COMPUTATION OF GAS AND MULTIPHASE SUPersonic JETS WITH NON-Equilibrium Processes

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ABSTRACT
A computational model for simulation of compressible multiphase supersonic jets with non-equilibrium physical and chemical processes is developed. Compared with the others, this model is distinguished by an extended system of non-equilibrium chemical reactions while taking into account the multiphase non-equilibrium. Lagrangian particle methodology was used. The particle phase change is simulated kinetically and included two solid Al₂O₃ crystalline structures: meta stable gamma and stable alpha forms. The simulation results were compared with the available results of the other authors. There was a satisfactory agreement regarding the results of the main gaseous component concentrations. Comparison of the simulation results with experimental data also showed their satisfactory agreement.

INTRODUCTION
Simulation of rocket exhaust flow fields is essential for assessments of the missile base heat transfer to ensure the motor's health and survival. Gas and multiphase gas/particle flow-field simulations are also an important element of efforts to predict liquid and solid-propellant rocket motor effluents for environmental studies including space debris.

The task for simulation of the gas-dynamic parameters of gas and two-phase jets was solved in the most rigorous formulation. Using the extended system of chemical reactions allowed us to obtain more accurate data on the concentrations of such important components of the gas mixture as NO, NO₂, ClO.

Usually at the altitudes below 15-20 km the assumption of equilibrium for a two-phase mixture and the chemical equilibrium is fairy true. In the range of heights 20-40 km the intensity of afterburning processes is drastically reduced. In this range there appears an effect of nonequilibrium flow of "gas + particle" mix. The non-equilibrium effects are greater if the combustion products mass flow (thrust) of the engines is lower.

Non-equilibrium flow of particles and gas delays the afterburning process and results in the shift of afterburning cessation. The use of the extended system of chemical reactions, i.e. introducing 12 reactions with chlorine components, results in temperature lowering in the jet and also in the shift of afterburning cessation. The lower mass flow, the lower is the altitude of afterburning cessation.

NOMENCLATURE

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Unit(s)</th>
<th>Description</th>
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<tbody>
<tr>
<td>a</td>
<td>[m/s]</td>
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</tr>
<tr>
<td>B_k, F_k</td>
<td>[-]</td>
<td>Backward and Forward reaction rate coefficients in reaction k</td>
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<tr>
<td>E</td>
<td>[m³/s]</td>
<td>Total energy</td>
</tr>
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<td>[m³/s]</td>
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<tr>
<td>h</td>
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</tr>
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<td>h_i</td>
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</tr>
<tr>
<td>J_x,i</td>
<td>[kg/(m³s)]</td>
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</tr>
<tr>
<td>K</td>
<td>[m³/s]</td>
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</tr>
<tr>
<td>L</td>
<td>[-]</td>
<td>Number of groups of particles</td>
</tr>
<tr>
<td>M_T</td>
<td>[-]</td>
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<tr>
<td>m_a</td>
<td>[kg]</td>
<td>The mass of one particle sized r_a</td>
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<tr>
<td>N_C</td>
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<tr>
<td>n_a</td>
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<td>number of particles sized r_a per unit volume</td>
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<tr>
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<td>[Pa]</td>
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</tr>
<tr>
<td>R</td>
<td>[J/(kmol K)]</td>
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<tr>
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<td>[m]</td>
<td>The radius of particle group α</td>
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<td>S</td>
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</tr>
<tr>
<td>S_i</td>
<td>[kg/(m³s)]</td>
<td>Species rate of production</td>
</tr>
<tr>
<td>S_C_r</td>
<td>[-]</td>
<td>Turbulent Schmidt number</td>
</tr>
<tr>
<td>T</td>
<td>[K]</td>
<td>Temperature</td>
</tr>
<tr>
<td>T_m</td>
<td>[K]</td>
<td>Temperature of particle group α</td>
</tr>
<tr>
<td>U</td>
<td>[-]</td>
<td>Conservative variable vector</td>
</tr>
<tr>
<td>u, v</td>
<td>[m/s]</td>
<td>Velocity components</td>
</tr>
</tbody>
</table>
The basic assumptions for the gas-dynamic model of the plume and simulation methods at the heights of 0-90 km are as follows:

1. The composite stream is replaced with an equivalent single axisymmetric jet.
2. The flow of gas in the jet is described by the complete system of Navier-Stokes [1] (see The governing gas-phase equations);
3. The extended system of chemical reactions is used for non-equilibrium chemical processes (for a system that contains C, O, H, N, C1, consisting of 42 reactions) [1-4] (see Table);
4. Non-equilibrium of particles and gas is considered in the complete statement: temperature, speed, phase for particles (liquid and solid states (α-, γ-phase)), crystallization for particles (see Particle flow equations).

