Supersonic nozzle profiling for supersonic aerospace testing in a view of high-temperature of properties of real gases

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Abstract. The paper presents the modified method for the supersonic nozzle profiling with respect to non-monotonic dependence of adiabatic index on temperature, as well as the results of nozzle profile calculation for two sets of input parameters, based on independently determined specific heat curve for molecular nitrogen $N_2$ and products of its thermal decomposition in the temperature range of $T = 260$–$100000$ K and atmospheric pressure.

1. Introduction
Combustion and non-transferred electrical arc heating is often used to expand the available temperature and Mach number ranges of the facilities aimed for aerodynamic testing of supersonic and hypersonic cruise vehicles (HCV) whereas chemical reaction of equilibrium dissociation and ionization take place producing high-enthalpy flow. However, with further acceleration the recombination reactions develop, leading to a sharp nonmonotonic behavior of adiabatic index function. Dissociation and ionization become also important while investigating the shock-compressed layer at the leading edge of HCV wing and the spark discharge propagation [1]. In order to modify classical one-dimensional nozzle profiling technique and to implement it for the case of variable adiabatic index, as well as for modeling in the industrial computational-fluid-dynamics (CFD) programs, we have performed an independent calculation of the heat capacity of nitrogen $N_2$ and its degradation products in a wide temperature range at the atmospheric pressure that will described in the following section.

2. Thermophysical parameters of molecular nitrogen for plasma flows calculation
To perform an accurate calculation of high-temperature fluid flows, one needs to take into account all the material parameters depending on the temperature. When the temperature increases above 5000 K, the endothermic process of equilibrium dissociation takes place in molecular gases; hereafter at higher temperatures the equilibrium ionization occurs, leading to the formation of ions of different multiplicity. These processes result in a sharp and non-monotonic variation of the transport coefficients of gas mixtures. Abrupt bursts of thermal...
conductivity and heat capacity of real gases during the dissociation and ionization, which also can be treated as an effect of competition between the the unbound states spectrum entropy and bond energy, are associated with the spatial transfer of chemical bond energy. These phenomena occur when the temperature is about one order less then dissociation energy, are associated with the spatial transfer of chemical bond energy. These phenomena occur when the temperature is about one order less than dissociation $D$ and ionization $I_i$, $i = 1 \ldots 5$ potentials.

The specific heat curve for molecular nitrogen $N_2$ and its thermal decomposition products was calculated in the temperature range of $260 \ldots 100000$ K and atmospheric pressure basing on the equilibrium dissociation and ionization equations for the following chain of reactions with corresponding energies $[2, 3]$:

$$
\begin{align*}
N_2 &\iff 2N & D &= 9.79 \text{ eV}, \\
N &\iff N^+ + e^- & I_1 &= 14.53 \text{ eV}, \\
N^+ &\iff N^{+2} + e^- & I_2 &= 29.611 \text{ eV}, \\
N^{+2} &\iff N^{+3} + e^- & I_3 &= 47.436 \text{ eV}, \\
N^{+3} &\iff N^{+4} + e^- & I_4 &= 77.468 \text{ eV}, \\
N^{+4} &\iff N^{+5} + e^- & I_5 &= 97.883 \text{ eV}.
\end{align*}
$$

Firstly the partition functions of the $N_2$ molecule (the maximum number of vibrational level was limited by dissociation potential and the rotational partition function took into account the statistical weights of ortho- and para- states of the nitrogen nucleus, corresponding to rotational modes with even and odd values of the total angular momentum $J$) and electronic levels of atomic species $N(NI)$, $N^+(NIII)$, $N^{+2}(NIV)$, $N^{+3}(NIV)$, $N^{+4}(NVI)$, $N^{+5}(NVI)$ were calculated using data from $[3–5]$, partly existing in the NIST database. It should be noted that the appearance of higher multiplicity ions is extremely difficult requiring the electron detachment from the $1s^2$ level with the ionization energy $I_6 = 552.0673 \text{ eV}$, which is hardly to be achieved in the up-to-date atmospheric plasma torches.

