Numerical simulation of the underexpanded plume spectral radiance using Monte-Carlo method

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Abstract. Numerical simulation of the tactical rocket plumes spectral radiance is performed. An influence of the chemical composition and temperature of the plume exhausts as well as the angle of sight and scattering on the solid particles is discussed. Numerical simulation results for homogeneous plume of tactical rocket are in a good agreement with published data.

1. Introduction
Most of the modern subsonic and supersonic vehicles produces plumes which radiate in the infrared region of the electromagnetic spectrum. Due to partial atmospheric opacity in this spectral region the radiance reaches the detector with some distortion. Particular shape of the spectrum depends on the type of the engine (solid or liquid), chemical composition of the engine fuel, radius of the nozzle exit, presence of solid particles, its phase and radius, altitude of the flight.

For this reason, numerical simulation of the plume spectral radiance is complex problem which requires the knowledge of large amount of data such as: spatial distribution of temperature and pressure in the plume, chemical composition, absorbance coefficients for different chemical species, complex refractive index of solid particles as well as physical and mathematical models[1–5] included different nonequilibrium processes proceeded in the plume. It is well known that the most universal algorithm to calculate spectral radiance is the Monte-Carlo method [1, 6, 7]. The main purpose of this work is to calculate spectral signature of the underexpanded plumes with the use of Monte-Carlo method and investigate its dependence on the plume characteristics: temperature, emitted volume, number density of solid particles and its size, imaginary part of the refractive index.

2. Spectral radiance of the plume with Al$_2$O$_3$ particles
The plume flowfield was modelled as a homogeneous cylinder. The cylinder size, temperature and pressure, as well as chemical composition was assumed to be the same as in [8]. It’s length is equal to L = 600 cm and radius r = 10 cm. The cylinder is isothermal with temperature T = 1000 K and pressure p = 1 atm. Gas and solid particle concentrations were uniform. All the particles are spherical and have the same radius. Chemical composition of the plume and its particle properties are given in table 1. The aspect angle was assumed to be equal to 90°.
Figure 1. Comparison of the imaginary part of the refractive indexes provided by different authors [9–15].

The absorption and scattering coefficients of the solid particles are calculated with the use of the Mie theory. So the spectral signature of the plume with scattering particles is significantly depends on the imaginary part of the refractive index which in its turn depends on the wavelength, temperature and phase of solid particles. Comparison of the values of imaginary part of the refractive index for $\text{Al}_2\text{O}_3$ particles given by different authors [9–15] is presented in figure 1. It can be seen that its values differ by several orders of magnitude for different temperature and phase of particles.

The influence of the imaginary part of the refractive index on the spectral radiance of the plume is given in figure 2. Numerical simulation of the signature performed for the particle radius $r = 1 \text{ mc}$ and different concentrations of solid $\text{Al}_2\text{O}_3$. Two approximations of the imaginary part of the refractive index were used provided by Dombrovskii [9] and Toon [12]. With the increase of the solid particle concentration difference in the spectral radiance of the plume for data [12] and data [9]

| Table 1. Chemical composition and solid particle properties of the plume. |
|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| Species         | Mole fraction   | Mole fraction   | Density, g cm$^{-3}$ | Concentration, cm$^{-3}$ |
|                 |                 |                 | R = 0.1 mc | R = 1 mc | R = 5 mc |
| HCL             | —               | 0.001           | 1.25E-06 | 8.08E+07 | 8.08E+04 | 6.46E+02 |
| HF              | —               | 0.01            | 1.26E-05 | 8.15E+08 | 8.15E+05 | 6.52E+03 |
| $\text{H}_2$    | 0.40            | 0.1             | 1.39E-04 | 8.96E+09 | 8.96E+06 | 7.17E+04 |
| $\text{H}_2\text{O}$ | 0.30    | 0.5             | 1.25E-03 | 8.07E+10 | 8.07E+07 | 6.45E+05 |
| CO              | 0.02            |                 |             |           |           |           |
| $\text{CO}_2$   | —               |                 |             |           |           |           |
| $\text{Al}_2\text{O}_3$ | (0.5)  |                 |             |           |           |           |
increases. The main change in spectrum is observed in the spectral range $\omega = 2400 \div 3000 \, \text{cm}^{-1}$ and
$\omega = 4100 \div 5000 \, \text{cm}^{-1}$ where optical depth is small. At the same time in the range $\omega = 2000 \div 2400 \, \text{cm}^{-1}$ and $\omega = 3000 \div 4100 \, \text{cm}^{-1}$ where the absorption coefficient for CO$_2$ and H$_2$O the differences in spectral radiance are insignificant.

![Spectral radiance calculated with the use of the different values of the imaginary part of the refractive index.](image)

**Figure 2.** Spectral radiance calculated with the use of the different values of the imaginary part of the refractive index.

