leads to the search for new mathematical models or calculation algorithm.

Table 1. Comparison of calculation results of the RPA and CEA(**CH_4/O_2** propellant) for RD-192 engine.

Parameters	Chamber RPA/CEA	Throat RPA/CEA	Exit RPA/CEA
Pressure, p_c, *bar*	205,940/ 205,940	118,823/ 117,31	0,647/ 0,64724
Temperature, T_c, *K*	1137,0131/ 1476,3800	1073,3577/ 1370,52	626,6064/ 808,01
Gamma, γ	1,23/ 1,1831	1,2264/ 1,1748	1,1834/ 1,1346
Sonic velocity, *a, m/s*	820,7198/ 1101,6	794,0866/ 1051,8	576,5509/ 741,8
Mach number, *M*		1,00	3,8388/ 3,853
Area ratio, A_e/A_{th}		1,00	34,4396/ 34,351

It is known that the main properties of the combustion product system in the LRE chamber are dynamic indicators that depend on many factors [16-19]:

- the physical and chemical properties of the initial fuel components,
- the unknown amount of combustion products of the previous chemical reactions,
- the reaction conditions at considered and previous points (temperature, pressure, density, speed),
- etc.

Thus, the gas mixture in the LRE chamber mathematically is a linear multi-component algebraic object (tensor). Tensor components written in a certain coordinate system in the matrix form are calculated by linear transformations when passing to another coordinate system. Moreover, in a special "own coordinate system" the tensor has the simplest structure in the form of a diagonal matrix. Consequently, the tensor description of the gas in the LRE chamber makes easy a study of its physical and chemical properties.

Therefore, it is necessary to apply the tensor calculus of the analytical model, which provides a solution stability and accurate determination of required thermochemical properties in a wide range of parameters α, T_c and ε ($\varepsilon = P_c / P_e, P_c, P_e$- pressure in the combustion chamber and at the nozzle exit) than in [10,12,13,20-23]. This approach will allow solving the following problems:

- more accurate determination of the gas characteristics in LRE and preburner chambers (also for pressurization system) using a single calculation model,
- more accurate determination of the gas parameters under various flow conditions (for example, in the boundary layer on the inner wall of the LRE chamber),
- more accurate determination of the emission of harmful substances.

Thus in order to determine the specific area variation along the LRE chamber, generalized tensor model (GTM) is applied at different total pressure values that are obtained by developing a linear distribution of it starting from the combustion chamber pressure until the nozzle exit pressure, which appears to be equal to the ambient pressure since the expansion is assumed to be ideal [5, 24, 25]. This approach has been implemented in the current paper in order to determine the pressure at the nozzle throat. However, since all the algebraic expressions for determination of such parameters as the mixture enthalpy and entropy, gas constant, average molecular weight, etc. are available in the sources presented in the bibliography [7-10], the current paper involves only the description of GTM. Research objective for the current research work only the chemical elements consisting of carbon $^{6}\mathbf{C}$, hydrogen $^{1}\mathbf{H}$, oxygen $^{8}\mathbf{O}$ and nitrogen $^{7}\mathbf{N}$ are considered. As mentioned previously, there are several methodologies that have been developed so far in order to solve for the various propellant configurations such as the combustion of liquid hydrogen $\mathbf{H}_2$ with liquid oxygen $\mathbf{O}_2$, liquid methane $\mathbf{CH}_4$ with liquid oxygen $\mathbf{O}_2$, hydrazine $\mathbf{N}_2\mathbf{H}_4$ with liquid $\mathbf{HNO}_3$, etc. At the same time, one of the main goals of these studies is to develop GTM that provides a stable solution for all cases where the fuel and oxidizer components consist of a large number of different compounds, i.e. multi-component fuel systems [10-13, 26]. Moreover, the development of a common algorithm for determination of the total pressure at the nozzle throat, which again depends on the formulation of a stable GTM, is, also, a question of major importance in the current article. Research limitations of TGDA of the combustion process are a combination of two scientific disciplines that are thermodynamics and gas dynamics. The thermodynamic branch of TGDA requires the implementation of the chemical information as well. The most significant chemical data required for TGDA is the values of the chemical equilibrium constants at different temperatures [23]. Due to the absence of the required laboratories and substances, only four chemical elements and the chemical equilibrium constants varying in the interval of 800K…4000K could have been taken into consideration. However, with the available information about the chemical equilibrium constants and accurate properties of other chemical elements as well, GTM developed in the current research work could be extended up to any desired number of chemical elements by, hence, extending the scope of application.

3. THE MATHEMATICAL MODEL FOR THERMOCHEMICAL CALCULATION OF COMBUSTION AND FLOW IN LRE CHAMBER

3.1. The Analytical Model for Thermochemical Calculation of the LRE

In general, for thermodynamic calculation of the LRE chamber is considered fuel with source elements **C**, **H**, **O** and **N**. For determining of the composition and temperature of the combustion products in each LRE chamber section a system of equations is composed using following laws and equations[1-9,14,27,28]:

1. The chemical equilibrium law,
2. The equation of material balance (law of conservation of matter),
3. The Dalton's law (partial pressure balance equation).

Thus, if the fuel consisting from m chemical components (in general $A^{(1)} = C$, $A^{(2)} = H$, $A^{(3)} = O$, $A^{(4)} = N$, $m = 4$) and the conditionally chemical formula of the fuel is shown as $A^{(1)}_{b_{1.y}} A^{(2)}_{b_{2.f}} ... A^{(i)}_{b_{i.f}} ... A^{(m)}_{b_{m.f}}$, and the formula for the j-th molecular compounds of the combustion products is shown in $A^{(1)}_{a_{1.j}} A^{(2)}_{a_{2.j}} ... A^{(i)}_{a_{i.j}} ... A^{(m)}_{a_{m.j}}$ form, then equations for the Fuel→Combustion Products chemical reactions can be shown in the form [4-7],

$$M_f (A^{(1)}_{b_{1.f}} A^{(2)}_{b_{2.f}} ... A^{(i)}_{b_{i.f}} ... A^{(m)}_{b_{m.f}}) \rightarrow \sum_{j=1}^{l} n_j M_j + \sum_{i=1}^{m} n_i A^{(i)} \quad (1)$$

where M_j -molecular compounds of combustion products, $CO, CO_2, H_2O, 0_2, H_2, H, O$ etc all.

1.The chemical equilibrium law [4-7],

$$K_j = \prod_i P_i^{a_{i.j}} \Big/ P_j \text{ or } \ln P_j + \ln K_j - \sum_{i=1}^{m} a_{i.j} \ln P_i = 0, \quad (2)$$

$$i = 1, 2, 3, ..., m, \; j = 1, 2, 3, ..., l.$$

2.The equation of material balance (law of conservation of matter) [4-7],

$$\sum_{j=1}^{l} a_{i.j} n_j + n_i = b_{i.y}, \; i = 1, 2, 3, ..., m, \; j = 1, 2, 3, ..., l \quad (3)$$

For M_f moles fuel

$$\sum_{j=1}^{l} a_{i.j} n_j + n_i = M_f b_{i.f} \text{ or } \ln(\sum_{j=1}^{l} a_{i.j} n_j + n_i) - \ln(M_f) - \ln(b_{i.f}) = 0 \quad (4)$$

3.The Dalton's law (partial pressure balance equation) [4-7],

$$\sum_{q}^{l+m} P_q = P, \ln \sum_{q}^{l+m} P_q - \ln P = 0, q = 1, 2, ..., l + m \quad (5)$$

where $a_{i.j}$ -atomic number of the chemical element $A^{(i)}$ in molecular product M_j, P_i - partial pressure of chemical element $A^{(i)}$ dissociated in dissociation, P_j - partial pressure of molecular product M_j exposed to dissociation, K_j -equilibrium constant, n_i -the number of moles of the chemical element $A^{(i)}$, n_j -moles of the molecular component M_j, $b_{i.f}$ - the number of atoms of the chemical element $A^{(i)}$ in the fuel, M_f - number of the fuel moles, P_q - partial pressure of the component in the mixture of the combustion

products, P - pressure of the mixture.

