Modeling of Relaxation Processes in Air Flows behind Shock Waves

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Abstract

Non-equilibrium flows of a reacting five-component air mixture consisting of N_2, O_2, NO, N, O behind shock waves at different altitudes from the earth's surface at different speeds of the incoming flow are numerically investigated. One-temperature mathematical model of non-equilibrium air flows is applied. The distributions of flow quantities behind the shock wave fronts are obtained and analyzed. The relaxation lengths of flow quantities are compared for various Mach numbers and altitudes.

Keywords 1

Hypersonic, chemical kinetics in air, shockwave

1. Introduction

An important problem in physical and chemical gas dynamics is the study of non-equilibrium kinetics in air flows behind shock waves. The impact of non-equilibrium kinetic processes on distributions of flow quantities is required, for example to correctly predict stand-off distance of shock wave in super- and hypersonic flows when spacecrafts enter the Earth's atmosphere.

Air is considered as a five-component mixture consisting of N_2, O_2, NO, N, O in which the various kinetic processes occur. These processes include chemical reactions of dissociation and recombination and chemical exchange reactions. They are as follows:

- Dissociation and recombination

$$N_2 + M \rightleftarrows N + N + M, \quad O_2 + M \rightleftarrows O + O + M, \quad NO + M \rightleftarrows N + O + M; \tag{1}$$

- Chemical exchange reactions

$$N_2 + O \rightleftarrows NO + N, \quad O_2 + N \rightleftarrows NO + O. \tag{2}$$

Here, $M = N_2, O_2, NO, N, O$.

There are various approaches to the description of non-equilibrium flows including one-temperature approach [1], multi-temperature approach [2, 3], and multi-level approach [4]. The most detailed description of non-equilibrium kinetics is given by the multi-level approach. However, the computational costs of this approach are extremely high due to the need to solve a large number of equations [5]. Therefore, the study uses a more simple from the computational point of view one-temperature approximation, which requires less time for calculations and is often used to solve applied problems of hypersonic flows [6, 7].

The sudy does not take into account the processes of ionization and electronic excitation, since the temperature ranges at which the influence of these processes on the flow parameters is weaker than the influence of vibrational excitation and chemical reactions is considered.

The vibrational energy ε_i^c of molecule c at level i is calculated based on the anharmonic Morse

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$$\varepsilon_c^0 + hc(\omega_e^c - \omega_e^c x_e^c - \omega_e^c x_e^c i)i, \qquad \varepsilon_c^0 = hc\left(\frac{1}{2}\omega_e^c - \frac{1}{4}\omega_e^c x_e^c\right),$$

where h is Plank constant, c is speed of light, ω_e^c and $\omega_e^c x_e^c$ are spectroscopic constants that characterize the frequency and anharmonicity of molecular vibrations, $c = N_2,\ O_2,\ NO.$

For the populations of the vibrational levels of air components, assuming that the distribution of molecules over the vibrational levels is quasi-stationary, and corresponds to the Boltzmann distribution, the flowing relationships are written

$$n_c^i(T) = \frac{n_c}{Z_c^{vibr}(T)}\exp\left(-\frac{\varepsilon_c^i}{kT}\right), \quad {}_c^{vibr} = \sum_i \exp\left(-\frac{\varepsilon_c^i}{kT}\right).$$

This study focuses on numerical simulation of non-equilibrium flows of a reacting five-component air mixture behind a shock wave at different heights from the earth's surface and at different velocities of the incoming flow. To assess the applicability of equilibrium thermodynamic models for calculating macro-parameters behind a shock wave, the lengths of relaxation zones are considered for various initial conditions.

2. Mathematical model

Within the framework of the one-temperature approach, the determining macro-parameters of the flow are the numerical densities of molecules and atoms n_{N_2}, n_{O_2}, n_{NO}, n_N, n_O, the gas temperature, T, and the macroscopic velocity, v.