The calculation of the respective dissociation $\alpha_D = n_N/(n_N + n_{N_2})$, and ionization $\alpha_{I_i} = n_{N^{+i}}/(n_{N^{+i}} + n_{N^{+(i-1)}})$, $i = 1 \ldots 5$ degrees was performed on the basis of the equilibrium equations for binary mixtures regardless the ionization potential lowering due to the Debye shielding – this correction was introduced at the next stages of the calculation. The reaction branch $N_2 \iff N_2^+ + e^-$, $N_2^+ \iff N + N^+$ has been excluded from reaction set, as at the time when $N_2$ ionization develops, the number of $N_2$ molecules becomes at least 3 orders less compared to other species, and the binding energy of this reaction $I_{N_2} = 15.580 \text{ eV}$ is greater than the nitrogen atom ionization potential. So, the total influence of this reaction was considered to be negligible.

Species concentrations were determined by solving a system of linear equations in matrix form at the pressure $P = 101325 Pa$ in the temperature range $T = 260 \ldots 100000$, $\Delta = 20K$ - step of calculation:

\[
\begin{array}{c|cccc|c|c|c}
1 & 1 & 2 & 3 & 4 & 5 & 6 & n_{N_2} \\
\hline
\alpha_D & \alpha_D - 1 & 0 & 0 & 0 & 0 & 0 & n_N \\
0 & \alpha_{I_1} & \alpha_{I_1} - 1 & 0 & 0 & 0 & 0 & n_{N^+} \\
0 & 0 & \alpha_{I_2} & \alpha_{I_2} - 1 & 0 & 0 & 0 & n_{N^{+2}} \\
0 & 0 & 0 & \alpha_{I_3} & \alpha_{I_3} - 1 & 0 & 0 & n_{N^{+3}} \\
0 & 0 & 0 & 0 & \alpha_{I_4} & \alpha_{I_4} - 1 & 0 & n_{N^{+4}} \\
0 & 0 & 0 & 0 & 0 & \alpha_{I_5} & \alpha_{I_5} - 1 & n_{N^{+5}}
\end{array}
\]

Thus, given the concentration of species, one can determine the internal energy per unit
volume of gas

\[ U = n_{N_2} \left( \frac{5}{2} k_B T + \langle \varepsilon_N(T) \rangle - k_B (D + 2 \sum_{i=1}^{5} I_i) \right) + n_N \left( \frac{3}{2} k_B T - k_B \sum_{i=1}^{5} I_i \right) + \sum_{i=1}^{4} n_{N^{i+1}} \left( \frac{3}{2} k_B T - k_B \sum_{j=i+1}^{5} I_i \right) + \frac{3}{2} k_B T n_{N^{i+5}} + \frac{3}{2} k_B \sum_{i=1}^{5} i \cdot n_{N^{i+1}}, \]  

the density \( \rho = M_N (2n_{N_2} + n_N + \sum_{i=1}^{5} n_{N^{i+1}}) \), the average molar mass, the specific internal energy \( u = U/\rho \). The specific heat \( C = du/dt \) was calculated by numerical differentiation of the internal energy curve. The specific heat at constant pressure we found from Mayer ratio \( C_p = C_V + R/\mu(T) \), where \( \mu = \mu(T) \) - average molar mass.

At the next stage according to the formula in [6] we calculated the correction to the “frozen” heat capacity, as well as a decrease in the ionization potential due to the Debye screening. Maximum potential lowering falls in the temperature range 6500 – 7000 K, which is associated with the dissociation reaction. Since the number of charged particles at given temperatures is small, so strong lowering \( \Delta I/I \approx 0.09 \) has no significant impact on the \( C_p \) and \( C_v \). Similarly, if the temperature \( T > 20000 \) K, the correction drops to \( \Delta I/I < 0.006 \), that also does not influence significantly the specific heat curve. At the final stage the 4th order virial corrections [6] to thermodynamic quantities including \( C_p \) and \( C_v \) were implemented and proved to be negligible.

Figure 1 shows the Gaussian-shaped relative concentrations of the different species of particles, which peak width at half height increases with rising temperature.

