MATHEMATICAL MODELING OF TWO-PHASE REACTING FLOW IN SUPERSONIC NOZZLE

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Abstract. *The prediction of the flow characteristics inside a nozzle of a rocket engine, both liquid and solid propellant types, is still an actual problem of mathematical modeling, mainly due to the complexities introduced by the local combustion products flow, which includes physical-chemical processes under high temperature and high pressure conditions. It is well known that using the ideal gas-flow model, each complex phenomenon, namely nonparallel flow in the nozzle outlet, non-equilibrium flow, viscosity and heat transfer, nonentrainment of the condensed particles by the gas and condensed particles division and coagulation, can be treated by a specific model, allowing a separated evaluation of its influence on the flow characteristics. In the present work, the most relevant specific models were selected to develop and compose a computer code package which can be used as a tool for practical evaluation of flow process in a nozzle. Five models were selected to compose the package and the most representative results obtained from the calculation are presented.*

Keywords: *Nozzle, combustion products, bi-phase flow, flow bidimensional, chemical kinetics.*

1. Introduction

The prediction of the flow characteristics inside a nozzle of a rocket engine, both liquid and solid propellant types, is still an actual problem of mathematical modeling, mainly due to the complexities introduced by the local combustion products flow, which includes physico-chemical processes under high temperature and high pressure conditions. Typically, such a flow occurs at sub and supersonic velocities, with shifting gas composition, heat and mass transfer among phases, interaction of gas flow with condensed particles, heat transfer and friction in the boundary layer, and so on. Due to the difficulties in predicting the nozzle's real performance, in the actual design situation certain correction factors, usually empirically obtained, are applied to the results derived from gas-flow calculations conducted for ideal conditions (Sutton, 1992). Among the factors which introduce deviation from ideal conditions, the following phenomena are significant: nonparallel flow in the nozzle outlet, nonequilibrium flow, viscosity and heat transfer, nonentrainment of the condensed particles by the gas and condensed particles division and coagulation.

It is well known that using the ideal gas-flow model (Alemassov et al., 1980 and Gordon & McBride, 1971), each phenomenon mentioned previously can be treated by a specific model, allowing a separated evaluation of its influence on the flow characteristics. In the present work, the most relevant specific models were selected to develop and compose a computer code package which can be used as a tool for practical evaluation of flow process in a nozzle.

Five models were selected to compose the package. Firstly, each model is presented and discussed separately, and the coupling methodology is presented in the sequence. Finally, the most representative results obtained from the calculation are presented.

2. Flow characteristics and description of the separated models

The transformation of chemical energy into thermal energy is obtained through the burning of propellant in the combustion chamber (Fig. (1)), where the flow velocity can be usually considered low (~100m/s), and the gas residence time long enough to yield almost complete combustion and chemical equilibrium at the nozzle inlet. These flow characteristics allow the application of a common initial condition for all the separated models (Alemassov et al., 1980). Under such a condition, following separated models were considered:

- ideal model (chemical equilibrium model);
- chemically nonequilibrated model;
- one-dimensional two-phase flow model with coagulation and particle division;
- two-dimensional flow model (single gas or two-phase); and

- boundary layer model.

This packed is enough to cover most of the usual parameters required for practical prediction of nozzle performance. For evaluating the most important parameter of a propulsion system for example, namely, specific impulse, following equation can be used:

$$I_{es} = I_{id}\left(1 - \xi_{dq} - \xi_{bf} - \xi_{np} - \xi_{at} - \xi_{ps}\right) \tag{1}$$

where: $\xi_i = \Delta I_i / I_{id}$; ΔI_i – specific impulse loss due to the *i-th* effect; ξ_{dq} – specific impulse loss due to the nonequilibrium process; ξ_{bf} - specific impulse loss due to the condensed-phase velocity reduction; ξ_{np} - specific impulse loss due to the non-paralel flow in the nozzle outlet; ξ_{at} - specific impulse loss due to the friction; ξ_{ps}. - specific impulse loss due to the effect of deflection of the condensed phase into the wall .

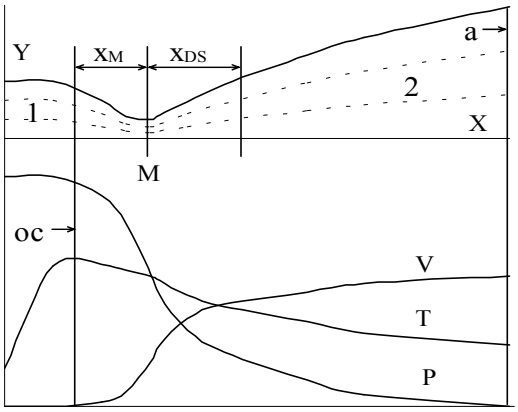

Figure 1. Variation of characteristics *V, T, P* in the chamber and in the nozzle:
1- combustion chamber; 2 - nozzle; *oc* – inlet section; *M* – minimum section (throat); *a* – outlet section.

2. Description of the separated models

2.1 Chemically equilibrated flow model

The ideal gas-flow model is based on the following assumptions:
- the reacting medium (A_q) includes *m*-types of molecules and radicals (j = 1...m) and *n*-types of atoms (i = 1...n), and they are in chemical equilibrium at a temperature (T) and a pressure (P) at any section in the nozzle;
- the condensed phases have velocity and temperature at the same level of the gas;
- the flow is one-dimensional, without friction and without heat transfer through the walls.