Numerical simulation results for the matrix of solid particle concentrations and radiiuses and its comparison to the data [8] are given in figure 3.

The are two sets of numerical simulation results. The first set (left column) is the total volume emission of the homogeneous plume and the second set (right column) is the emission only for a path through the diameter of the radiative cylinder. The numerical simulation results with the use the values of the refraction index provided by Toon [12] give satisfactory agreement with the data [8].

3. **Spectral radiance of the plume with B$_2$O$_3$ particles**

As in previous section the plume flowfield was modelled as a homogeneous cylinder. The cylinder size, temperature and pressure, as well as chemical composition was assumed to be the same as in [16]. It’s length is equal to $L = 1500 \, \text{cm}$ and radius $r = 75 \, \text{cm}$. The cylinder is isothermal with temperature and pressure given in table 2. The temperature is assumed to be equal to $T = 1000 \, \text{K}$ (variant 1) and $T = 1600 \, \text{K}$ (variant 2) and pressure $p = 1 \, \text{atm}$ (both cases). Its gas and solid particle concentrations were uniform. All the particles are spherical and have the same radius. It was assumed that B$_2$O$_3$ are the scattering solid particles in this case. Values of the complex refractive index for B$_2$O$_3$ particles were taken from [16]. Chemical composition of the plume and its particle properties are given in table 2. The aspect angle was assumed to be equal to 90°.
Figure 3. Total volume emission of the plume (a) and the emission for a path through the diameter of the cylinder (b) and its comparison to data [8].

Numerical simulation results for the matrix of solid particle concentrations and radiuses and its comparison to the data [16] are given in figure 4. There are two sets (variant 1 and variant 2) of numerical simulation results. The conditions for any case are given in table 2. A good agreement with the data [16] is obtained for all considered cases.

| Mole fraction | Density, g * cm⁻³ | Concentration, cm⁻³ | CO₂ | H₂O | CO | HBO₂ | N₂ |
|---------------|--------------------|---------------------|-----|-----|----|------|----|
|               | R = 0.1 mcm        | R = 1 mcm           |     |     |    |      |    |
| Variant 1     |                    |                     |     |     |    |      |    |
| 0.00011       | 9.53E-08           | 1.26E+07            | 1.26E+04 |
| 0.00025       | 2.14E-07           | 2.84E+07            | 2.84E+04 | 0.140 | 0.060 | 0.030 | 0.001 | 0.579 |
| 0.00100       | 8.58E-07           | 1.14E+08            | 1.14E+05 |
| Variant 2     |                    |                     |     |     |    |      |    |
| 0.00011       | 5.95E-08           | 7.90E+06            | 7.90E+03 |
| 0.00025       | 1.34E-07           | 1.78E+07            | 1.78E+04 | 0.30  | 0.020 | 0.020 | 0.020 | 0.790 |
| 0.00100       | 5.36E-07           | 7.11E+07            | 7.11E+04 |
Figure 4. Spectral radiance of the plume with $\text{B}_2\text{O}_3$ particles and its comparison with data [16].

In figure 5 comparison of the spectral signature for different angles of observation is given ($\theta = 90^\circ$ and $\theta = 45^\circ$). Numerical simulation results are presented for the Variant 2 (see table 2) for concentration of solid particles $N = 7.11 \times 10^4$ and its radius $r = 1 \text{ mcm}$. With the decrease of the angle between the axis of the cylinder and the line of sight from $\theta = 90^\circ$ to $\theta = 45^\circ$ the local maximum in the spectral radiance in the range $\omega = 3300 - 4000 \text{ cm}^{-1}$ (which corresponds to $\text{H}_2\text{O}$ emission) is decreased.

Figure 5. Spectral radiance of the plume for different angles of observation.
4. Spectral radiance of the nonhomegeneous plume of tactical rocket

The plume flowfield in this section is calculated from a system of a Navier-Stokes equations for compressible chemically reacting gas [2,17,18]. The system of equations is formulated in two-dimensional axisymmetric geometry:

\[
\frac{\partial f}{\partial t} + \frac{\partial E}{\partial r} + \frac{\partial G}{\partial z} = \frac{\partial E_\mu}{\partial r} + \frac{\partial G_\mu}{\partial z} + H
\]

\[
f = \begin{bmatrix} \rho \\ \rho U^r \\ \rho U^z \\
\end{bmatrix} ;
E = \begin{bmatrix} \rho U^r \\ \rho U^r U^r + P \\ \rho U^z U^r \\
\end{bmatrix} ;
G = \begin{bmatrix} \rho U^z \\ \rho U^z U^z + P \\ \rho U^z U^r \\
\end{bmatrix} ;
\]