2.1. Governing equations

The system of governing equations for macro-parameters contains the equations of one-temperature non-equilibrium chemical kinetics, the equations of conservation of momentum and total energy. In the case of a stationary one-dimensional flow of an inviscid and non-heat-conducting mixture, these equations have the form [7]

$$v\frac{dn_M}{dx} + n_M\frac{dv}{dx} = R_M^{2\leftrightarrow 2} + R_M^{2\leftrightarrow 3}; \tag{3}$$

$$\rho v\frac{dv}{dx} + \frac{dp}{dx} = 0; \tag{4}$$

$$v\frac{dE}{d\sim} + (p+E)\frac{dv}{dx} = 0. \tag{5}$$

Here, $\rho = \sum_M n_M m_M$ is density of the mixture, $p = nkT$ is pressure, $n = \sum_M n_M$ is numerical density of the mixture, E is total energy of a unit of volume. The total energy is represented as

$$E = E^{tr} + E^{rot} + E^{vibr} + E^f,$$

where $E^{\langle r}, E^{rot}, E^{vibr}, E^f$ are translational, rotational, vibrational energy and the energy of formation of particles of the mixture per unit volume.

2.2. Initial conditions

The one-temperature approach assumes that only the chemical composition is preserved at the shock wave front, so the relation on the shock wave are valid. The equations take the form

$$\rho v = \rho^{(0)} v^{(0)}; \tag{6}$$

$$\rho v^2 + p = \rho^{(0)}\left(v^{(0)}\right)^2 + p^{(0)}; \tag{7}$$

$$\frac{E+p}{\rho} + \frac{v^2}{2} = \frac{E^{(0)}+p^{(0)}}{\rho^{(0)}} + \frac{\left(v^{(0)}\right)^2}{2}. \tag{8}$$

The superscript 0 indicates the parameters before the shock front.

2.3. Relaxation terms

To close the system (3)-(5) it is necessary to express the relaxation terms in terms of macro-parameters, $R_M^{2\leftrightarrow 2}$ and $R_M^{2\leftrightarrow 3}$. The terms $R_M^{2\leftrightarrow 2}$ describe changes in the numerical densities of molecules due to exchange reactions (2) and have the following form [7]:

$$R_{N_2}^{2\leftrightarrow 2} = n_{NO} n_N k_{NO\to N_2}^{N\longrightarrow O} - n_{N_2} n_O k_{N_2\to NO}^{O\longrightarrow N}, \quad R_{O_2}^{2\leftrightarrow 2} = \varnothing_{NO} n_O k_{NO\to O_2}^{O\longrightarrow N} - n_{O_2} n_N k_{O_2\to NO}^{N\longrightarrow O},$$

$$R_{NO}^{2\leftrightarrow 2} = -R_{N_2}^{2\leftrightarrow 2} - R_{O_2}^{2\leftrightarrow 2}, \quad R_N^{2\leftrightarrow 2} = -R_{N_2}^{2\leftrightarrow 2} + R_{O_2}^{2\leftrightarrow 2}, \; R_O^{2\leftrightarrow 2} = R_{N_2}^{2\leftrightarrow 2} - R_{O_2}^{2\leftrightarrow 2},$$

where $k_{N_2\to NO}^{O\longrightarrow N}$ and $k_{O_2\to NO}^{N\longrightarrow O}$ are temperature-dependent coefficients of the rate of direct exchange reactions, $k_{NO\to N_2}^{N\longrightarrow O}$ and $k_{NO\to O_2}^{O\longrightarrow N}$ are coefficients of the rate of reverse reactions (2).