THE GOVERNING GAS-PHASE EQUATIONS

The set of Favre averaged equations for high Reynolds two-dimension turbulent reacting flow can be cast in the following compact form:

\[
    \frac{\partial u}{\partial t} + \frac{\partial F_a}{\partial x} + \frac{\partial F_y}{\partial y} = \frac{\partial G}{\partial x} + \frac{\partial G}{\partial y} + \frac{\partial F}{\partial x} + \frac{\partial F}{\partial y} + \frac{\partial H}{\partial x} + \frac{\partial H}{\partial y} = S, \tag{1}
\]

where

\[
    U = \left[ \rho, \rho u, \rho v, \rho E, \rho Y_1, ..., \rho Y_{Nc}, \rho K, \rho \varepsilon \right]^T,
\]

\[
    F_a = \begin{pmatrix} \rho u \\ \rho u^2 + p \\ \rho v \\ \rho v + p \\ u \left( \rho E + p \right) \end{pmatrix},
    G = \begin{pmatrix} \rho v \\ \rho v u \\ \rho v^2 + p \\ \rho v \left( \rho E + p \right) \end{pmatrix},
    H = \begin{pmatrix} \rho \varepsilon \\ \rho \varepsilon u \\ \rho \varepsilon v \\ \rho \varepsilon \left( \rho E + p \right) \end{pmatrix}.
\]

\[
    S = \left[ 0, S_x, S_x, S_y, ..., S_x, S_y, S_{K}, S_{\varepsilon} \right]^T.
\]

The Reynolds stress tensors and the enthalpy, species, K, ε turbulent fluxes are closed by the classical Boussinesq-like formulation for non-zero divergence flows:

\[
    T_{xx} = \frac{2}{3} \mu_t \left[ \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right] - \frac{2}{3} \rho K, \tag{2}
\]

\[
    T_{xy} = \frac{2}{3} \mu_t \left( \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) + \frac{2}{3} \frac{\partial \varepsilon}{\partial y},
    T_{yy} = \frac{2}{3} \mu_t \left( \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right) - \frac{2}{3} \rho K, \tag{3}
\]

\[
    Q_x = \frac{\mu_t}{\rho} \frac{\partial h}{\partial x} + \mu_l \sum_{i,j} \left( \frac{1}{\Pr_T} \frac{1}{S_{c_{ij}}} \right) h_i \frac{\partial Y_i}{\partial x}, \tag{4}
\]

\[
    Q_y = \frac{\mu_t}{\rho} \frac{\partial h}{\partial y} + \mu_l \sum_{i,j} \left( \frac{1}{\Pr_T} \frac{1}{S_{c_{ij}}} \right) h_i \frac{\partial Y_i}{\partial y}.
\]

\[
    J_{x,x} = \frac{\mu_t}{\sigma_x} \frac{\partial K}{\partial x},
    J_{x,y} = \frac{\mu_t}{\sigma_x} \frac{\partial \varepsilon}{\partial y},
    J_{y,y} = \frac{\mu_t}{\sigma_x} \frac{\partial \varepsilon}{\partial y}, \tag{5}
\]

Additional equations:

\[
    \sum_{i=1}^{Nc} Y_i = 1, \quad h = \sum_{i=1}^{Nc} h_i Y_i,
    H = \sum_{i=1}^{Nc} h_i Y_i + \frac{1}{2} \left( u^2 + v^2 \right), \quad E = H - \frac{p}{\rho}.
\]

\[
    F = \begin{pmatrix} 0 \\ -T_{xx} - T_{xy} \\ -T_{xy} - T_{yy} \end{pmatrix},
    G = \begin{pmatrix} 0 \\ -u T_{xx} - v T_{xy} \\ -u T_{xy} - v T_{yy} \end{pmatrix},
    H = \begin{pmatrix} 0 \\ -u T_{xx} - v T_{xy} \end{pmatrix}.
\]
For a high temperature, chemically reacting flow, the gas is assumed to be thermally perfect:

\[ p = \rho T R \sum_{i=1}^{N_s} \frac{Y_i}{W_i} \]  

(7)