Assuming gases as ideal, the relationship between partial pressures and moles can be considered as

$$n_\Sigma = \sum n_i \ , \ P = P_\Sigma = \sum P_i \ , \ n_i = P_i \ , \ n_\Sigma = P_\Sigma \tag{6}$$

The system of non-linear equations is solved accurately using the Newton method [29]. As already noted, in order to more accurately design of the engine chamber, it is necessary to take into account changes in the specific heat values (c_v , c_p) and the isentropic index γ along the LRE chamber length [30-34].

Taking into account the noted features of the matrix calculus, in the next paragraph is considered the solution of the analytical model (Eq.'s 1-6) in tensor form.

3.2. The Tensor Model for Elementary Composition of Propellant

Introduce the tensor $\mathbf{E}_i$ consisting of several chemical elements that are included in TGDA of the combustion process [1-7]. For example, in case, if TGDA involves the existence of four chemical elements such as carbon $^6\mathbf{C}$, hydrogen $^1\mathbf{H}$, oxygen $^8\mathbf{O}$ and nitrogen $^7\mathbf{N}$, then $1 \le i \le 4$ and the tensor $\mathbf{E}_i$ represents the chemical elements respectively. Besides, introduce the tensor $^{(k)}\mathbf{U}_i$ that represents any chemical compound in general, where $1 \le k \le 2$ indicating the fuel and oxidizer components, respectively. For example, $^{(2)}\mathbf{U}_3$ represents the number of atoms of $\mathbf{E}_3$ in the oxidizer component. Allowing the number of compounds involved in the fuel and oxidizer mixtures to be υ_k , the fuel and oxidizer mixtures can be written as,

$$^{(k)}\mathbf{\Lambda}_{ij} = \left[\begin{array}{cccc} ^{(k)}\mathbf{U}_1 & ^{(k)}\mathbf{U}_2 & \dots & ^{(k)}\mathbf{U}_{\upsilon_k} \end{array} \right] \tag{7}$$

Let the tensor $^{(k)}\mathbf{G}_j$ represent the mass fractions and tensor $^{(k)}\mathbf{M}_j$ represent the molecular weights of the compounds involved in component k. Then, the elementary composition of any compound can be written as,

$$^{(k)}\mathbf{\Pi}_i = {}^{(k)}\phi_1 \, {}^{(k)}\phi 2 \tag{8}$$

where

$$^{(k)}\phi_1 = \left[\sum_{j=1}^{\upsilon_k} {}^{(k)}\mathbf{G}_j \left[{}^{(k)}\mathbf{M}_j \right]^{-1} \right]^{-1} \tag{9}$$

and

$$^{(k)}\phi_2 = \sum_{j=1}^{\upsilon_k} {}^{(k)}\mathbf{G}_j \, {}^{(k)}\mathbf{\Lambda}_{ij} \left[{}^{(k)}\mathbf{M}_j \right]^{-1} \tag{10}$$

where, $1 \le k \le 2$, $1 \le i \le N$, $1 \le j \le \upsilon_k$, $i,j, k \in Z$ and N corresponds to the number of chemical elements involved in TGDA. There after taking into account the oxidizer excess

coefficient α ($\alpha = k_m / k_m^0$, k_m, k_m^0-actual and stoichiometric mixture ratio) and molar stoichiometry ratio λ_0, the elementary composition of the propellant can be written as,

$$\mathbf{\Gamma}_i = {}^{(k=1)}\mathbf{\Pi}_i + \alpha\lambda_0^{(k=2)}\mathbf{\Pi}_i \tag{11}$$

where

$$\lambda_0 = \sum_{i=1}^{N} {}^{(k=1)}\mathbf{\Pi}_i\mathbf{V}_i \left[\sum_{i=1}^{N} {}^{(k=2)}\mathbf{\Pi}_i\mathbf{V}_i\right]^{-1} \tag{12}$$

The tensor $\mathbf{V}_i$ holds the valences of elements included in $\mathbf{E}_i$, respectively. Based on Eq.12, the mass stoichiometric ratio can computed as,

$$k_0 = \lambda_0^{(k=2)}\phi_1\left[{}^{(k=1)}\phi_1\right]^{-1} \tag{13}$$

The mass stoichiometric ratio of the propellant components is eventually used to determine the propellant enthalpy.

3.3. The Tensor Model for Chemical Equilibrium

It is obvious that the combustion products will consist of the elements presented by $\mathbf{E}_i$. Moreover, the recombination and dissociation reactions can be written for these products. Let the tensor $\mathbf{R}_z$ store all the reactions occurring during the combustion process, where $1 \le z \le N_r$ and N_r corresponds to the number of chemical reactions presented in the system. Thereafter, the chemical equilibrium constant based equations representing the recombination and dissociation reactions can be in a general fashion as,

$${}^{(k)}\mathbf{K}_{\mathbf{R}_z} = \prod_{i=1}^{{}^{(z)}\upsilon_p} {}^{(z)}P_i^{\,{}^{(z)}C_i} \left[\prod_{j=1}^{{}^{(z)}\upsilon_r} {}^{(z)}P_j^{\,{}^{(z)}C_j}\right]^{-1} \tag{14}$$

where, υ_p-number of reaction products, υ_r-number of reactants, P_i and P_j – partial pressures of the reaction compounds with the corresponding coefficient C_i and C_j, respectively, $1 \le i \le \upsilon_p$, $1 \le j \le \upsilon_r$, $1 \le z \le N_r$ and $i, j, z \in Z$. Moreover, it is known that the chemical equilibrium constant of any chemical reaction is a function of temperature,

$${}^{(k)}\mathbf{K}_{\mathbf{R}_z} \propto T^{-1} \tag{15}$$

The first seven equations which GTM is based on can be constructed by applying Eq.14 for all the reactions appearing to be in the combustion model, respectively.

3.4. The Tensor Model for Material Balance

For analyzing processes in the LRE chamber, the mass conservation equation is expressed taking into account

- the number of atoms of elements in the elementary composition of the propellant;
- number of propellant of required for the equilibrium phase;

- partial pressures, moles of combustion products;
- number of atoms of considered elements in combustion product.

In a general fashion, the mass conservation based equations for initially selected N number of elements can be written as,

$$^{(k)}\psi\mathbf{\Gamma}_i = \sum_{j=1}^{\upsilon} {}^{(k)}N_j \, {}^{(k)}P_j \tag{16}$$

where, ψ – number of propellant moles required for the equilibrium phase, P_j – partial pressures of the combustion products involving the element $\mathbf{\Gamma}_i$, N_j – number of atoms of $\mathbf{\Gamma}_i$ in the product, the partial pressure of which is given by P_j , υ – number of the combustion products involving the element $\mathbf{\Gamma}_i$, $1 \leq k \leq N_{E_i}$, $1 \leq j \leq \upsilon$, $i = k$, $i, j, k \in Z$ and N_{E_i} corresponds to the number of individual chemical elements involved in TGDA.