\[
E_\mu = \begin{bmatrix} 0 \\
2 \mu \left( \frac{\partial U^r}{\partial r} - \frac{2}{3} \mu \text{div}(U) \right) \\
\mu \left( \frac{\partial U^z}{\partial r} + \frac{\partial U^r}{\partial z} \right) \\
\end{bmatrix} ;
G_\mu = \begin{bmatrix} 0 \\
\mu \left( \frac{\partial U^z}{\partial r} + \frac{\partial U^r}{\partial z} \right) \\
2 \mu \left( \frac{\partial U^z}{\partial z} \right) - \frac{2}{3} \mu \text{div}(U) \\
\end{bmatrix} ;
\]

\[
H = \begin{bmatrix} \frac{-\rho U^r}{r} \\
2 \mu \left( \frac{\partial}{\partial r} \left( \frac{U^r}{r} \right) \right) - \frac{\rho (U^r)^2}{r} \\
\mu \left( \frac{\partial U^z}{\partial r} + \frac{\partial U^r}{\partial z} \right) - \frac{\rho U^z U^r}{r} \\
\end{bmatrix} ;
\]

Diffusion equation for chemical species:

\[
\frac{\partial \rho_i}{\partial t} + \text{div} \rho_i U = \text{div} J_i + \dot{\omega}_i
\]

Heat equation:

\[
\rho c_p \frac{\partial T}{\partial t} + \rho c_p U \text{grad} T = \text{div} \left( \lambda \text{grad} T \right) + \frac{\partial p}{\partial t} + \text{grad} p + \Phi_\mu - \sum_{i=1}^{N_s} h_i \dot{\omega}_i
\]

where \( \Phi_\mu \) is dissipative function; \( t \) – is time; \( z, r \) – orthogonal cylindrical coordinates; \( U^r, U^z \) are the projections of the velocity vector \( U \) on the axis \( r \) and \( z \); \( p, \rho \) are pressure and density; \( T \) is temperature of the gas; \( \mu, \lambda \) are viscosity and conductivity coefficients; \( c_p \) is the specific heat capacity; \( h_i, \rho_i \) are the enthalpy and density of i-th component; \( \dot{\omega}_i \) is the mass production of the i-th component; \( J_i \) is the density vector of the diffusion flow for i-th component; \( D_i \) is the diffusion coefficient for the i-th component; \( Y_i \) is mass fraction for i-th component; \( N_s \) is the number of chemical species.
The algebraic Penner-Haselman-Edwards model of turbulent transfer [19] (PHE), were used to consider the effects of turbulent mixing in the model:

\[
\mu_I = \frac{1}{2} \rho l^2 \left( \frac{\partial U'}{\partial r} + \frac{\partial U'}{\partial z} \right)^2 + 2 \left[ \left( \frac{\partial U'}{\partial r} \right)^2 + \left( \frac{\partial U'}{\partial z} \right)^2 + \left( \frac{U'}{r} \right)^2 \right]^{1/2}
\]

\[
l = K \left( \frac{\left( U' \right)^2 + \left( U' \right)^2}{B} \right)^{1/2} \left( \frac{1}{B} \left( \frac{\partial^2 U'}{\partial r^2} + \frac{1}{r} \frac{\partial U'}{\partial r} \right)^2 + \left( \frac{U'}{r} \right)^2 \right) + \left( \frac{\partial^2 U'}{\partial z^2} \right)^2 + \left( \frac{\partial^2 U}{\partial r^2} + \frac{1}{r} \frac{\partial U}{\partial r} \right)^2 + \left( \frac{\partial^2 U}{\partial z^2} \right)^2 \right)^{1/2}
\]

\[
B = \left( \frac{\partial U}{\partial r} \right)^2 + \left( \frac{\partial U}{\partial z} \right)^2 + \left( \frac{\partial U}{\partial r} \right)^2 + \left( \frac{\partial U}{\partial z} \right)^2 + \left( \frac{U'}{r} \right)^2
\]

where \( K \) is an empirical constant with recommended value of 0.125 [19]. Its value is varied in calculations.

For the numerical simulation of the afterburning processes in the plume the following kinetic scheme was used:

1) \( \text{OH} + \text{H}_2 \leftrightarrow \text{H}_2 \text{O} + \text{H} \)
2) \( \text{OH} + \text{O} \leftrightarrow \text{H} + \text{O}_2 \)
3) \( \text{H} + \text{H} + \text{M} \leftrightarrow \text{H}_2 + \text{M} \)
4) \( \text{H} + \text{OH} + \text{M} \leftrightarrow \text{H}_2 \text{O} + \text{M} \)
5) \( \text{OH} + \text{OH} \leftrightarrow \text{H}_2 \text{O} + \text{O} \)
6) \( \text{O} + \text{H}_2 \leftrightarrow \text{OH} + \text{H} \)
7) \( \text{H} + \text{O} + \text{M} \leftrightarrow \text{OH} + \text{M} \)
8) \( \text{O} + \text{O} + \text{M} \leftrightarrow \text{O}_2 + \text{M} \)
9) \( \text{CO} + \text{OH} \leftrightarrow \text{CO}_2 + \text{H} \)
10) \( \text{CO} + \text{O} + \text{M} \leftrightarrow \text{CO}_2 + \text{M} \)

Rate coefficients for the processes (1)–(8) were taken from the [20]. Rate coefficients for the reaction (9) – (10) were taken from the [21].