The species specific heat and enthalpies are obtained from the following equations [9]:

\[ C_{P,i}(T) = a_{i,1} + a_{i,2} T + a_{i,3} T^2 + a_{i,4} T^3 + a_{i,5} T^4, \]

\[ h_i(T) = \frac{a_{i,1}}{RT} + \frac{a_{i,2} T^2}{2} + \frac{a_{i,3} T^3}{3} + \frac{a_{i,4} T^4}{4} + \frac{a_{i,5} T^5}{5} + \frac{b_{i,1}}{T} \]  

(8)

The members \( S_v, S_s, S_k \) comprised in the source S take into account the effect of particles on the gas parameters:

\[ S_v = \sum_{a=1}^{l} f_{a,v}; \quad S_s = \sum_{a=1}^{l} f_{a,s}; \]

\[ S_k = \sum_{a=1}^{l} (q_{a,conv} - f_{a,u_x} u_x - f_{a,u_y} v_y) \]  

(described in Particle flow equations section).

The members \( S_1, ..., S_{N_w-1} \) are defined by species rates of production (see Chemical Kinetics). And, at last, \( S_k, S_s \) are defined by the turbulence model (see Turbulence model).

**TURBULENCE MODEL**

The transport equations for \( K \) and \( \varepsilon \) for high Reynolds numbers are as follows [1]:

\[ \frac{\partial}{\partial t} (\overline{\rho K}) + \frac{\partial}{\partial x_j} (\overline{\rho u_j K}) = \frac{\partial}{\partial x_j} \left[ \mu + \frac{\rho K}{\sigma_k} \right] \frac{\partial K}{\partial x_j} \]

\[ + P_k - \left[ 1 + \phi(M_T) \right] \overline{\rho e} \]  

(10)

\[ \frac{\partial}{\partial t} (\overline{\rho e}) + \frac{\partial}{\partial x_j} (\overline{\rho u_j e}) = \frac{\partial}{\partial x_j} \left[ \left( \frac{\mu + \mu}{\sigma_j} \right) \frac{\partial e}{\partial x_j} \right] \]

\[ + \frac{\varepsilon}{K} (C_{\alpha} \overline{P_{\alpha}} - C_{\varepsilon} \overline{\rho e}) \]

which use standard constant pool:

\[ \sigma_k = 1; \quad \sigma_e = 1.3; \quad C_{\alpha} = 1.44; \quad C_{\varepsilon} = 1.92 \]  

(12)

In these equations \( P_k \) is the production term, \( M_T \) - Mach turbulent number

\[ M_T = \frac{\sqrt{2} K}{a} \]  

(13)

\( a \) - local sound speed. \( \phi(M_T) \) - compressibility function:

\[ \phi(M_T) = C_{\mu} M_T \]  

(14)

Assuming that diffusion and convection are balanced in these equations, the following formula for turbulent viscosity can be obtained

\[ \mu_t = \frac{(1 - C_{\varepsilon}) V^*}{C_i} \frac{\rho K^2}{\varepsilon} = C_{\mu} \rho \frac{K^2}{\varepsilon}, \]  

(15)

where

\[ C_{\mu} = \frac{(1 - C_{\varepsilon}) V^*}{C_i} \]  

(16)

\( V^* \) - velocity fluctuation normal to the streamlines, for which it is true:

\[ \frac{V^*}{K} = \frac{2}{3} \left( 1 - \frac{(1 - C_{\varepsilon})}{C_i} \right) \left( \frac{1 + \phi(M_T)}{1 + \phi(M_T)} \right) \]  

(17)

The following numerical constants are used:

\[ C_1 = 1.8; \quad C_2 = 0.6 \]  

(18)

Thus, unlike standard \( K-\varepsilon \) turbulence model, the presented model firstly includes supplementary dissipation dependable on the turbulent Mach number \( M_T \), and secondly the coefficient \( C_{\mu} \) in formula (15) of turbulent viscosity is no longer constant but dependable on \( M_T \) as well.

The following constant is used in formula(14) for this model:

\[ C_{\mu} = 0.4 \]  

(19)

**CHEMICAL KINETICS**

Finite rate chemical kinetics is used to track chemical reactions in the present work. This method is based on the Law of Mass Action.

The production rate of each species is given by:

\[ S_i = W_i \sum_{k=1}^{N_S} \left( \nu_{i,k}^r - \nu_{i,k}^s \right) R_k \]  

(20)

The Law of Mass Action for \( k \)-th reaction is:

\[ R_k = \left( F_k \prod_{l=A,B}^{N_f} [I]^r - B_k \prod_{l=A,B}^{N_f} [I]^s \right) \]  

(21)

It is very important to select properly chemical reaction rate coefficients. The available data on these coefficients were obtained in the conditions that are considerably different from those of rocket engines jets having a greater dispersion characterized by the uncertainty factor.