The terms $R_M^{2\leftrightarrow 3}$ describe the processes of dissociation and recombination (1) and take the form

$$R_{N_2}^{2\leftrightarrow 3} = \sum_M n_M \left(n_N^2 k_{rec,N_2}^M - n_{N_2}^M k_{N_2,diss}^M\right), \quad R_{O_2}^{2\leftrightarrow 3} = \sum_M n_M \left(n_O^2 k_{rec,O_2}^M - n_{O_2}^M k_{O_2,diss}^M\right),$$

$$R_{NO}^{2\leftrightarrow 3} = \sum_M n_M \left(n_N n_O k_{rec,NO}^M - n_{NO}^M k_{NO,diss}^M\right), \quad R_N^{2\leftrightarrow 3} = -2R_{N_2}^{2\leftrightarrow 3} - R_{NO}^{2\leftrightarrow 3},$$

$$R_O^{2\leftrightarrow 3} = -2R_{O_2}^{2\leftrightarrow 3} - R_{NO}^{2\leftrightarrow 3},$$

where $k_{N_2,diss}^M$, $k_{O_2,diss}^M$, $k_{NO,diss}^M$ are gas temperature-dependent coefficients of the rate of dissociation of molecules $N_2,\ O_2,\ NO$ in collision with a particle M, k_{rec,N_2}^M, k_{rec,O_2}^M, $k_{rec,NO}^M$ are coefficients of the rate of recombination of atoms to form molecules $N_2,\ O_2,\ NO$.

To calculate the one-temperature coefficients of the rate of direct exchange and dissociation reactions, the Arrhenius law was used, which is valid in a thermally equilibrium gas

$$k_{c,eq}^M = A_M T^n \exp\left(-\frac{E_\alpha}{kT}\right),$$

where $E_\alpha(D_c)$ is activation energy in the case of exchange reactions and dissociation energy in the case of decay reactions, A_M and n are constant factors that are determined in a number of studies based on experimental data or detailed numerical calculations. The dissociation rate coefficients recommended in [8] are used.

The coefficients of the rate of recombination and reverse exchange reactions are calculated using the relations following from the principle of detailed balance [7]. These relations are as follows

$$k_{rec,N_2}^M = k_{N_2,diss}^M \left(\frac{m_{N_2}}{m_N^2} \frac{h^2}{2\pi kT}\right)^{3/2} Z_{N_2}^{rot}(T) Z_{N_2}^{vibr}(T) \exp\left(\frac{D_{N_2}}{kT}\right),$$

$$k_{rec,O_2}^M = k_{O_2,diss}^M \left(\frac{m_{O_2}}{m_O^2} \frac{h^2}{2\pi kT}\right)^{3/2} Z_{O_2}^{rot}(T) Z_{O_2}^{vibr}(T) \exp\left(\frac{D_{O_2}}{kT}\right),$$

$$k_{rec,NO}^M = k_{NO,diss}^M \left(\frac{m_{NO}}{m_N m_O} \frac{h^2}{2\pi kT}\right)^{3/2} Z_{NO}^{rot}(T) Z_{NO}^{vibr}(T) \exp\left(\frac{D_{NO}}{kT}\right),$$

$$k_{NO\to N_2}^{N\to O} = k_{N_2\to NO}^{O\to N} \left(\frac{m_{N_2} m_O}{m_{NO} m_N}\right) \frac{Z_{N_2}^{rot}(T) Z_{N_2}^{vibr}(T)}{Z_{NO}^{rot}(T) Z_{NO}^{vibr}(T)} \exp\left(\frac{D_{N_2} - D_{NO}}{kT}\right),$$

$$k_{NO\to O_2}^{O\to N} = k_{O_2\to NO}^{N\to O} \left(\frac{m_{O_2} m_N}{m_{NO} m_O}\right) \frac{Z_{O_2}^{rot}(T) Z_{O_2}^{vibr}(T)}{Z_{NO}^{rot}(T) Z_{NO}^{vibr}(T)} \exp\left(\frac{D_{O_2} - D_{NO}}{kT}\right),$$

where $\boldsymbol{Z_c^{rot}(T)}$ is statistical sum of rotational degrees of freedom, $\boldsymbol{Z_c^{vibr}(T)}$ is statistical sum of the vibrational degrees of freedom.