The initial data for the numerical simulation were assumed to be the same as in [22]. The temperature is equal to \( T = 2070 \text{K} \) and pressure is equal to \( p = 1.069 \text{K} \). Chemical composition is given in table 3.

| Table 3. Chemical composition. |
|-----------------------------|
| Chemical component: | Mass fraction |
| CO\(_2\) | 0.103 |
| H\(_2\)O | 0.0124 |
| CO | 0.169 |

The rocket radius is equal to \( r = 8 \text{ cm} \). The nozzle exit radius is assumed to be equal to \( r = 3.81 \text{ cm} \). The nozzle exit velocity isn’t given in the paper [22] so it has been varied. Numerical simulation results for the plume flowfield are presented in figure 6. Spatial two-dimensional distribution in the plane through the axis of the plume for the density, temperature, and mass fraction of chemical species are presented in this figure. This results were obtained for the nozzle exit velocity \( V = 1476 \text{ m/s} \). Comparison of the axial distributions of temperature and mass fraction of chemical species for different nozzle exit velocities ( \( V = 1476 \text{ m/s} \) and \( V = 3000 \text{ m/s} \) ) is given in figure 7.
Figure 6. Spatial distribution of the density (a), temperature (b), $\text{H}_2\text{O}$ (c) and $\text{CO}_2$ (d) mass fractions.

Figure 7. Axial distributions of the temperature (top) and mass fractions of chemical species (bottom) for different values of the nozzle exit velocities ($V = 1476$ m/s (a) and $V = 3000$ m/s (b)).

Spectral signature of the plume for the different angles of observation (broadside and nose on) are given in figure 8. It is considered that in the case of the nose on signature ($\Theta = 0^\circ$) the rocket body partially obscure the radiative plume.
Numerical simulation results for the plume flowfields for different altitudes are given in figure 9. With the increase of the altitude plume significantly expands and the absolute value of temperature on the plume axis is decreased. Comparison of the plume radianc for different altitudes are presented in figure 10.

Figure 9. Comparison of the temperature (left) and H$_2$O mass fraction spatial distribution calculated at H = 5 km (a), H = 10 km (b), H = 20 km (c) altitudes.

Figure 8. Broadside (a) and nose on (b) spectral radianc of the tactical rocket plume.
Figure 10. Spectral radiance of the plume with $\text{B}_2\text{O}_3$ particles and its comparison with data [5].

5. Spectral radiance of the Atlas plume

Numerical simulation of the Atlas rocket plume flowfield was performed with the use of the technique described in the previous section. The boundary conditions for the freestream and nozzle exit regions were taken from the [23]. The specified boundary conditions are given in the table 4.

| Freestream | Nozzle exit |
|------------|-------------|
| Velocity (m/s) | 1476 | 2960 |
| Pressure (Pa) | 278 | 68850 |
| Temperature (K) | 251 | 2230 |
| Mass Fractions: | | |
| $\text{CO}_2$ | 0.000458 | 0.302262 |
| $\text{H}_2\text{O}$ | 0.000000 | 0.272443 |
| $\text{CO}$ | 0.000000 | 0.412135 |
| $\text{N}_2$ | 0.766388 | 0.000000 |
| $\text{O}_2$ | 0.233154 | 0.000028 |
| $\text{H}_2$ | 0.000000 | 0.012194 |
| $\text{OH}$ | 0.000000 | 0.000127 |

Spatial distributions of temperature and density in the Atlas plume are presented in figure 11. Comparison of the axial and spatial distributions calculated with those obtained in the [23], for perfect and chemically reacting gas is given in figure 12. Numerical simulation results presented in this figure were obtained for the laminar case. There is a satisfactory agreement for both (perfect gas and chemically reacting gas) cases.

Comparison of the spectral signature with those obtained by [24] is given in figure 13.
6. Conclusion

Numerical simulation of the plume flowfields and spectral signatures for different altitudes, chemical composition, altitudes and solid particle properties were performed. A satisfactory agreement with published results are obtained. An influence of the altitude and imaginary part of the refractive index on the plume spectral signature was shown.

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Figure 11. Spatial distribution of the temperature(left) and pressure(right) in the plume.

Figure 12. Comparison of the axial (top) and spatial (bottom) distributions with the data [23] for perfect(a) and chemically reacting gas(b).
Spectral signature of the Atlas plume and its comparison to data [24].

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