![Figure 1. Relative concentrations \( n_i/n \) of \( N_2, N, N^+, N^{+2}, N^{+3}, N^{+4}, N^{+5} \) as functions of temperature at pressure \( P = 101325 \) Pa.](image)

The results of present study are in reasonable agreement with data obtained by IVTANTHERMO program (see figure 2), contrary to the results of [1]. One can see a substantial
shift $\Delta T \approx 1000 \, K$ of dissociation and ionization peaks to lower temperatures along with a sufficiently small peak of ionization.

Turning to a wider temperature ranges shown in figure 2, one can see that the behavior of the specific heat curve depends significantly on the amount of chemical reactions under consideration. In particular, the calculation of the first two reactions (dissociation and primary ionization) causes the heat capacity curve to converge to the monatomic gas value already at $T \approx 20000 \, K$. This leads to excessively high temperatures in the local domains of intense heat release (the electric arc simulation). The model overheating of the gas can cause in some cases the development of the numerical instability and malfunction of CFD algorithm. This disadvantage is reflected in figure 3 in the behavior of the curves: (3) - the present study; (2) - the results of the IVTANTHERMO that performs the minimization of the Helmholtz free energy functional to find thermodynamic parameters. Considering larger number of reactions (curves 4 and 5 of the present study) allows calculating more accurately the behavior of the specific heat curve at $T = 20000 \ldots 100000 \, K$. Deficient values of transport coefficients of argon, nitrogen and other gases necessary for modeling high-temperature gas flows and plasma can be also borrowed from the well-known papers [7, 8]. Utilizing the results obtained one can find the adiabatic index $k$ dependence on temperature that has several remarkable properties, pointed out by numerals in figure 4: 1 is the region of diatomic gas specific heat without internal degrees of freedom, 2 shows the internal degrees of freedom excitation region, abrupt drops depicted by 3, 4 manifest an isothermal mode due to the high thermal conductivity in the dissociation and ionization ranges. It is worth noting the adiabatic index tends to 1 during the dissociation or ionization. Hence, in some sections of the flow the quasi-isothermal process $PV \approx const$ can be realized leading to certain difficulties when implementing classical gasdynamic functions, since high-speed plasma flow (especially through the nozzle) represents the non-adiabatic and even non-polytropic process. This brings us to a simple iterative nozzle profiling method based on the temperature dependence curve for the gas enthalpy.
3. Plasma torch supersonic nozzle profiling

Numerical simulation of the immersed plasma jets plays a substantial role in plasma physics and physical gas dynamics, as one need to account for the effects of the high-speed flows (compression shocks), the significant number of molecular reactions, the material-radiation interaction and its impact in heat transfer along with of the electrodes and channel walls destruction and plasma turbulence. Consequently, the solution of such problems involving wide temporal and spatial range phenomena requires considerable computing power.

Reynolds number at the plasma torch exit at the certain flow rates reaches $Re \sim 10^3$, if the characteristic size of the cross section is $L \sim 10^{-2}$ m, then according to Kolmogorov microscale turbulence theory, the computational cell size should be about $l \sim 10^{-5}$ m. Evidently, the three-dimensional unsteady turbulent plasma jet calculation taking into account the radiation is a time consuming task, in terms of both algorithm complexity and the computational resources required.

The design of nozzles with known flow rate characteristics and thermodynamic parameters at the nozzle exit is an important issue in supersonic and hypersonic aerodynamic testing. One can solve the inverse problem of the nozzle theory [9] using a well-developed numerical methods for nozzles with characteristic dimensions $l \approx 0.1$ m. Among of them is widely used method of characteristics [10] that can be employed while calculating two-dimensional supersonic and one-dimensional unsteady gas flows and also for the flows with physico-chemical transformations, such as the vibrational excitation of the molecules, chemical reactions, and gas flows with superimposed electromagnetic fields. Alternative methods are the shock-capturing method (Godunov scheme), and the relaxation approach which is used for solving stationary problem basing on non-stationary equations of gas dynamics. A steady solution is obtained as the asymptotic state of non-stationary process if $t \to \infty$.