The main equations of the model are:
- of molecules (and radicals) dissociation to form atoms:

$$\frac{\prod r_i^{a_{ij}}}{r_j} = \frac{K_j}{P^{\left(\sum a_{ij} - 1\right)}} \tag{2}$$

- of atoms conservation:

$$\sum a_{ij} r_j + r_i = F_c b_{ip} / P \tag{3}$$

- of Dalton:

$$\sum r_q = 1 \tag{4}$$

where: a_{ij} – the amount of the *i-th* atom in *j-th* molecule; K_j – the dissociation constant of *j-th* molecule; b_{ip} – the quantity of the *i-th* atom in conditional formula of propellant; F_c – the unknown coefficient; r_q – the molar fraction of the *q-th* substance.

Additionally, the energy equation is used for determining the nozzle entrance characteristics (r_q^{oc}, T_{oc}):

$$h_p - \frac{\sum_q H_q^{oc} r_q^{oc}}{\mu_m^{oc}} = 0 \qquad q = 1, ..., (m + n); \tag{5}$$

where: h_p – the enthalpy of propellant; H_q – the molar enthalpy of the *q-th* substance; μ_m - the molecular mass average; subscript *oc* corresponds to the entrance section of nozzle.

For an isentropic flow process, the Eqs. (2, 3 and 4) can be used together with the isentropic expansion equation, yielding the determination of the properties at any nozzle sections (including the exit section), for a given known local pressure *P*:

$$S(P,T) - S_{oc} = 0 \tag{6}$$

$$h_p - \frac{\sum_q H_q r_q}{\mu_m} - \frac{V^2}{2} = 0 \tag{7}$$

where *S(P,T)* – the entropy of combustion products at each section; S_{oc} – the entropy in the combustion chamber; and V – the flow velocity.

For calculating the properties at the minimum section (throat), additional equations are required:

$$S(P_M, T_M) - S_{oc} = 0; \qquad \sqrt{2(h_{oc} - h_M)} - a_e = 0 \tag{8}$$

where: h_{oc} – the enthalpy in the combustion chamber; *M* refers to the minimum section at the throat; a_e – the "equilibrated" sound velocity; and P_M, and T_M are unknown variables.

For calculating the composition and the temperature by using the ideal model, Newton's methods can be applied (Alemassov et al, 1980). In this case, it is obtained: in the inlet: r_q^{oc}, T_{oc}; in the throat: P_M, T_M, r_q^M, h_M; in any given section (including the exit section): r_q, T. Subsequently, thermodynamics and thermophysics properties can be determined in each section: c_{pe}, c_{pf} - frozen and equilibrated specific heats; a_e, a_f - frozen and equilibrated sound velocities in each section; and flow velocity:

$$V = \sqrt{2 \cdot (h_{oc} - h)}; \tag{9}$$

- the specific impulse in vacuum, in each section:

$$I_{es} = V + P/(\rho \cdot V); \tag{10}$$

- the mean adiabatic coefficient:

$$n = \ln\left(\frac{P_{oc}}{P_a}\right) \Big/ \ln\left(\frac{P_{oc} \cdot R_a \cdot T_a}{P_a \cdot R_{oc} \cdot T_{oc}}\right) \tag{11}$$

where the subscript *a* refers to the exit section.

To account the condensed phase formation in the combustion products, big molecules (BM) method, proposed by Khudiakov em (Alemassov et al, 1973), was adopted. In this method, each condensed phase is considered as a conjunct of BM, which contains a definite number of usual molecules (for instance, 1 BM of carbon C* may contain 1000 molecules C). The values of enthalpy and entropy of BM correspond to those of solid state condition and at the same time, it is supposed that BM obey the ideal gas law. Therefore, above mentioned equations can be used for the cases involving heterogeneous reagents medium.

2.2 Model for chemically nonequilibrated flow

Following the methodology for "decompose" a complex phenomenon, the model considers that the gaseous flow is one-dimensional and the viscosity is negligible. Besides, following simplifying hypotheses are adopted: the combustion products are a mixture of ideal gases and the condensed phase and the gas have the same temperature and velocity. In the nozzle inlet, chemical equilibrium is established and reactions in the flow obey the detailed chemical kinetic. The base of the model is the chemical kinetic equations represented in an exponential form:

$$\frac{d\gamma_i}{dx} = -\frac{1}{V}\left(e^{\gamma_i} \sum_j \nu_{ij} \Omega_j + \sum_s \sum_j \nu_{sj} \Omega_j\right); \qquad i, p, s = 1...n; \quad j = 1...2m; \tag{12}$$

where: $\Omega_j = k_j \left(P/R_0T\right)^{\overline{m}_j} \exp(-\sum_p n_{pj}\gamma_p)$; $\overline{m}_j = m_j - 1 + \sum_p n_{pj}$; $\gamma_i = -\ln r_i$; m – the number of reactions in the reacting medium; R_0 – the universal gas constant; m_j – the index representing the level of participation of a catalytic particle in the *i-th* reaction; ν_{ij}, n_{pj} – the stoichiometric coefficients of *j-th* reaction.