3. Results and discussion

The results are obtained using numerical methods. At the beginning, a system of equations (6)–(8), is solved to find the gas-dynamic parameters of the mixture behind the shock wave front. Further, the obtained values are used as initial data for solving the system of equations (3)–(5) using the implicit Geer method [9].

To determine the parameters at different altitudes of flight, data from standard atmosphere [10] are applied. They set the average numerical values of the main atmospheric parameters for altitudes from -2 000 m to 1 200 000 m or latitude 45°32′33″, corresponding to the average level of solar activity.

The considered flight speeds vary from M=10 to M=16. The upper limit is due to the fact that at Mach numbers above M=16 the temperature and pressure immediately behind the shock layer have values at which the ionization processes begin to significantly affect the flow [11].

Figures 1–7 show the dependences of temperature and velocity on the distance behind the shock wave front, respectively, at different flight altitudes. Fragments a correspond to altitude of *h*=0 km, fragments b correspond to altitude of *h*=10 km, fragments c correspond to altitude of *h*=24 km, and fragments d correspond to altitude of *h*=60 km.

It can be seen from Figures 1 and 2 that with an increase in the Mach number of the incoming flow, the changes in temperature and velocity become much more significant and pass much faster. As the altitude increases, the temperature and velocity values behind the shock wave decrease.

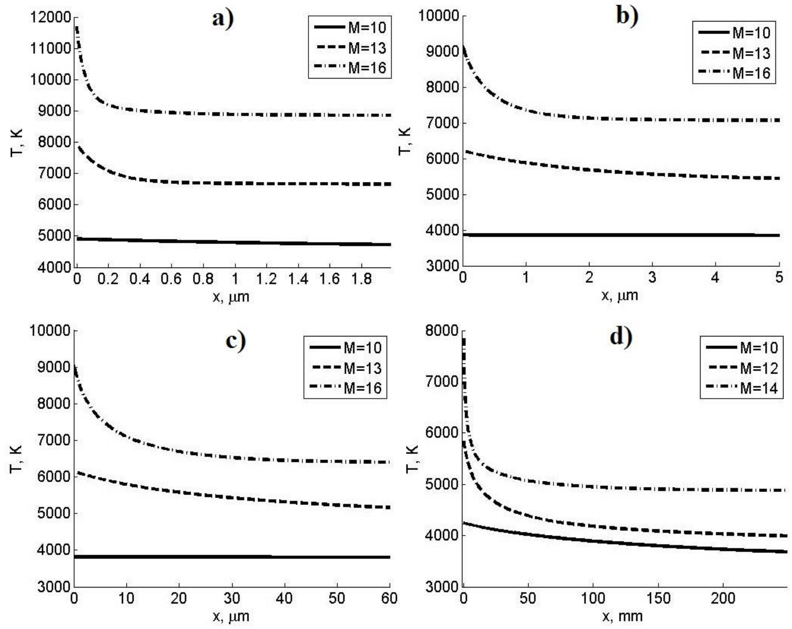

Figure 1: The dependence of the temperature on the distance behind the shock wave front for altitudes *h*=0 km (a), *h*=10 km (b), *h*=24 km (c), *h*=60 km (d)