The flow in the nozzle regardless its application is often assumed to have an axisymmetric structure that can be divided into three characteristic regions: the subsonic flow region in the

Figure 4. Temperature dependence of adiabatic index of and products of its high-temperature decomposition.
tapered portion, transonic region in the vicinity of the critical cross section and the supersonic region in an expanding part of the nozzle. In present study we deal with sufficiently small nozzle with the characteristic dimensions \( l \approx 0.01 \, \text{m} \) that urges to reject due to technological reasons the complex curved profiles, so the consideration is restricted by conical-wall nozzle. Conical nozzles are widely used in propulsion systems, wind tunnels, as well as in studies of various nonequilibrium processes. Profile conjugating characteristics of various nozzle sections can have a significant impact on the flow structure. For example, the flow deceleration [10] in the vicinity of radius-conical conjugation at the critical nozzle portion under certain conditions can give a rise to the stationary shock wave that is repeatedly reflected from the symmetry axis and the nozzle profile. Elementary nozzle profiling in the case of constant adiabatic index is based on the given flow rate and stagnation parameters. The idea of method proposed is that for the case of variable adiabatic index one can use the law of conservation of enthalpy and its temperature dependence calculated in advance. Enthalpy is a thermodynamic system functional and can be reckoned from some arbitrary value. In particular case, it is defined as a primitive function of the heat capacity from a certain temperature value

\[ h(T) = \int_{T_0}^{T} C_p(T') dT'. \]

Using one of the elementary consequences of the law of energy conservation

\[ h(T_{stag}) = h(T) + \frac{v^2}{2}, \]

where \( T_{stag} \) is a stagnation temperature, one can profile conical-wall nozzle resting upon the inlet, critical and outlet cross-sections, given the mass flow rate \( G \), static inlet pressure \( p_1 \), temperature \( T_1 \) and diameter \( D_1 \) in the settling chamber, as well as Mach number \( M_{out} = 4 \) of the outlet flow. At the first stage the calculation of missing parameters in the inlet section subscripted as “1” was performed (molar mass \( \mu_1 \), sound speed \( a_1 \), Mach number \( M_1 \), enthalpy \( h_{T_1} \)), which were then used for stagnation enthalpy

\[ h_{stag} = h_{T_1} + \frac{1}{2} \left( \frac{GRT_1}{\mu_T P_1} \right)^2 \]

and stagnation temperature determination \( T_{stag} = h^{-1}(T_{stag}) \). Involving the adiabatic equation with an exponent index \( k = k_{stag} \) one can determine other required thermodynamic variables. For the critical section calculation it is necessary to find the minimum of the function \( \Delta = (h_{stag} - h(T)) \mu(T) - k(T) \cdot RT \) with appropriate temperature and also the average adiabatic index \( k_{avg} \) for input and critical sections, where \( R \) is the universal gas constant. Next basing on the adiabatic equation in the region between the inlet and outlet sections one can find the pressure \( P_c \), density \( p_c \), the critical sound speed \( a_c \), and throat area \( F_c = G/(\rho_c a_c) \).

Similarly, minimizing the function \( \Delta = \frac{1}{2} \left( \frac{GR}{\mu_T} (h_{stag} - h(T)) \mu(T) - k(T) \cdot RT \right) \), we find the corresponding temperature and the average adiabatic index \( k_{out} \) for outlet and critical sections. In the iterative approach which is more precise we find at first the inlet section flow parameters, as well as stagnation parameters, then, assuming a linear growth of the Mach number \( M \), the difference \( \Delta = \frac{1}{2} \left( h_{stag} - h(T) \right) \mu(T) - k(T) \cdot RT \) is minimized. At the final stage we calculated the average adiabatic index of the previous and the current section of the nozzle, as well as others gas-dynamic parameters.

Enthalpy curve of molecular nitrogen and its products shown in figure 5 is the basis of suggested approach.

The proposed profiling method was used to calculate the supersonic nozzles for two sets of the thermodynamic parameters at the nozzle inlet. The first calculation was performed at the
Figure 5. The dependence of the supersonic nozzle diameter on Mach number (assuming the linear growth) at the inlet pressure: $P_1 = 4$ bar, temperature $T_1 = 10020$ K and gas flow rate $G = 0.016$ kg/s (marked in black). The black curve shows the results of 200 sections calculation, and the sign ★ marks a non-iterative implementation for the critical and outlet cross-sections, the sign ▲ marks the calculation results based on [11]. Grey solid and dashed lines indicate the supersonic nozzle diameter dependency on the Mach number at a higher temperature $T_1 = 14020$ K. Gray circle shows the non-iterative results for the critical and outlet cross-sections, the sign △ - results of calculations based on [11].