3.5. The Tensor Model for Dalton's Law

Introducing the tensor $\mathbf{P}_i$ consisting of the partial pressures of the combustion products the number of which can be presented as N_p, Dalton's law can be written as,

$$\sum_{i=1}^{N_p} \mathbf{P}_i = P \tag{17}$$

stating that the total pressure of a gas mixture is equal to the sum of the partial pressures of the gas compounds that build up the mixture and where P – local sectional total pressure. Dalton's law is the last concept that is applied in the system of non-linear algebraic equations.

3.6. System of Equations

At this stage of TGDA, Eq.'s 14, 16 and 17 can be gathered together to form a system of non-linear algebraic equations $^{(0)}\mathbf{D}_i$ which can be eventually solved by applying appropriate numerical methods [4,7,9,24,29]. Let Eq.'s 14, 16 and 17 be indicated as $\mathbf{D}_1$, $\mathbf{D}_2$ and $\mathbf{D}_3$, respectively. Taking the logarithm of these equations yields,

$$^{(1)}\mathbf{D}_i = \ln \begin{bmatrix} \mathbf{D}_1 \\ \mathbf{D}_2 \\ \mathbf{D}_3 \end{bmatrix} = 0 \tag{18}$$

Eq.18 represents the matrix equation which can be solved through the methods such as Gauss-Jordan method, Gauss-Seidel method, etc., yielding the corresponding values for the partial pressures of the combustion products and number of propellant moles according to [29]. Note that, the unknowns are the logarithmic changes of the parameters that are being solved for, such as,

$$\mathbf{X}_i = \Delta \ln \begin{bmatrix} \mathbf{P}_1 \\ \vdots \\ \mathbf{P}_{N_p} \\ \psi \end{bmatrix} \tag{19}$$

This concludes the brief description of GTM. It can be applied to yield the partial pressures of the combustion products and number of propellant moles for any type of propellant configuration. Thereafter, based on the partial pressure and number of moles, the rest of thermogasdynamic parameters including the enthalpy and entropy of the mixture, molar fractions, gas constant, average molecular weight of the mixture, combustion temperature, density of the mixture, characteristic speed, specific area, local Mach number, etc. can be determined using straightforward algebraic equations retrieved from thermodynamics and gas dynamics.

4. IMPLEMENTATION OF THE GENERALIZED TENSOR MODEL

LREs based on methane and oxygen are very perspective [35-37]. RD-192 engine (JSC "NPO Energomash n.a. V.P.Glushko") can be shown as an example. Consequently, the thermodynamic calculation of thrust chambers of such engines is relevant. RD-192 ($\mathbf{CH_4/O_2}$) has been designed based on the configuration of RD-191 ($\mathbf{RP\text{-}1/O_2}$). The comparison of the enginesmain characteristics has been presented in Tab.2 [36].

Table2. Comparison of the RD-191 and RD-192characteristics [36].

LRE parameters	RD-191	RD-192
	$\mathbf{RP1+O_2}$	$\mathbf{CH_4+O_2}$
Pressure in the combustion chamber, *kPa*	25693	20594
Thrust: at sea level, *kN* in vacuum,*kN*	1922 2085	1938 2101
Specific impulse: at sea level, *s* in vacuum,*s*	 309.0 337.0	 333.4 358
Mixture ratio	2.72	3.5
Nozzle exit diameter, *mm*	1445	1445

Consider an example combustion problem, in which as the fuel and oxidizer components liquid methane $\mathbf{CH_4}$ and liquid oxygen $\mathbf{O_2}$ are presented, respectively. Methane contains the largest percentage of hydrogen in comparison with other hydrocarbon fuels and, as a rocket fuel, occupies an intermediate position between hydrogen and kerosene in terms of its physical and chemical properties: molecular weight - (16.047); density at boiling point - (0.424 g/cm^3); boiling point - (-161.52°C); melting point - (-184°C); corrosiveness - not active; toxicity - slightly toxic; shock sensitivity - not sensitive.

The enthalpies of the components appear to be -5566kJ/kg and -398kJ/kg, respectively. Moreover, the mass fraction of each component is given to be 1. Besides, the combustion chamber and ambient (or nozzle exit) pressures are provided to be 210atm. and 0.1 atm., respectively. As the last given data, the oxidizer excess coefficient

is given to be 1. It is required to apply GTM at the major nozzle sections;those are the combustion chamber, nozzle throat and nozzle exit, in order to yield the required thermogasdynamic parameters. Taking all the significant recombination and dissociation reaction occurring in the combustion chamber, GTM can be applied in order to observe the variation of the partial pressures of the combustion products in the combustion chamber for the temperature range $3000 \le T_c \le 4000K$.

4.1. Analysis of the Equilibrium in the Combustion Chamber

The energy potential of the gas is formed in the combustion chamber of the LRE and design of this part requires scientifically proven calculations. Considering the experience of LRE design based on CH_4 and O_2 proposed GTM is applied at the combustion chamber with the local section total pressure of 210 atm. with the temperature interval of [3000, 4000]K.

Methane-engines have been studied in the PhD thesis of Klepikov [36]. The choice of this temperature range in the combustion chamber is confirmed by numerical and experimental data from tests of LRE based on the propellant components liquid methane and liquid oxygen [36-39].

Fig.1 represents the variation of the partial pressures values of different combustion products and number of propellant moles, obtained through using GTM with P_c=210 atm., $\alpha = 0.8$, $k_m = 3.2$ for the combustion chamber, with temperature in the combustion chamber. As observed, the partial pressures of some of the products increase, whereas the partial pressures of other ones decrease. The reason for such an observation lies behind the expression presented in Eq.15. It can be seen that changes of partial pressures of combustion products in the range $3000 \le T_c \le 3500K$ is less intense than in the range $3500 \le T_c \le 4000K$. With an increase in the considered total pressure in the chamber, changes of partial pressures (i.e., mole fractions) of the combustion products become more intense. Due to the high temperatures, the dissociation degree increases. Hence, the partial pressures of the major complex compounds such as $\mathbf{CO}_2$ and $\mathbf{H}_2\mathbf{O}$ decrease with increasing temperature, whereas the partial pressures of the minor products increase, since the minor products occur from dissociation of $\mathbf{CO}_2$ and $\mathbf{H}_2\mathbf{O}$ and some minor reactions that occur between the minor combustion products themselves. As observed, the increase in the gas temperature (and enthalpy) in the initial section of the combustion chamber of the LRE at 210 atm. is provided by the increase of molar fractions of $\mathbf{OH}^-, \mathbf{O}_2, \mathbf{H}^+, \mathbf{O}^{-2}, \mathbf{CO}, \mathbf{CO}_2, \mathbf{H}_2, \mathbf{OH}$. This circumstance requires efficient atomization of fuel components and correct organization of mixture formation processes. A poor-quality working process in the combustion chamber of a LRE strongly affects the loss of specific impulse. Consequently, in order to increase the molar fractions of indicated combustion products an effective organization of mixture formation processes at the initial section of the combustion chamber is required.

Thereafter, variation of the mixture enthalpy can be found by applying corresponding algebraic equation [5,7]:

$$H_m = \frac{\sum_{i=1}^{N_p} H_i \mathbf{P}_i}{\sum_{i=1}^{N_p} \mu_i \mathbf{P}_i} \tag{20}$$

Where H_m -mixture enthalpy, N_p -number of combustion products, H_i - enthalpies of combustion products, $\mathbf{P}_i$ -partial pressures of combustion products, μ_i -molecular weights of combustion products.