From the chemical equilibrium model, the dependence $P = P(x)$ can be derived, resulting in equation:

$$\varphi(x) = -\ln(P/P_{oc}) \tag{13}$$

therefore, the equation of linear momentum is given by:

$$\frac{dV}{dx} = \frac{R_0 T}{V\mu_m}\varphi'(x) \tag{14}$$

Equations (7, 12 and 14), with initial data V_{oc}, γ_i^{oc}, T_{oc}, P_{oc} in the nozzle inlet complete the current model. Details on integration of these equations were already described in a previous work (Krioukov et al, 1997). Dependencies of $V(x), \gamma_i(x), T(x), f_a(x)$ through the nozzle are obtained during the calculation; here f_a is the nozzle expansion ratio.

The adapted Khudiakov method for non-equilibrium process (Krioukov et al., 1997), with inclusion of BM concept in the chemical reaction mechanisms, was used to account the heterogeneous medium in the current model. For instance, the reaction:

$$\mathrm{B}^* + \mathrm{B} \Leftrightarrow 1{,}001\mathrm{B}^* \tag{15}$$

reflects the condensation of a gaseous molecule B in a big molecule B*. The reaction rate constants for this type of reaction can be obtained using one of the following procedures:

- prescribe a big value of k^+ for simulating an equilibrated condensation process, or
- determinate the value of k^+ through the corresponding state theory (Hirschfelder et all, 1966) for condensation.

2.3 One-dimensional two-phase flow model with coagulation and particle division

The aim of this model (Tishin and Khairutdinov, 1971) is to determine the size changing of the condensed particles, their velocities and temperatures throughout the nozzle flow. The main hypothesis are: no composition change in the gaseous phase; the two-phase flow is one-dimensional; the particles are spherical; the particles distribution is discrete and is represented by group of particles; each group is composed by particles having uniform size; and the temperature of a particle is uniform.

The model takes account of the following phenomenon in the flow: division and coagulation of particles due to the collisions; difference in the temperatures of the gaseous phase and the particles (each group of particles has a specific temperature); difference in the velocities of the gaseous phase and the particles; and specific impulse losses due to the previously mentioned differences.

Some of the initial data of model (T_{oc}, z (condensed phase mass fraction), μ_m, and n (mean adiabatic coefficient)) are obtained from other models such as those for chemical equilibrium or for chemically non-equilibrated processes. The model is represented by the following ordinary differential equation systems:

$$\frac{dW_i}{dx} = \frac{3}{4} C_{x_i} \rho \frac{|V - W_i|(V - W_i)}{W_i \rho_i d_i}; \tag{16}$$

$$\frac{dT_i}{dx} = \frac{6\alpha_i (T - T_i)}{d_i \rho_{ci} W_i c_i}; \tag{17}$$

$$\rho V \frac{dV}{dx} + \frac{dP}{dx} + \frac{z}{1-z}\rho V \sum_{i=1}^{n} g_i \frac{dW_i}{dx} = 0; \tag{18}$$

$$c_p \frac{dT}{dx} + V\frac{dV}{dx} + \frac{z}{1-z}\sum_{i=1}^{n}\left(c_i \frac{dT_i}{dx} + W_i \frac{dW_i}{dx}\right) g_i = 0; \tag{19}$$

$$\frac{1}{p}\frac{dp}{dx} + \frac{1}{T}\frac{dT}{dx} - \frac{1}{\rho}\frac{d\rho}{dx} = 0; \tag{20}$$

$$\frac{dm_i}{dx} = \frac{1}{W_i}\sum_{j=1}^{i-1} k_{ij}\, n_j\, m_j\ ; \tag{21}$$

$$\frac{dn_i}{dx} = -\frac{n_i}{W_i}\sum_{j=i+1}^{n} k_{ij}\, n_j\ ; \tag{22}$$

$$\frac{dg_i}{dx} = \frac{(1-z)W_i^2}{z\,\rho V}\left(n_i\frac{dm_i}{dx} + m_i\frac{dn_i}{dx}\right); \tag{23}$$

where: $C_{x_i} = \frac{21{,}12}{\mathrm{Re}_i} + \frac{6{,}3}{\sqrt{\mathrm{Re}_i}} + 0{,}25$; $\alpha_i = \mathrm{Nu}_i\lambda/d_i$; $\mathrm{Nu}_i = 2 + 0{,}46\,\mathrm{Re}_i^{0{,}55}\cdot\mathrm{Pr}^{0{,}33}$; T_i, W_i – temperature and velocity of the *i-th* group particles; m_i, n_i, and g_i – mass, particle numbers and mass fraction of the *i-th* group particles, respectively; $C_{x_i}, \alpha_i\, d_i, \mathrm{Re}_i, \rho_{ci}, c_{ci}$ - friction coefficient, heat transfer coefficient, diameter, relative Reynolds number, particle density and specific heat of the *i-th* group, respectively; k_{ij} – constant for *i-th* and *j-th* groups particles interaction; ρ, V, λ - density, velocity and heat conductivity of the gaseous phase. The particle diameters must satisfy the condition We$_i$ < 17, where $We_i = \rho_{ci}(V - W_i)^2\, d_i/\sigma_{ci}$, σ_{ci} – superficial tension of the *i-th* group particles.