Figure 5 shows the relationship between the diameter of the supersonic nozzle and the Mach number. The graph illustrates the dependence of the nozzle diameter on Mach number at an inlet pressure $P_1 = 4$ bar, temperature $T_1 = 10020$ K, and a gas flow rate $G = 0.016$ kg/s. The black curve represents the results of a 200-section calculation, and the symbol ★ denotes a non-iterative approach for critical and outlet cross-sections. The symbol ▲ represents the calculation results based on [11]. The grey solid and dashed lines indicate the supersonic nozzle diameter dependence on the Mach number at a higher temperature $T_1 = 14020$ K. The grey circle symbolizes the non-iterative results for critical and outlet cross-sections, while the symbol △ represents the results of calculations based on [11].

In the second calculation, the higher inlet temperature value $T_1 = 14020$ K was used. In addition, the satisfactory comparison of obtained profiles for 100 nodes (grey solid line in figure 5) and for 200 nodes (grey dashed line in figure 5) was performed. Similarly, we obtained a good agreement in the critical diameter calculation between iterative and non-iterative methods. Using a constant (the critical section value) or averaged adiabatic exponent yields significantly higher value. In addition to the above results, the reduced pressure as a function of Mach numbers was obtained (not shown in the figures), in particular, if $T = 10020$ K, the flow can be accelerated only up to $M \approx 1.6$, otherwise the static pressure becomes lower than atmospheric one, resulting in permanent shock slapping along the nozzle generating line. Obviously, to increase the flow velocity one need to decrease the pressure in the outlet chamber.

Enthalpy curve can also serve as the basis for an elementary method of determining the average plasma temperature at the nozzle exit. As in nozzle profiling procedure, firstly we find
all the gas dynamic parameters of the inlet section and stagnation parameters. Then determining experimentally the average gas velocity in the outlet section one can easily calculate the enthalpy value $h(T_2)$ of the output stream and corresponding temperature $T_2$.

4. Supersonic nozzle velocity characteristics measurements
To verify the acceleration characteristics of supersonic nozzle profiled, as well as to determine the gas velocity, a series of measurements of stagnation pressure was conducted. As a source of high-enthalpy plasma flow we used a plasma torch with a rated power of 50 kW (subsonic channel diameter – 10 mm) with a swirl stabilization and expanding channel providing high flow rates, efficient heating of the working medium and small thermal losses in the water-cooled anode surface. The use of such low-temperature plasma generator allows to obtain plasma flow temperature in the range of thousands to tens of thousands of degrees that is of particular interest in plasma thermodynamics and chemistry.

As the heated gas accelerated up to the outlet of critical portion of the nozzle discharges to the atmosphere, it is exposed to the abrupt deceleration passing via compression shock that results in the subsonic outflow at high temperature. According to our spectroscopic measurements the corresponding temperatures are $T_1^{\text{out}} = 5000 \pm 250$ K at the current $I_1 = 150$ A (power $W \approx 14.45$ kW) and $T_2^{\text{out}} = 5500 \pm 250$ K at $I_2 = 200$ A (W $\approx 18$ kW). The flow rate in both cases was $G = 1$ g/s. Principal scheme of the experimental setup is depicted in figure 6.

The stagnation pressure measurements were performed using a Pitot tube consisting of a curved capillary tube, enclosed in a copper water-cooled body frame. The probe itself was mounted on the three-degree-of-freedom traversing gear with a positioning accuracy of $\delta x = \delta y = \delta z = 0.1$ mm. The stagnation pressure was measured by current Honeywell Eclipse OEM Pressure Transducer with an operating range $p = 0 \ldots 20.413$ bar, base current of $i_0 = 4$ mA and a linear pressure-current characteristics $dp/di = 1.2927 \cdot 10^8$ Pa/A. The current and temperature measurement errors are estimated as $\delta T = 1$ and $\delta T = 250$ K correspondingly.