After comparing the simulated and experimental data on the characteristics of jets of real and model rocket engines, the coefficients for reactions 1-20 were selected, within the limits of the uncertainty factor (see table), which provided the best agreement between the simulation and experimental data.
The system of non-equilibrium chemical reactions

<table>
<thead>
<tr>
<th>No.</th>
<th>Reaction</th>
<th>No.</th>
<th>Reaction</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>CO+OH=CO₂+H</td>
<td>22</td>
<td>N₂O₅=O₂+NO</td>
</tr>
<tr>
<td>2</td>
<td>OH+H₂=H₂O+H</td>
<td>23</td>
<td>N+OH=H+NO</td>
</tr>
<tr>
<td>3</td>
<td>H+O₂=OH+O</td>
<td>24</td>
<td>H+O+M=OH+M</td>
</tr>
<tr>
<td>4</td>
<td>O+H₂=OH+H</td>
<td>25</td>
<td>N₂+O=NO+M</td>
</tr>
<tr>
<td>5</td>
<td>H+O₂+M=HO₂+M</td>
<td>26</td>
<td>O₂+N₂=2NO</td>
</tr>
<tr>
<td>6</td>
<td>OH+HO₂=H₂O+O₂</td>
<td>27</td>
<td>HO₂+NO=NO₂+OH</td>
</tr>
<tr>
<td>7</td>
<td>H+HO₂=2OH</td>
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<td>O+NO₂=NO+O₂</td>
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<td>O+HO₂=O₂+OH</td>
<td>29</td>
<td>NO₂+H=NO+OH</td>
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<tr>
<td>9</td>
<td>2OH=O+H₂O</td>
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<td>Cl₂+NO=NO₂+Cl</td>
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<td>10</td>
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<td>Cl₂+Cl₂=Cl₂O₂</td>
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<tr>
<td>11</td>
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<td>Cl₂+OH=HO₂+Cl</td>
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<td>12</td>
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<td>41</td>
<td>HOCl+OH=H₂O+ClO</td>
</tr>
</tbody>
</table>

Figure 1 shows a comparison of calculation results of the combustion products mass flow rates along the jet axis (solid lines) with the calculations given in [3] (dashed lines) for the intermediate-thrust rocket ~ 80 ton.

As seen, there are significant differences from the basis computation of concentrations of HO₂, ClO, NO and NO₂. Comparing with [3] with the altered system of chemical reactions showed a good agreement of distribution of components mass flow rate of NO and NO₂ (compare dashed lines NOₓ in Figure 1 and NO, NO₂ in Figure 2).

The use of the extended system of reactions led to the fact that a considerable part of components NO transfer into NO₂ when molecules NO interacted with ClO in the jets of solid-fuel rocket engines containing chlorine-containing components (i.e., "Space-Shuttle" launch vehicle and "Titan" launch vehicle). This transfer of NO into NO₂ did not happen in the jets of liquid rocket engines (i.e., "Proton" launch vehicle) due to the absence of chlorine-containing components.

Based on the computation results of distribution of component concentrations in the end of the jet of "Space-Shuttle" and "Titan" Professor I.L. Karol performed computations of concentration component variance in the jet wake, which were presented in [5]. The results were compared with the data of [6] on the variance of Cl₂ concentration in the wake. For the "Titan" the computation results for night launch are shown in Figure 3. There was a good agreement with the variance of Cl₂ concentration (marked by (*) in Figure 3).
PARTICLE FLOW EQUATIONS

Polydisperse mixture of particles is represented as a set of
L groups of particles, each of which is characterized by the
values of the radius rα, density ρα = nα · mα, velocity
components uα, vα, and temperature Tα.

For each of L groups (α=1,2,...,L), under the assumptions
that the particles are spherical, chemically inert to the gaseous
phase, and do not interact with each other, equations describing
the motion of Al2O3 particles can be written as:

1) Particle continuity:

\[ \frac{\partial}{\partial x} (\rho_u u) + \frac{\partial}{\partial y} (\rho_v v) = 0, \] (22)

2) Particle momentum in x direction:

\[ \rho_u u \frac{\partial u}{\partial x} + \rho_v v \frac{\partial u}{\partial y} = f_{a,x}, \]

3) Particle momentum in y direction (α=1,2,...,L):

\[ \rho_u u \frac{\partial v}{\partial x} + \rho_v v \frac{\partial v}{\partial y} = f_{a,y} \]

4) Particle energy:

\[ \rho_u u C_s \frac{\partial T}{\partial x} + \rho_v v C_s \frac{\partial T}{\partial y} = q_{\text{phase},\alpha} - q_{\text{conv},\alpha} - q_{\text{rad},\alpha} \]

As a result of crystallization, the following is true for a

heat flow:

\[ q_{\text{phase},\alpha} = 3q_{cr} \frac{r_{cr}^2}{r_0} \]

where qcr - the heat of crystallization, Vcr - crystallization
rate, rcr,α - the position of the crystallization front.