The system includes ($5k$ + 3) equations (k – is the number of groups) and the same quantity of unknowns: W_i, T_i, m_i, n_i, g_i, V, T, ρ, which are prescribed in the nozzle inlet; additionally, pressure distribution throughout the nozzle flow is known. To solve the system, fourth order Runge-Kutta methods is applied.

2.4 Two-dimensional flow model

The aim of this model is to determine the two-phase flow field characteristics in the nozzle, including both convergent (M <1) and divergent (M > 1) parts. The following simplifying hypothesis are adopted: no change in the combustion product composition; near-wall viscosity and thermal conductivity effects are neglected; condensed particles are spherical with constant diameter and without phase transitions; gaseous phase and particles are at the same velocities and temperatures at the beginning of the flow.

The following phenomenon are considered in the model: interaction (involving velocity and temperature) between the gaseous phase and the particles; separation of the gas and the particles field lines (M = 1); possibility of the condensed particles separation from the flow, reaching the nozzle wall; and specific impulse loss due to the non-parallelism of the exhaust gases in the nozzle outlet.

The mean size of the condensed particles (d_p^m) are obtained from two-phase flow model (item 2.3). Equations for the gaseous phase flow are represented by a system of partial derivative equations, developed and introduced by (Richkov, 1988):

$$\frac{\partial\vec{F}}{\partial\bar{x}} + \frac{\partial\vec{G}}{\partial\theta} = \vec{E}\ ; \tag{24}$$

where:

$$F = \begin{bmatrix} \bar{m}\,\theta\,\bar{Y}_k^2 \\ \left(\bar{m}^2/\bar{\rho} + B\,\bar{P}\right)\theta\,\bar{Y}_k^2 \\ \dfrac{\bar{m}\,\bar{n}}{\bar{\rho}}\,\bar{Y}_k^2 \\ H_0\,\bar{m}\,\theta\,\bar{Y}_k^2 \end{bmatrix}; \qquad G = \begin{bmatrix} A\,\theta\,\bar{Y}_k \\ \left(A\dfrac{\bar{m}}{\bar{\rho}} - B\,\bar{P}\,\theta\,\bar{Y}_k\right)\theta\,\bar{Y}_k' \\ \left(A\dfrac{\bar{n}}{\bar{\rho}} + B\bar{P}\right)\bar{Y}_k \\ A\,H_0\,\theta\,\bar{Y}_k \end{bmatrix}; \qquad E = \begin{bmatrix} 0 \\ 0 \\ -\dfrac{\bar{n}}{\theta\bar{\rho}} \\ 0 \end{bmatrix};$$

$$\bar{m} = \bar{\rho}\cdot\bar{V}_x; \quad \bar{n} = \bar{\rho}\cdot\bar{V}_y; \quad A = \bar{n} - \bar{m}\,\theta\,\bar{Y}_k^{-1}; \quad H_0 = \frac{n}{n-1}\frac{\bar{P}}{\bar{\rho}} + \frac{\bar{m}^2 + \bar{n}^2}{2B\,\bar{\rho}^2}; \quad \bar{Y}_k' = \frac{d\bar{Y}_k}{d\bar{x}};$$

$$B = (n+1)/n; \quad \theta = \frac{\bar{Y}}{\bar{Y}_k}; \quad \bar{x} = x/r_M; \quad \bar{Y} = Y/r_M; \quad \bar{\rho} = \rho/\rho_{oc}; \quad \bar{P} = P/P_{oc}; \quad \bar{V}_x = V_x/a_{cr}; \quad \bar{V}_y = V_y/a_{cr};$$

x_k, Y_k – coordinates of the nozzle contour; r_M – minimum radius of the nozzle; a_{cr} – critical sound velocity; V_x, V_y – axial and radial velocities; n – mean adiabatic coefficient.

The following prescribed conditions for the nozzle contour are given:

- in the nozzle inlet: distribution of the properties $\bar{\rho}$, $\bar{V}_x$, $\bar{V}_y$, $\bar{P}$;

- in the nozzle axis: $\overline{n}=0;\quad \frac{\partial\overline{m}}{\partial\theta}=\frac{\partial\overline{\rho}}{\partial\theta}=\frac{\partial\overline{P}}{\partial\theta}=0;$

- in the contour (wall) of the nozzle: $\overline{n}=\overline{m}\cdot\overline{Y}_k$; (impermeability condition).

The equations for two-phase flow are described in (Richkov, 1980). The integration area are preliminarily transformed in rectangle. In the zone $x < X_{DS}$ (Fig. (1)) the calculation is made using the Mc-Cormak scheme (for gaseous phase) and the Richkov (1980) scheme for the condensed phase. In the supersonic region $x > X_{DS}$, the Mc-Cormak scheme are also used.