As a preliminary procedure Pitot tube alignment along the jet axis and zero point adjustment was undertaken. After that the probe was positioned 100 mm below the nozzle exit to measure the stagnation pressure sequentially with a spatial step mm at two different current values $I_1 = 150$ A and $I = 200$ A. Basing on the current measurements obtained and the spectroscopic data on temperature, it is possible to determine the density $\rho = p\mu(T)/(RT)$ ($p$ - static (atmospheric) pressure, $T$ - temperature, $\mu = \mu(T)$ -average molar mass of the mixture at given temperature, $R$ - the universal gas constant), and the velocity $v = \left(\frac{2p_0 - p}{\rho}\right)$, where $p_0 - p$ is measured by the transducer. In addition, defining the speed of sound at the nozzle exit $a^{\text{out}} = \sqrt{\frac{k\rho^{\text{out}}}{\mu(T^{\text{out}})}}$ equal to $a_1^{\text{out}} = 1291.3$ m/s in the first case and $a_2^{\text{out}} = 1359.6$ m/s in the second one we plot the superficial velocity $\lambda = v/a^{\text{out}}$ versus the distance from the nozzle exit measured in calibers.

It worth noting that due low $N_2^+$ spectral lines intensity even at a pretty small distance from nozzle exit we managed to obtain temperature only as the average domain value in the vicinity of the nozzle exit. Thus, the respective densities are: $\rho_1^{\text{out}} = \rho(T_1^{\text{out}}) = 0.0666 \text{ kg/m}^3$, $\rho_2^{\text{out}} = \rho(T_2^{\text{out}}) = 0.576 \text{ kg/m}^3$.

Two graphs were constructed both in dimensional $(v, z)$ and dimensionless $(\lambda, z')$, $z' = z/a^{\text{out}}$, coordinates, where $d^{\text{out}} = 6$ mm - of the outlet section diameter. The corresponding fitted curves were determined by the least square method. Relative experimental errors of calculated velocity are $\sigma_{v_1} = 0.033$ at $I_1 = 150$ A and $\sigma_{v_2} = 0.043$ at $I_1 = 200$ A. The experimental data are easily approximated by a decreasing exponential function. As expected, increasing heat emission (or electric arc power) leads to the rise of gas flow velocity at the central axis of the nozzle. Turning
Figure 6. Schematic diagram of the experimental setup. Numbers indicate: 1 - plasma torch facility, 2 - supersonic nozzle, 3 - Pitot tube, introduced across the flow, 4 pressure transducer, 5 amperemeter, 6 - power supply.

Figure 7. Supersonic nozzle operation at $I = 150$ A.

Figure 8. Axis superficial velocity versus the dimensionless distance from nozzle exit

Figure 9. Axis velocity versus the distance from nozzle exit

to figure 4 one can see that at the nozzle exit the transonic regime is implemented, as in this domain the superficial velocity equals to the Mach number $M$. We also assume that at large distances from the nozzle exit the transonic regime persists because of the jet cooling leading to the sound speed reduction. This speculation has not yet been verified experimentally in view of the low radiation intensity of the molecular ion $N_2^+$, which may require to come over to other
spectral ranges. The differences in the arrangement of the curves at various power consumptions almost disappear at a distance of 10 calibers, which is probably caused by the temperature drop and mixing of the jet with the ambient air.

5. Conclusion
In present paper the calculations of certain thermophysical parameters of \(\text{N}_2^+\) in the temperature range \(T = 260 \ldots 100000 \text{ K}\) basing on the equations of equilibrium dissociation and ionization and in a view of the effects of real gases (4th order virial corrections) and plasma (Debye correction), as well as the comparison of the obtained results with other researchers are presented. The authors also propose a modified technique of one-dimensional nozzle profiling including variable adiabatic index that utilizes the dependence of the gas enthalpy on temperature. According to the results of profiling we developed a supersonic nozzle and measured the gas velocity at various distances from the nozzle outlet. Relay on findings, one can conclude that at the vicinity of nozzle exit a transonic flow mode exists that can be preserved at large distances from the nozzle.

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