It is supposed that particles start crystallizing when their
temperature is equal to 0.82T_L (T_L - the equilibrium melting
point of γ-phase equal to 2300 K).

According to [7] the crystallization rate of Al2O3 particles is
calculated by the formula

\[ V_{cr} = 0.64 \cdot 10^{-6} (T_L - T)^{1.8}, m/s \]

and the position of crystallization front is defined from the
equation

\[ \frac{dr_{cr,\alpha}}{dt} = -V_{cr}, \]

(crystallization front moves toward the center of the
particle).

The liquid phase is assumed to transfer initially to the
metastable solid γ-phase for all conditions. The transition
process from the γ-phase to the stable α-phase begins as soon as
any portion of the γ-phase has appeared.

To determine the portion of solid substance in the α-phase
(fα) the following equation is applied [8]:

\[ \frac{df}{dt} = A \cdot \exp \left( -B / T_\gamma \right), \quad 0 < f < 1 \]

where A=1.03·10^12 s^{-1}, B=58368 K.

PARTICLE EFFECT ON AFTERBURNING

Fig. 4 demonstrates the axis distributions of the estimated
gas temperature with and without considering the particle effect
in a jet of typical solid rocket engine with thrust 12 ton at the
attitude of 31 km. At that attitude the estimated gas temperature
without considering particle effect is so low that chemical
reactions do not occur (see dashed line on fig. 4).

When considering the particle effect on gas, the gas
estimated temperature increases, which leads to afterburning of
products exhausting from the nozzle. At that attitude the effect
of chemical reactions with chlorine-containing components on
the gas temperature is also noticeable; considering those results
in reducing the estimated temperature in the jet (see solid and
dashed lines on Figure 4).
For an engine with thrust of 85 ton, non-equilibrium is noticeable at the altitudes H= 40-45 km, and particularly at the altitude H = 40 km (Figure 5), where the jet ceases burning without considering particles on the gas. This brings down the temperature drastically (ΔT ≈ 300-600 K) and considerably (in times and orders) change in combustion products concentration.

For very large missiles, such as “Space Shuttle”, afterburning does not cease during the mid-course burn of rocket engine (H < 50 km). According to computations taking into account the effect of particles, the concentrations of gas components changed by 25-30%.

Particles intensify afterburning process in the jets and lead to the increase in the attitude of afterburning cessation by 5-10 km depending on engine thrusts; on the contrary chemical reactions with chlorine-containing components lead to the decrease in the attitude of afterburning cease by 1-5 km depending on the engine thrust.

Conclusions
A computational model for simulation of compressible multiphase supersonic jets with non-equilibrium physical and chemical processes is developed.

The simulation results were compared with the available data obtained by the other authors specializing in chemically non-equilibrium jets. There was a satisfactory agreement of the results by the basis gas components of the jet. Comparing the simulation results with the experimental data also showed their good agreement.

Using the extended system of chemical reactions allowed us to obtain more accurate data on the concentrations of such important components of the gas mixture as NO, NO2, ClO.

The range of altitudes (H = 30-50 km) was determined where the particles and chlorine-containing components reactions effect on the parameters of the gas phase is the most essential. It was shown that the particles intensify the process of burning in jets and increase the altitude of afterburning cessation (5-10 km, depending on the engine thrust); and on the contrary, the chlorine-containing components chemical reactions reduce the altitude of afterburning cessation (1-5 km depending on the engine thrust).

In this altitude range the effect of particles on the gas flow-field can lead to substantial increase (~300-600 K) of the jet temperature and great (in times and orders) changes in component concentrations.

The altitude range where the effect of particles on temperature and species concentrations is significant is highly dependent on the combustion products mass flow. The lower mass flow, the lower is the altitude of afterburning cessation. For very large rockets, such as the “Space Shuttle”, the gas-particle interaction causes the change of the component concentrations by 25-30%.

REFERENCES