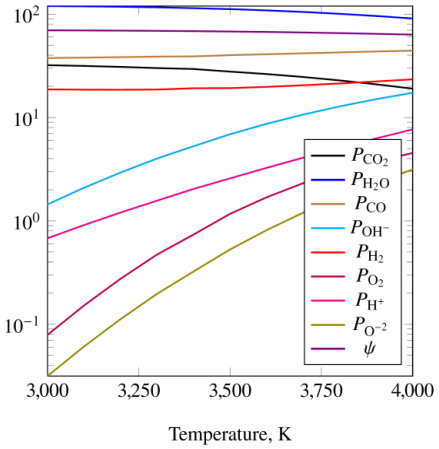

Figure 1. Variation of $\mathbf{P}_i$ in combustion chamber.

Thus on Fig.2 variation of the mixture enthalpy has been presented. Determination of the temperature at which the enthalpy of the mixture appears to be equal to the propellant enthalpy, which is -1.6285MJ/kg, yields the combustion temperature to be 3659.8K. Retrieving the partial pressure values of the combustion products and number of propellant moles at the given temperature from Fig.1 yields the actually observed values in the combustion chamber.

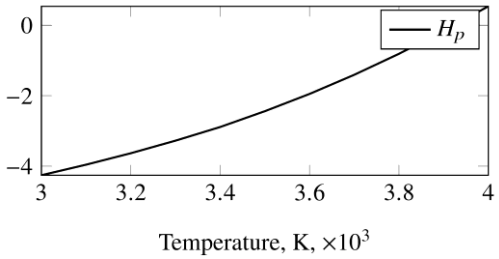

Figure 2. Variation of mixture enthalpy, MJ/kg.

Based on the corrected partial pressure values of the combustion products, the entropy, average molecular weight and gas constant of the gas mixture in the combustion chamber are computed to be 11.9383kJ/kgK, 21.3419g/mol and 389.6J/kgK, respectively. The rest of the parameters are computed based on these main thermodynamic parameters.

4.2. Analysis of the Equilibrium at the Nozzle Throat

In order to determine the parameters at the nozzle throat, initially, the total pressure at given section has to be determined. In specific area approach, the total pressure at the nozzle throat appears to be the one at which the specific area is minimum. In order to determine the minimum specific area, primarily, GTM is applied at the nozzle throat for an array of different pressure values with the starting value equal to the total pressure in the combustion chamber and final value equal to the total pressure at the nozzle exit, which, in fact, appears to be the ambient pressure in the ideal expansion case. Let 10 total pressure values to be applied in GTM.

Figs.3 and 4 represent the variation of partial pressures of the combustion products $\mathbf{P}_i$ for a linear distribution of the local sectional total pressure from the combustion chamber until the nozzle exit (in the perfect expansion case the ambient pressure is accounted). Taking the partial pressure values at each section with the local sectional total pressure for different temperatures in the given temperature interval, the variation of entropy of the mixture can be presented as well. As can be seen from Fig. 3 and 4, with an increase in pressure value the formation of heat is more intensely influenced by reactions with releasing of products $\mathbf{H_2O}, \mathbf{CO}, \mathbf{CO_2}, \mathbf{H_2}, \mathbf{OH^-}$. Wherein a strong decrease in the intensity of reactions with formation of products $\mathbf{OH^-}, \mathbf{O_2}, \mathbf{H^+}, \mathbf{O^{-2}}$ has a positive effect on the efficient conversion of heat into kinetic energy.

The variation of entropy of the mixture with temperature can be observed from Fig.5. This figure represents the variation of entropy of the mixture with temperature for different local sectional total pressure values. Despite the fact that the entropy is directly proportional to the temperature (i.e., the entropy of a mixture increases with increasing temperature), it tends to decrease as the local sectional total pressure increases. However, the results presented in Fig.5 are not enough in order to complete the nozzle throat analysis. It is known that the flow in the rocket nozzle is, theoretically, assumed to be isentropic – $\Delta S=0$. Recall, that the entropy for this propellant configuration and problem formulation appeared to be S=11.9383 kJ/kgK. Fig.5 is corrected using the cancellation principle. The entropy values are rechecked for the entropy value computed previously. The intervals not involving the given entropy value are cancelled out and only the values holding 11.9383 kJ/kgK within itself remain. Corrected variation of entropy at the nozzle throat is given in Fig.6.The temperature values at which the entropy of the mixture appears to be equal to 11.9383 kJ/kgK are retrieved from Fig.6. Thus, the variation of temperature at the nozzle throat for the given problem can be presented as well. Using appropriate algebraic equations, from the temperature variation with the local sectional total pressure at the nozzle throat, corresponding enthalpy of the mixture, flow velocity, average molecular weight, gas constant and density values can be computed as well. The variation of thermodynamics properties of the gas mixture at nozzle throat can be observed from Fig.7 and Fig.8.The specific area for any section of the LRE nozzle can be computed based on the flow velocity and density of the mixture values in this section - $f = A/\dot{m} = 1/(\rho V)$. Therefore, variation of the specific area with the local sectional total pressure can be presented as well. It can be observed that the nozzle throat corresponds to the section at which the specific area appears to be minimum- $f_{th.} = f_{th.\min}$ (see Fig.9a). Hence, from Fig.9a, it can be concluded,

that the total pressure at the nozzle throat is 140.03 atm. GTM is applied taking this value as the total pressure input and the partial pressures of the combustion products are yielded. The temperature value corresponding to the minimum specific area is 3491.8K. Applying GTM using the interpolated coefficient values at this temperature with the mentioned total pressure yields the partial pressures of the combustion products and number of propellant moles at the nozzle throat. Note that, the partial pressures of hydroxide $\mathbf{OH}^{-}$, oxygen gas $\mathbf{O}_2$, hydrogen $\mathbf{H}^{+}$ and oxygen $\mathbf{O}^{-2}$ approach to zero as the local sectional total pressure decreases.

Further, the area of each section of the chamber and nozzle is determined based on the mass flow rate $A = \dot{m}f$, $\dot{m} = F / I_{sp}$ - where I_{sp}-specific impulse, which is determined from the thermochemical calculation of processes in the LRE chamber, F -thrust (see Fig.9b).

4.3. Analysis of the Equilibrium at the Nozzle Exit

For the nozzle exit, observing the variation of the partial pressures of the combustion products, it can be assumed, that the partial pressures of the mentioned secondary combustion products get too close to zero, so that they can be neglected. Furthermore, it can, also, be assumed, that carbon monoxide $\mathbf{CO}$ at relatively lower temperatures after the nozzle throat recombines back to produce carbon dioxide $\mathbf{CO}_2$. Using this assumption and applying GTM at the nozzle exit, the partial pressures of carbon dioxide $\mathbf{CO}_2$, water vapor $\mathbf{H}_2\mathbf{O}$ and hydrogen gas $\mathbf{H}_2$ can be obtained. At the nozzle exit GTM is applied for the temperature range of $800 \le T_e \le 3000K$. Computing the entropy of the mixture at each temperature, the variation of entropy of the gas mixture at the nozzle throat can be presented. Taking the temperature at which the entropy appears to be 11.9383 kJ/kgK (recall, that the flow is assumed to be isentropic), the total pressure equal to the ambient pressure (perfect expansion is assumed) and applying GTM yields the corrected partial pressures of the combustion products at the nozzle exit (Fig.10).