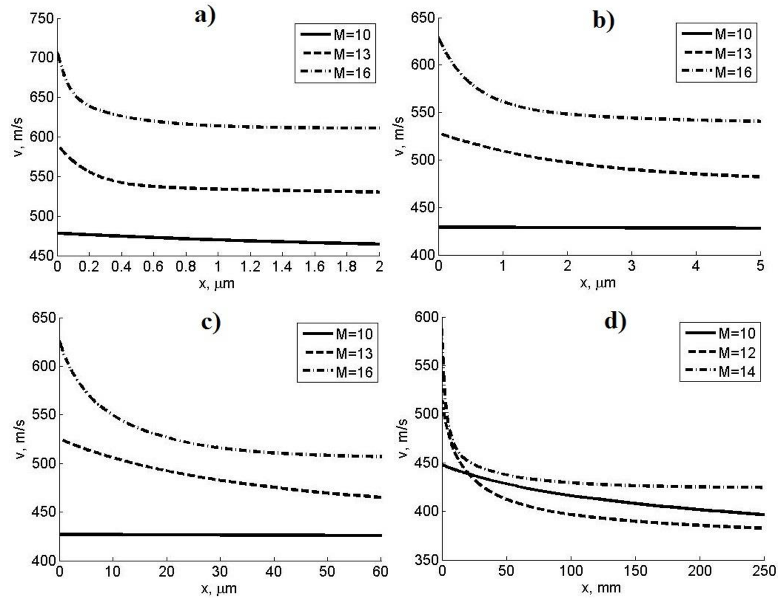

Figure 2: The dependence of the velocity on the distance behind the shock wave front for altitudes *h*=0 km (a), *h*=10 km (b), *h*=24 km (c), *h*=60 km (d)

When moving away from the wave front, the numerical densities of the molecules N_2 and O_2 decrease, as can be seen in Figures 3 and 4. With an increase in the Mach number, the concentration of components in the air mixture N_2 and O_2 falls behind the shock wave, the sharpness of the concentration change increases. At an altitude of 10 km (Figure 3b and 4b), the concentration of components increases, but already at an altitude of 24 km (Figures 3c and 4c), the concentration of components decreases and continues to decrease with increasing altitude.

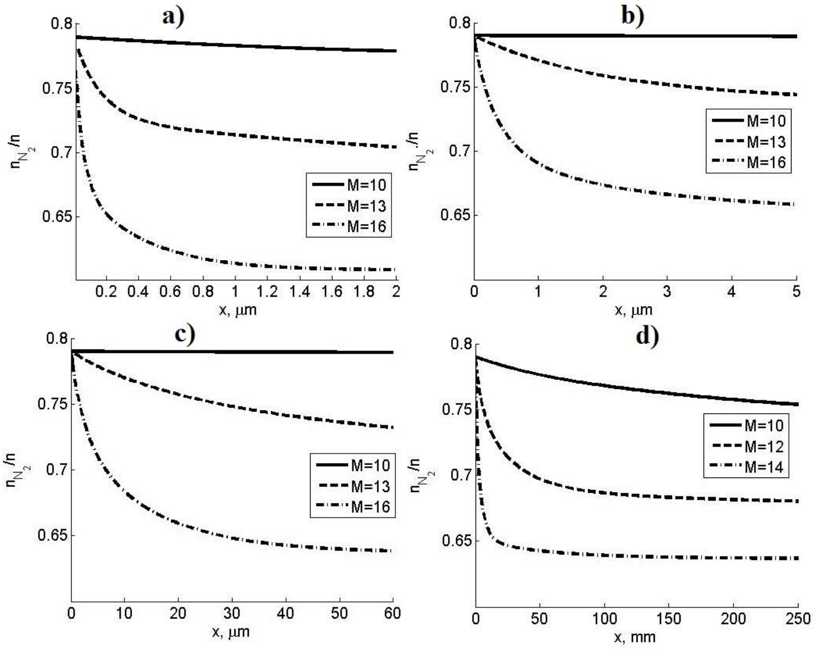

Figure 3: The dependence of the N_2 concentration on the distance behind the shock wave front for altitudes *h*=0 km (a), *h*=10 km (b), *h*=24 km (c), *h*=60 km (d)