2.5 Boundary-layer model

The aim of this model is to determine the boundary layer thickness (δ^{**}) and the specific impulse losses ξ_{at} throughout the nozzle wall. For this purpose, the Avduevski (1962) method, whose boundary layer theory was applied to the curved contour of a nozzle (*S*), was used. It is supposed that only gas phase is present in the layer. The initial data of the model *M(S)* (Mach number through the line S), *P(S)*, *T(S)*, *n* (mean adiabatic coefficient), μ_m (mean molecular mass) are obtained from the two-dimensional flow model results. Equations for obtaining δ^{**} and specific impulse losses due to the friction are presented below:

$$\overline{\delta}_a^{**}=\frac{\left(\frac{2}{n-1}\right)^{0,1}}{\mathrm{Re}_{W_0}^{0,2}}\cdot\left[\frac{0{,}015}{f_{at}^{0,5}}\right]^{0,8}\cdot\frac{\left(1+\frac{n-1}{2}M_a^2\right)^{\frac{n+1}{2(n-1)}}}{M_a^{\gamma+1}}\cdot\frac{\overline{S}^{0,2}}{\overline{Y}_a^2}\cdot\left\{\int_0^{\overline{S}}\frac{(\overline{r})^{5/4}\cdot M^{\left(1+\frac{5}{4}\gamma\right)}\,d\overline{S}}{\left(1+\frac{n-1}{2}M^2\right)^{\left(\frac{1{,}36n-0{,}36}{n-1}\right)}}\right\} \tag{25}$$

where: $\delta_a^{**}=\overline{\delta}_a^{**}Y_a;\quad \gamma=\frac{18}{7}f_{at}-\frac{2}{7};\quad \mathrm{Re}_{w0}=V_{\max}\,x_a\,\rho_{oc}/\eta_{pr};\quad V_{\max}=\sqrt{\frac{2n}{n-1}RT_0};\ \overline{S}=\frac{S}{r_M};$

x_a – nozzle length; $f_{at}=T_{pr}/T_{oc}$ - heat transfer factor; T_{pr} – mean temperature of the nozzle wall (prescribed value); M_a e Y_a – Mach number and radius in the nozzle outlet; η_{pr} – gas viscosity at $T_{pr.}$

The impulse loss due to the friction is given by:

$$\xi_{at}=\frac{2\overline{\delta}_a^{**}}{1+1/\left(nM_a^2\right)} \tag{26}$$

3. Summary of the code "Tubeira" package

The models presented previously were coupled in a package named "Tubeira" and coded in Fortran 90. Each model's code was identified by a symbol, namely:

T – chemically equilibrated flow (item 2.1);

K – chemically nonequilibrated flow (item 2.2);

G – two-phase flow with coagulation and particle division (item 2.3);

D, S – two-dimensional two-phase (or eventually single phase) flow (item 2.4) with same and constant particle diameter d_p^m (subsonic parts D: up to the section X_{DS}, in Fig. (1); supersonic parts S: after the section X_{DS} in Fig. (1)).

No symbol was defined for the boundary layer code, since the application of this code is always associated with D or S. The coupling among the codes was made through the input and output data. Disconnected use of the codes T, K, G, D and S can be made by a special characterization of the initial data (adding the symbol * for the two phase flow case). Under these conditions, the initial data are:

- for T: x_k, Y_k, P_{oc}, b_{ic}, b_{iox}, H_c, H_{ox}, α_{ox}, A_q (symbols for substances of reacting medium);
- for K: initial information for T + R_j (refers to the chemical reaction mechanisms);
- for G: x_k, Y_k, P_{oc}, d_{in}^m (if the standard data are not used), n, μ_m, $\sigma_c(T)$, $\rho_c(T)$, $c_c(T)$;
- for D, S: x_k, Y_k, P_{oc}, d_p^m, n, μ_m, f_{at}, and the velocity distributions (V_{x0}, V_{y0}, W_{x0}, W_{y0}); if the distributions are uniforms, no prescription is required for W_{x0} and W_{y0} (axial and vertical components of the velocity of condensed phase).

For a coupled calculation however, the result from a code is used as an input data for the next code by reducing the number of initial data. For instance, for the most complex case (TKGDS*), the initial data are equivalent to those for K + f_{at} code because:

- the values of n and μ_m for the codes G, D or S results from the codes T or K;
- the dependences $\sigma_c(T)$, $\rho_c(T)$ and $c_c(T)$ are obtained from the data of substances A_q;

- the value d_p^m for the codes D and S are obtained from the code G.

The codes T and K can be applied to the reacting medium (A_q, R_j) which can include condensed phases. Following properties are calculated in the codes:
- in the code T: r_i, I_{es}, z, T, P, μ_m and other thermophysics and thermodynamics properties;
- in the code K: the same parameters as before (but using nonequilibrated model) and ξ_{dq};
- in the code G: d_i, ΔV_{ci}, ΔT_{ci}, ξ_{bf}, where $\Delta V_{ci} = V - W_i$; $\Delta T_{ci} = T - T_i$.
- in the code D, S: V_x, T_x, ρ_x, V_y, T_y, ρ_y (gas), W_x, T_{cx}, W_y, T_{cy} (condensed phase), δ^{**}, ξ_{np}, ξ_{at}, ξ_{ps};
- the final specific impulse by applying Eq. (1).

The afore mentioned models and codes have been already tested separately by many author in the past (Alemassov et al., 1980; Krioukov et al., 1997; Tishim & Khairutdinov, 1971; Richkov, 1988; Avduevskii, 1962).