4.4. Combined Application of Equilibrium Analysis, Method of Characteristics and Navier-Stokes equations

Final partial pressures of the combustion products are given in Fig.11 for different significant sections along the engine. Based on the partial pressure values of the combustion products at the significant engine sections, an approximate variation of the partial pressures can be defined by writing an approximate function relation the partial pressure to the relative position for each combustion product. Fig.12 represents the variation of the partial pressures of the combustion products with respect to the relative position along the engine. Based on the final values of the partial pressures, the variation of different thermogasdynamic parameters, including the flow velocity, gas constant, temperature and Mach number with respect to the relative position x / x_0 along the engine chamber can be presented. Fig.13 represents the variation of the main thermogasdynamic parameters with respect to the relative position along the engine. The mixture is cooled down. Moreover, due to the pressure drop of the individual compounds, the gas constant drops as well. Also, note that, the average specific heat ratio along the engine appears to be 1.1942.

A preliminary analysis shows that the combined application of the method of characteristics and the Navier-Stokes equations based on the obtained results (Fig.10-Fig.13) makes it possible to accurately determine the full geometry, including optimal contour and length of the LRE chamber. Accurate determining of these data allows to increase the specific impulse of the engine by 2.5%.

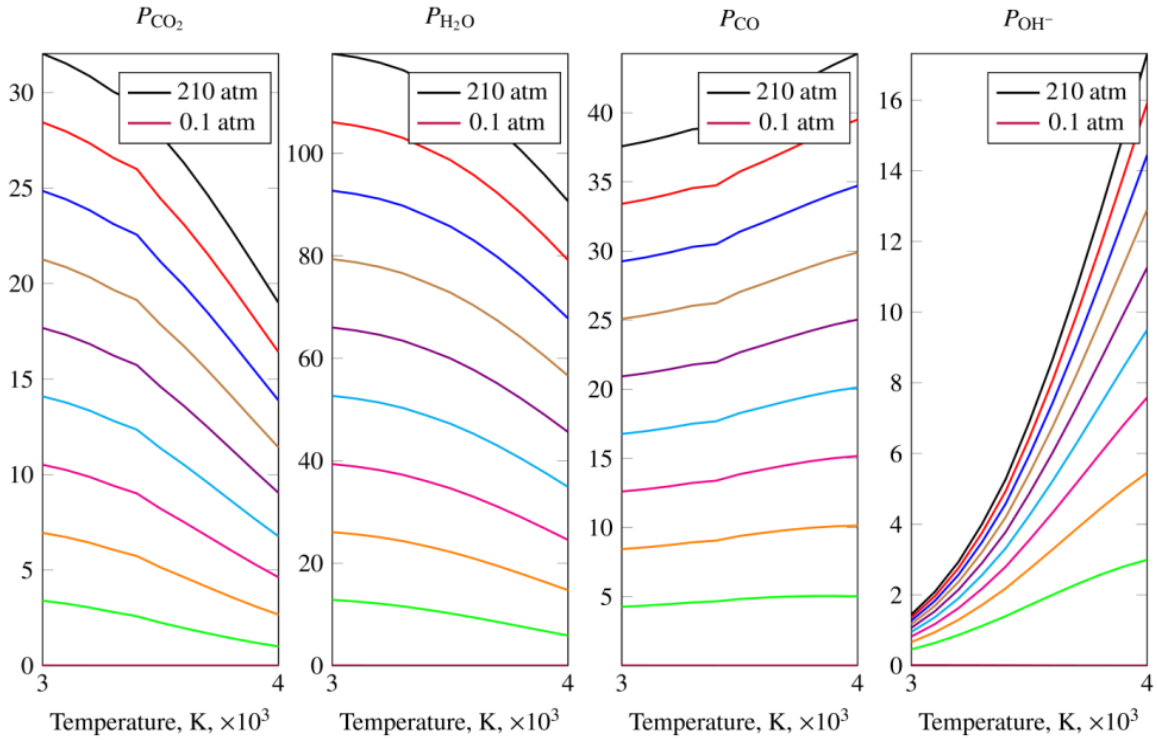

Figure 3. Variation of P_{CO_2}, P_{H_2O}, P_{CO} and P_{OH^-} for different local sectional total pressure values.

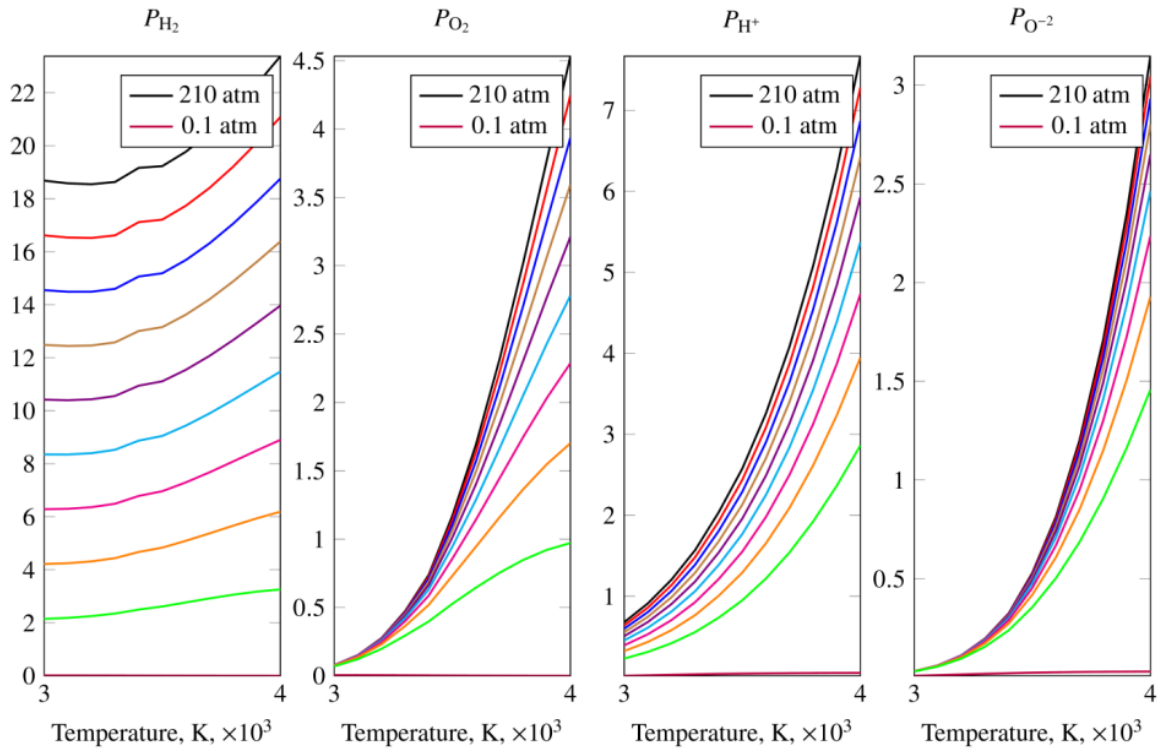

Figure 4. Variation of P_{H_2}, P_{O_2}, P_{H^+} and $P_{O^{-2}}$ for different local sectional total pressure values.