4. Some relevant results from numerical simulations and discussion

To test the possibilities of the coupled package "Tubeira", the following conditions were defined: a bipropellant: "O2 (liquid) + [Kerosene (60%)+Aluminum powder (40%)]"; a nozzle (values of coordinates x_k, Y_k are presented in Tab. (1) operating at pressure $P_{oc} = 5{\cdot}10^6$ Pa and expansion ratio $f_a = 49$ ($r_M = y_M = 25$ mm). Aluminum powder was added in the propellant in order to test the presence of a condensed phase in the combustion product.

Table 1 Coordinates of the nozzle contour.

x_k(mm)	0	50	75	100	110	139	177	262	320	472
Y_k(mm)	75	50	30	25	31	49,3	71.1	110	132	174

Figures (2) and (3) show the effects of α_{ox}, (0.4 to 1.4), on some main properties of the combustion products, obtained from the code T. In the calculation, 24 substances, including AL_2O_3*, were considered. It can be seen that the maximum values of I_{es} (ideal) and T_{oc} are not clearly defined, but occur in the interval $\alpha_{ox} = 0.5$ to 0.9. Both values are rather high, when compared with already known conventional "O_2 + Kerosene" bipropellant system calculation, due to the inclusion of aluminum in the fuel. From Figure (3) it is possible to realize that the combustion product compositions change significantly during the flow through the nozzle. For instance, for $\alpha_{ox} = 0.8$ the molar fraction r_{H2O} increases from $r_{H2O}^{oc} = 0.2$ up to $r_{H2O}^{a} = 0.35$, resulting in a big difference between I_{es} (in equilibrium) and I_{es} (frozen), which can be expressed in a relative form $\delta I_{es} = 6.8\%$. This figure shows also the variation of z throughout the nozzle flow (for example, for $\alpha_{ox} = 0.8$, $z_{oc} = 0.264$ and $z_a = 0.284$).

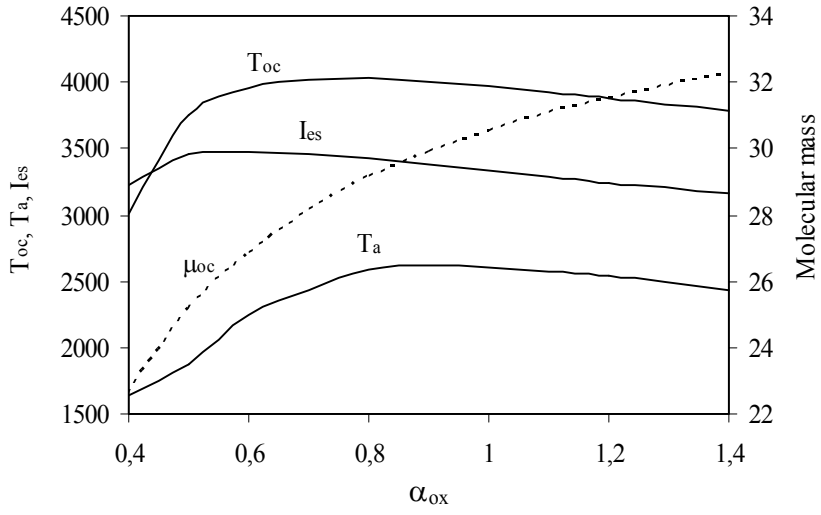

Figure 2. Variation of T_{oc}, T_a and I_{es} with α_{ox} (code T; $P_{oc} = 50$ atm; $f_a = 49$).

Figure (4) shows a comparison of the results obtained from the codes T and K (for $\alpha_{ox} = 0.8$). The mechanism of chemical transformations R_j required by code K includes 55 reactions. Significant difference can be seen in the temperature and composition in the nozzle outlet, leading to an impulse loss of nearly $\xi_{dq} = 0.78\%$. Therefore, for the currently selected data, it can be concluded that the flow in the nozzle is quasi equilibrated expansion since $\xi_{dq} << \delta I_{es}$. The values of $n = 1.107$ and $\mu_M = 29.55$ obtained from code K are used in the subsequent codes.

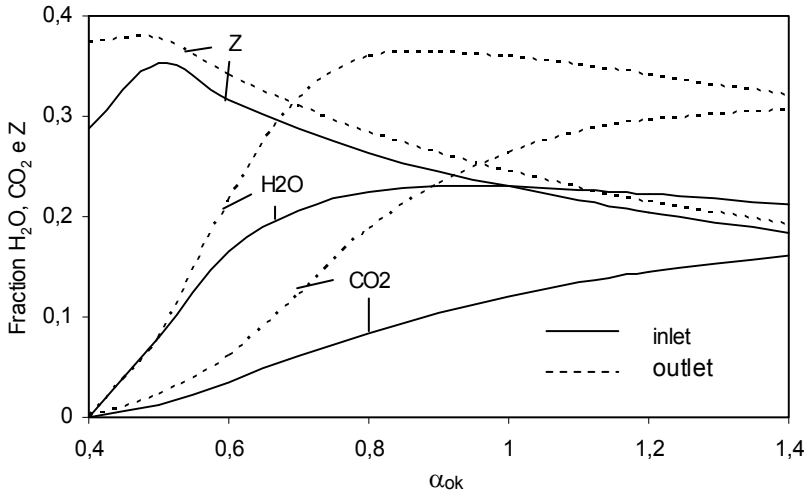

Figure 3. Variation of z, r_{H2O} and r_{CO2} with a_{ox} (code T; — *oc*; – – – *a*).

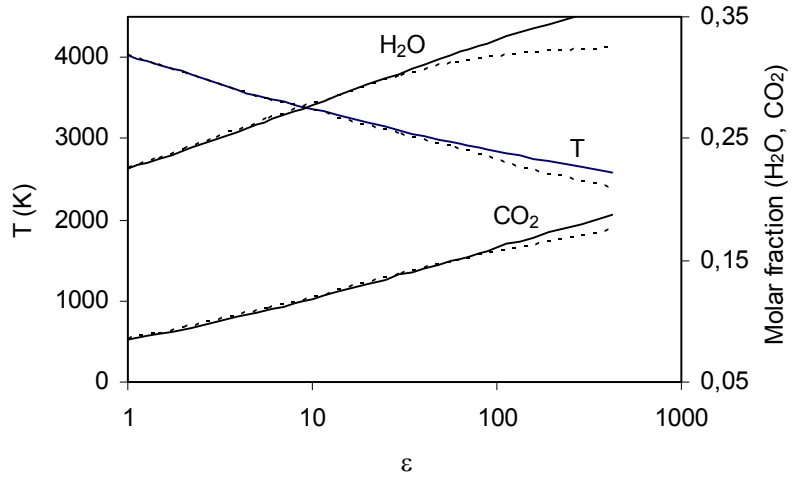

Figure 4. Variation of r_{H2O}, r_{CO2} and T in the nozzle (— code T; – – – code K).

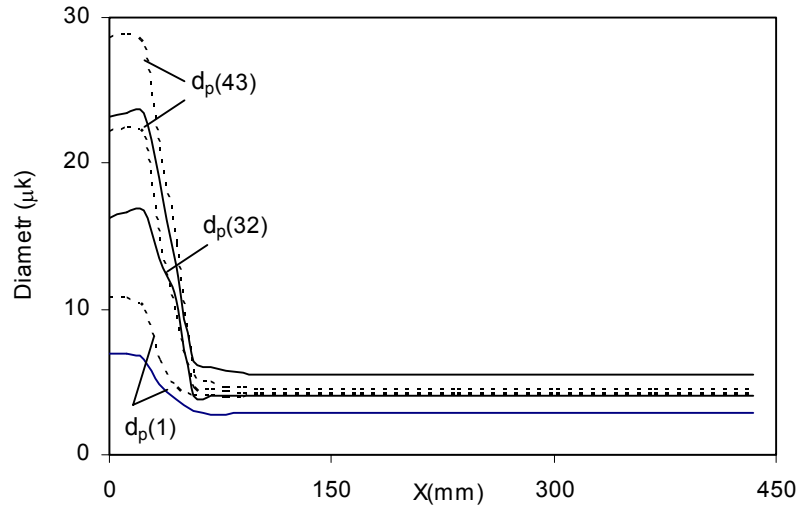

Figure 5. Variation of the mean diameters d_1, d_{32} and d_{43} in the nozzle (code G; — d_{in}^m = 5 μk; – – – d_{in}^m = 8 μk;)

Figures (5, 6) show some representative results obtained from the code G simulation, using the following diameters for the condensed particles: d_{min} = 1 μk; d_{max} = 50 μk; with the two initial average diameters d_{in}^m = 5 μk and d_{in}^m =8μk; σ_s = 2 (mean quadratic deviation); and N_p = 10 for the number of the group particles. Figure (5) shows the evolutions of the mean diameters: d_1 by the number of particles; d_{32} by the surface of particles and d_{43} by the mass of particles. In the initial part of the subsonic regime, some effect of coagulation can be observed; subsequently, in the transonic regime

(0.7 < M < 1.2) drastic division of particles occurs and finally, in the supersonic regime, an equilibrium is attained between the coagulation and division processes. Additionally, it can be observed that the mean sizes d_1, d_{32}, and d_{43} of the particles in the nozzle outlet are nearly equivalents, showing that the impulse loss ξ_{bf} does not depend on the initial diameter of the particles.

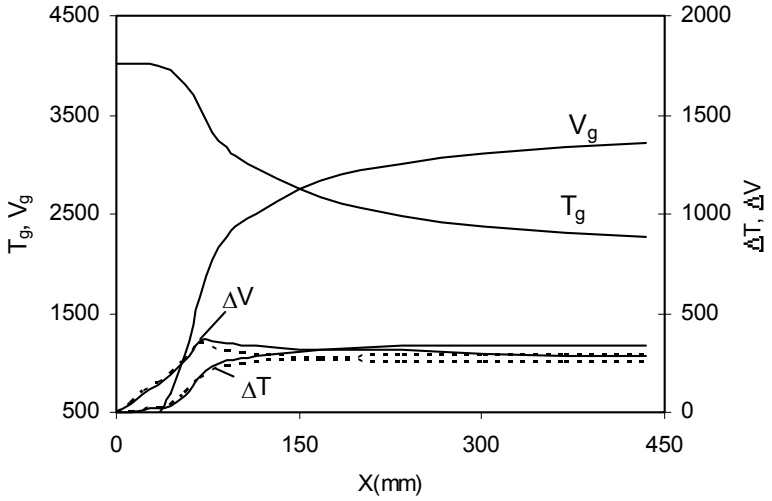

Figure 6. Variation of V, T, ΔV_c and ΔT_c in the nozzle (code G; — d_{in}^m = 5 μk; – – – d_{in}^m = 8 μk)

Behavior of the velocity difference $\Delta V_c = |V - W|$ and temperature difference $\Delta T_c = |T - T_c|$ in a gas–particles flow is illustrated in Fig. (6). In the nozzle inlet, ΔV_c and ΔT_c are reduced but increase quickly as the minimum section is attained, and become nearly constants (ΔV_c = 250 m/s; ΔT_c = 300 K) at the supersonic region. For the present conditions, the loss in the impulse is significant (ξ_{bf} = 2,295%).