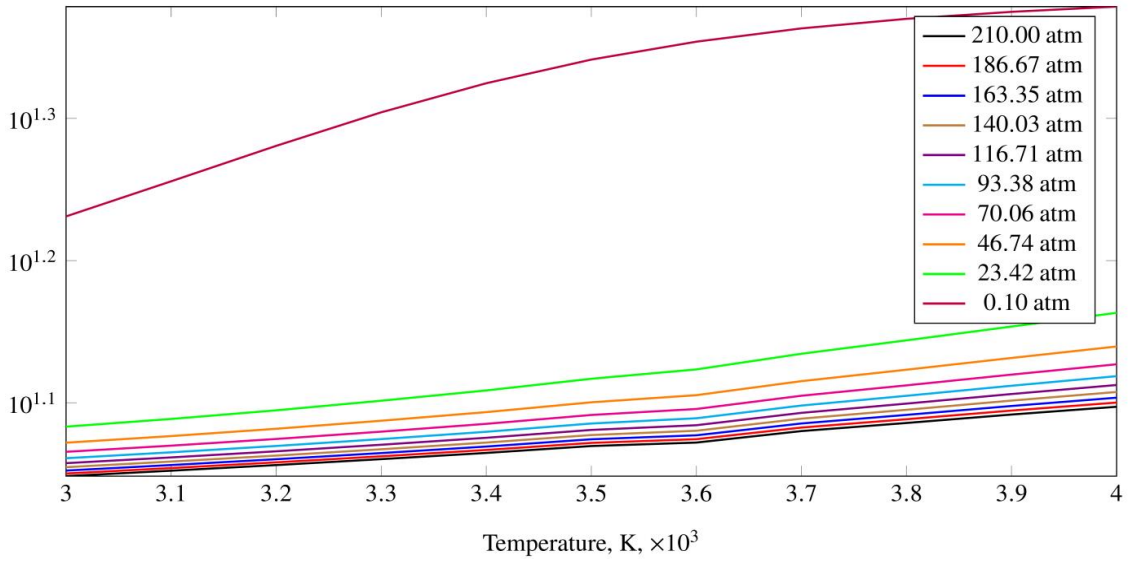

Figure 5. Variation of entropy of mixture with temperature.

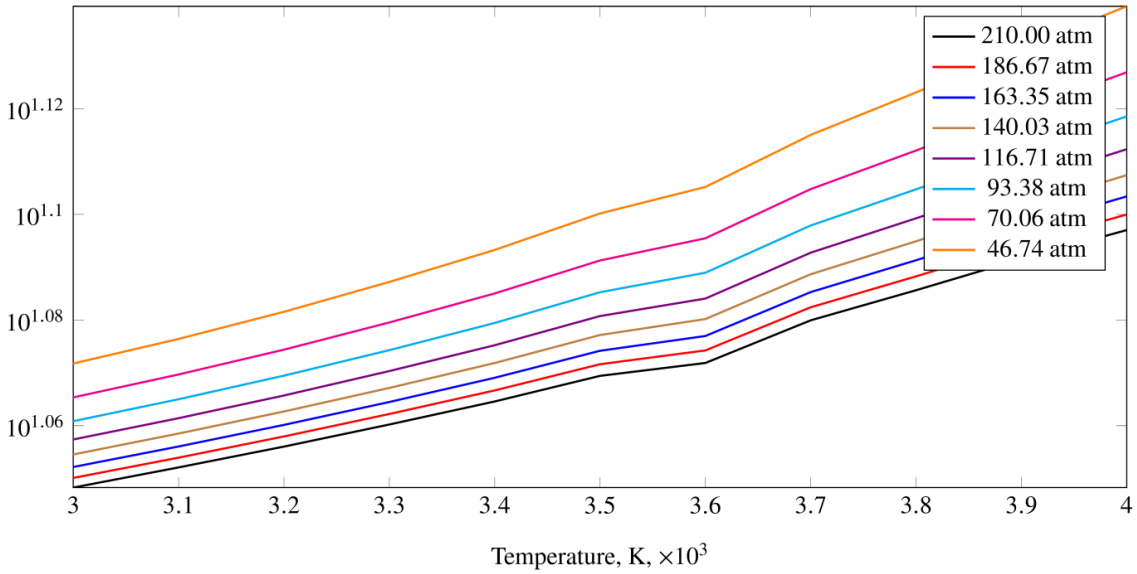

Figure 6. Corrected variation of entropy of mixture with temperature.

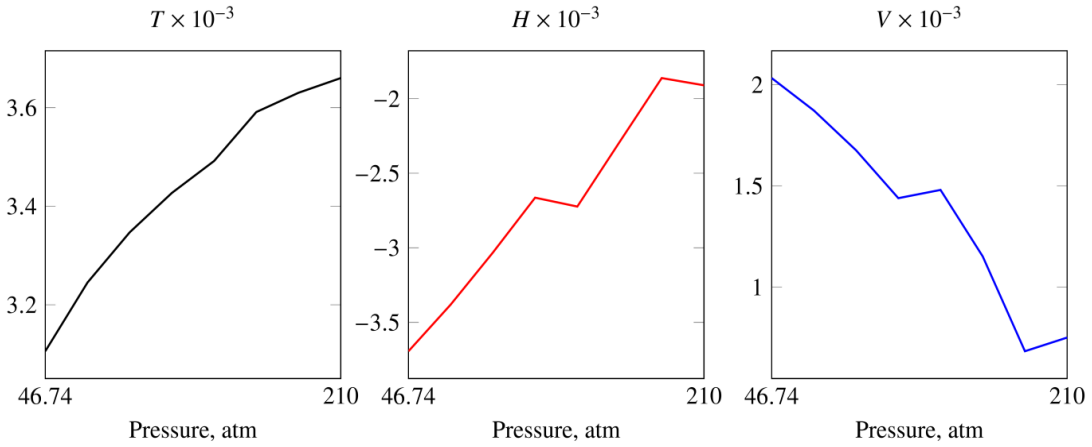

Figure 7. Variation of thermogasdynamic properties at nozzle throat (temperature, enthalpy, flow velocity).

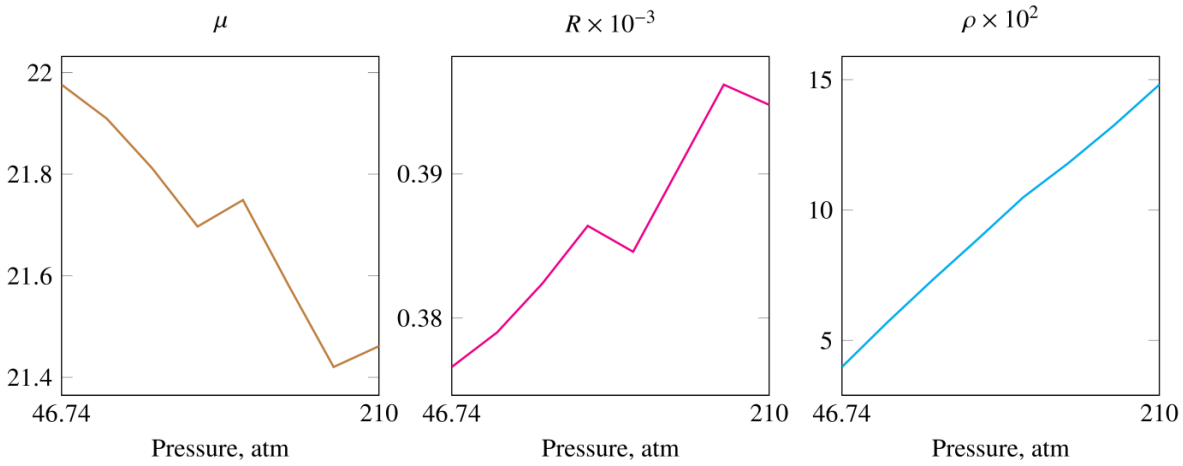

Figure 8. Variation of thermogasdynamic properties at nozzle throat (mixture molar weight, gas constant, mixture density).