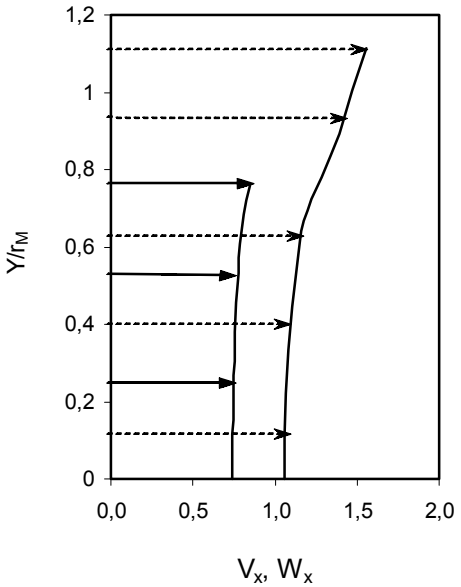

Figure 7. Axial velocity distributions.
V_x and W_x in the section X_{DS}.
(code D; arrows – – – for $\overline{V}_x$; — for $\overline{W}_x$)

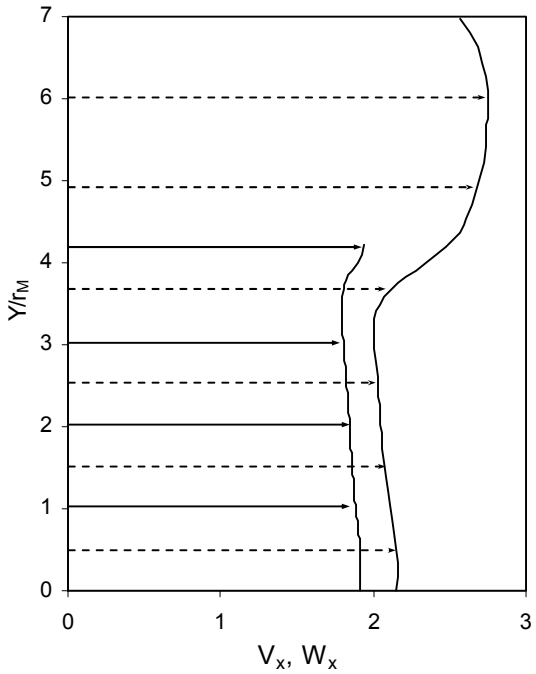

Figure 8. Axial velocity distributions.
V_x and W_x in the nozzle outlet.
(code S; arrows – – – for $\overline{V}_x$; — for $\overline{W}_x$)

The simulations with codes D and S were performed with n = 1.107 and μ_M = 29.55, obtained from code K. The mean size of the condensed particles d_{43} was obtained from code G. The value f_{at} = 0.5 was prescribed. Figures (7, 8) show the distributions of the axial velocities of the gas V_x (relative) = $\overline{V}_x$ and of the condensed phase W_x (relative) =

$\overline{W}_x$, for the cross section X_{DS} (Fig. (7)) and at the nozzle outlet (Fig (8)), respectively. The section X_{DS} is selected automatically in the code D calculation: $\overline{X}_{DS} = X_{DS}/r_M$ = 0.2601. Figure (7) allows observe that:

- the velocities $\overline{V}_x$ in the central parts ($\overline{V}_x$ = 1.05) and in the periphery ($\overline{V}_x$ = 1.5) of the flow are quite different;

- the condensed phase flow partially occupies the cross section $\overline{Y}_{DS} = Y_{DS}/r_M$ = 0.75 and the sonic velocity was not attained yet ($\overline{W}_x$ = 0.8).

Evolution of the flow at the nozzle outlet is shown in Fig. (8). In this case, the condensed phase flow forms a core of particles in the central zone of the nozzle, resulting in a loss coefficient ξ_{pc} = 0%. Additionally, coefficients ξ_{np} = 1.402% and ξ_{at} = 0.903% were also calculated. Finally, the real specific impulse value I_{es} = 3238 m/s was determined as a result of TKGDS* coupled mode calculations.

5. Conclusion

In the present work, a code package "Tubeira" was developed in order to estimate the characteristics of combustion products in a De Laval type nozzle. The models and the codes included in the package took account of chemical nonequilibrium and nonequilibrated transfer among the phases; effects of the presence of condensed particles on velocity and temperature in the flow; coagulation and division of particles; two-dimensional characteristics of two-phase flow in the nozzle; and presence of boundary layer in the nozzle wall.

The numerical simulations conducted for the bipropellant O_2 + Kerosene with addition of Aluminium powder showed that the package can be useful to predict many fundamental characteristics required for practical projects and researches on both liquid or solid propellant rocket engine.

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