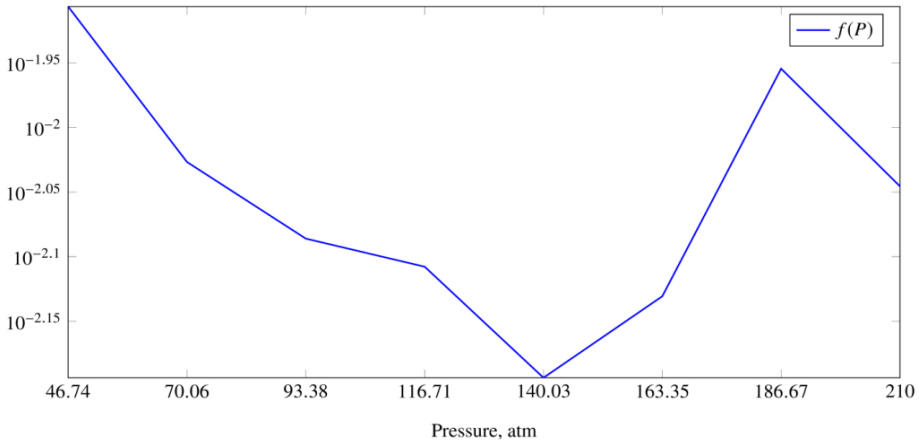

Figure 9a. Variation of specific area with local sectional total pressure.

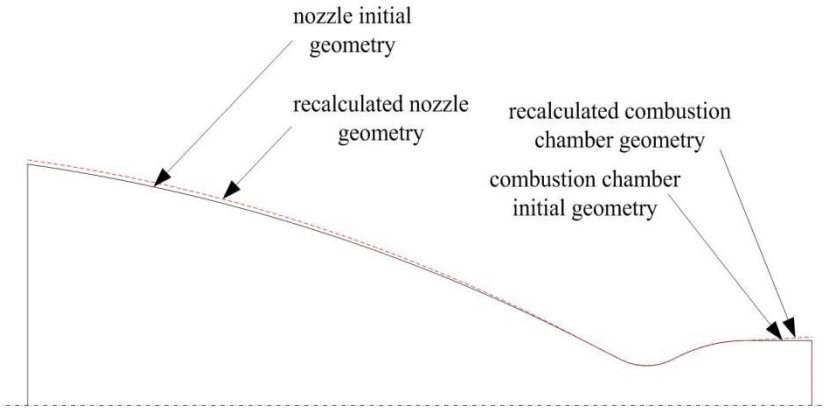

Figure 9b. Recalculated thrust chamber geometry of LRE RD-192. (CH_4/O_2).

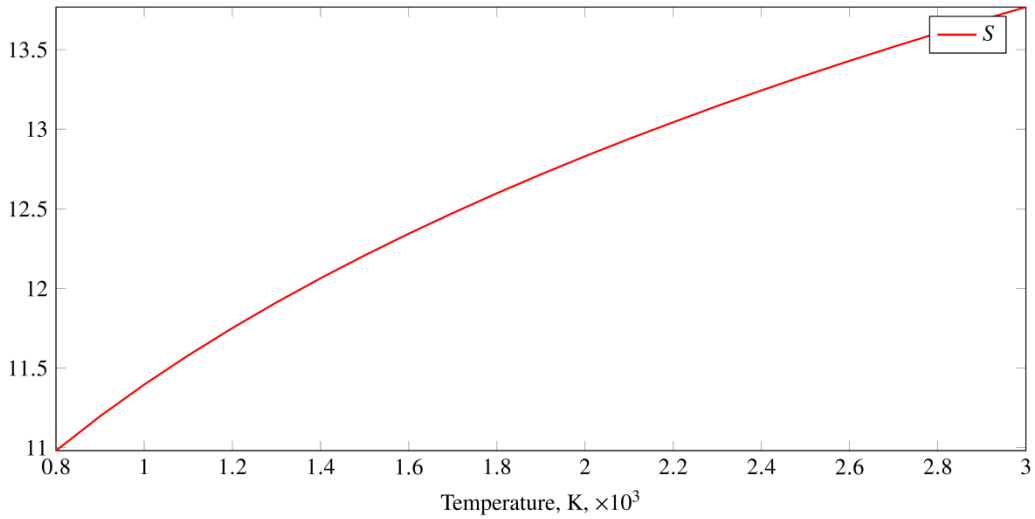

Figure 10. Entropy variation at nozzle exit.

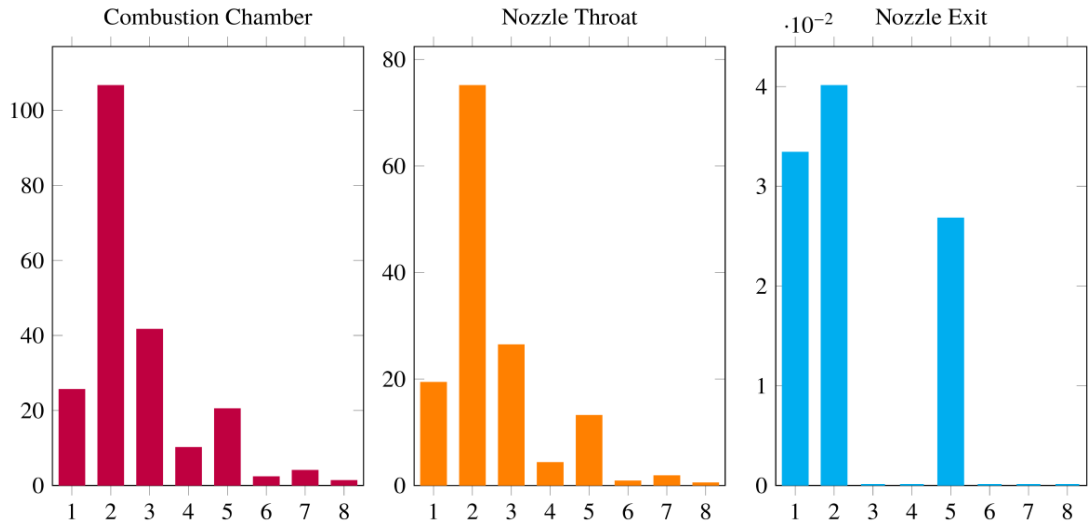

Figure 11. Partial pressures of combustion products at major sections of the nozzle: 1- P_{CO_2}, 2- P_{H_2O}, 3- P_{CO}, 4- P_{OH^+}, 5- P_{H_2}, 6- P_{O_2}, 7- P_{H^+}, 8- $P_{O^{-2}}$

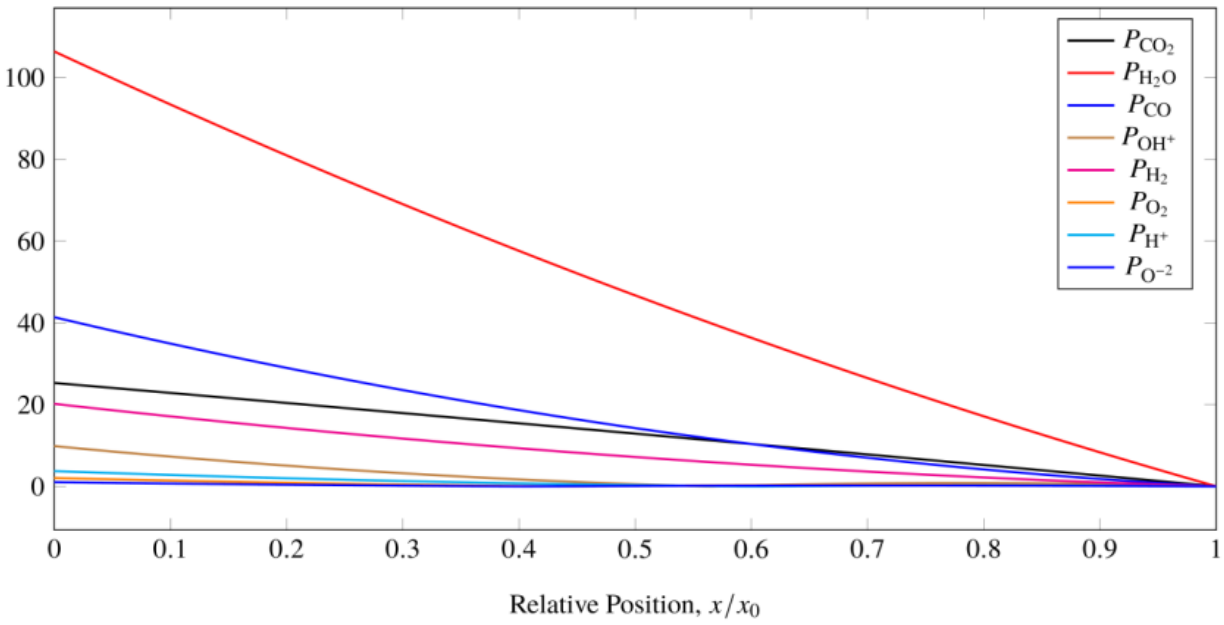

Figure 12. Variation of partial pressures of combustion products with relative position of LRE nozzle.

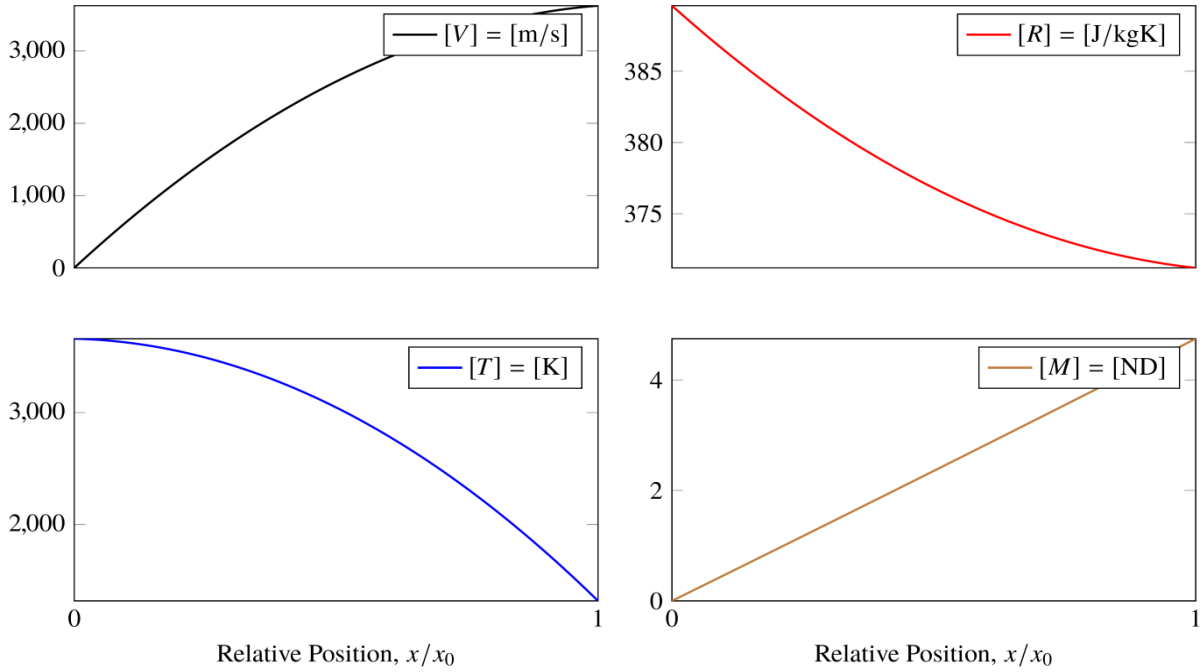

Figure 13. Variation of thermogasdynamic properties at nozzle throat. (flow velocity, gas constant, temperature, enthalpy, mixture molar weight).

5. CONCLUSION

In the current paper a generalized tensor model has been studied (combustion chamber, 3000K…4000K) and researched. These results are important for gas generators (or preburners), fuel tank pressurization systems design and calculation of the boundary layer on the inner wall of the LRE chamber.

As seen, the model consists of the stages such as the elementary composition of the propellant, construction of a system of equations considering all the recombination and dissociation reactions and solving a linearized system of equations in order to obtain the partial pressures of the combustion products and number of propellant moles required to reach the equilibrium phase. As the main research purpose, construction of a generalized model, that would be universal and have unique solutions for each individual case, has been considered. Using the example problem involving combustion of liquid methane $\mathbf{CH_4}$ with liquid oxygen $\mathbf{O_2}$, in LRE, it has been proved, that the model behaves stably meaning that the solution does not diverge. The results for the partial pressures of the combustion products and their variation along the engine chamber with respect to the relative position together with the thermodynamic outcomes and major parameters have been presented. Furthermore, as mentioned before, a specific area approach used to determine the parameters at the nozzle throat has been extensively demonstrated through the example problem presented in the paper.

Thus, the analysis of the conducted studies results shows that for considered fuel components the accuracy of parameters estimations of the LRE chamber depends on the correct choice of the composition of the combustion products and specified step for the iterative calculation. In addition, the concept of the cylindrical shape of the LRE combustion chamber and other chambers in which combustion and flow processes occur with small values of the parameter k_m should be revised.

The uniqueness of GTM is that it can be applied not only for the LRE, but, also, for the other types of engines as well, including the internal combustion engines, turbofan, turbojet, etc., since all these engines use the combustion of the hydrocarbon fuel component. Therefore, it can be concluded, that GTM can be applied in any chamber geometry that involves the combustion of the fuel component. The main advantage of considered GTM is that it yields appropriate results and is stable. Moreover, such GTM can be applied for the other elements combination (**N**, **F**, **Cl**, **Al**, **Mg**, **B**, **Be**, **Li**, etc.) as well. In other words, the current mathematical model does not limit itself to the certain amount of elements. All the available elements can be implemented in GTM. In addition, GTM takes into account all the recombination-dissociation reactions occurring in the engine and any phases (gas, liquid, condensed) of combustion products. Therefore, the model can be accounted as unique.

The reliability of the developed model is confirmed by ensuring the convergence of the numerical solution with a given level of error in the entire range of k_m (or α) parameter values. The results obtained for the considered k_m (or α) range correspond to the theory of the combustion chemistry at high temperatures, data of the reference books and CEA, RPA software packages.

6. FUTURE WORKS

Since the tensor model is generalized, it can be combined with all the other mathematical models as well. For example, while dividing the solution domain into small control volumes while solving Navier-Stokes equations, GTM can be applied at every control volume taking the pressure found from the solution of Navier-Stokes equations as the total pressure input and yielding the partial pressures of the combustion products throughout the entire solution domain. The combined application of the thermochemical tensor model and Navier-Stokes equations will make it possible to determine the local composition and properties of combustion products at any considered point of the flow.

On the other hand, the model can, also, be combined with the method of characteristics while designing the LRE nozzle. Although, the problem is 1D, still GTM can be useful in some sense while combined with the method of characteristics.

Using GTM the nodal combustion model can be developed as well. The major purpose of the nodal combustion model for LRE is to observe the behavior of the combustion products along the LRE thrust chamber length in 2D and make optimal design decision accordingly.

Equilibrium analysis demonstrates that the combustion chamber of a LRE should be design in a non-cylindrical configuration.

Results of the combined application of thermochemical tensor model, method of characteristics and Navier-Stokes equations will be presented in the next paper.

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