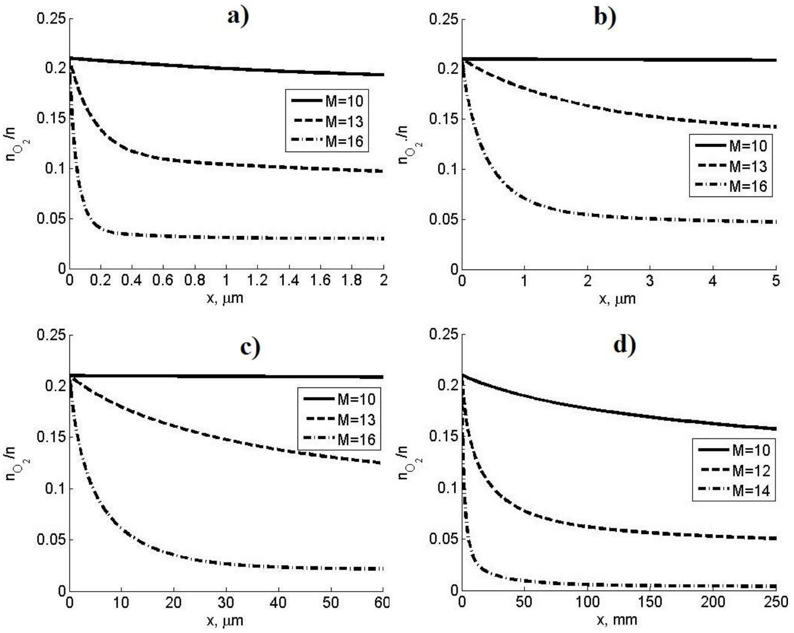

Figure 4: The dependence of the O_2 concentration on the distance behind the shock wave front for altitudes *h*=0 km (a), *h*=10 km (b), *h*=24 km (c), *h*=60 km (d)

Figures 5 and 6 demonstrate that the numerical densities of N and O components increase with distance from the shock front. An increase in the Mach number leads to an increase in the concentration of N and O components in the air mixture behind the shock wave, the sharpness of the concentration change increases. As the altitude increases, the concentration of nitrogen atoms N decreases, and the concentration of oxygen atoms O decreases at 10 km, but already at 24 km there is an increase in the concentration.

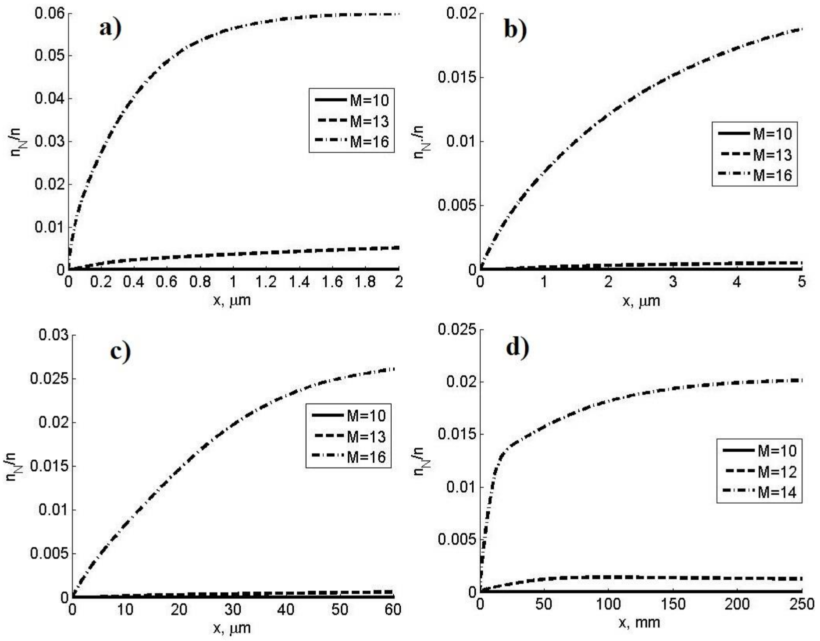

Figure 5: The dependence of the N concentration on the distance behind the shock wave front for altitudes h=0 km (a), h=10 km (b), h=24 km (c), h=60 km (d)

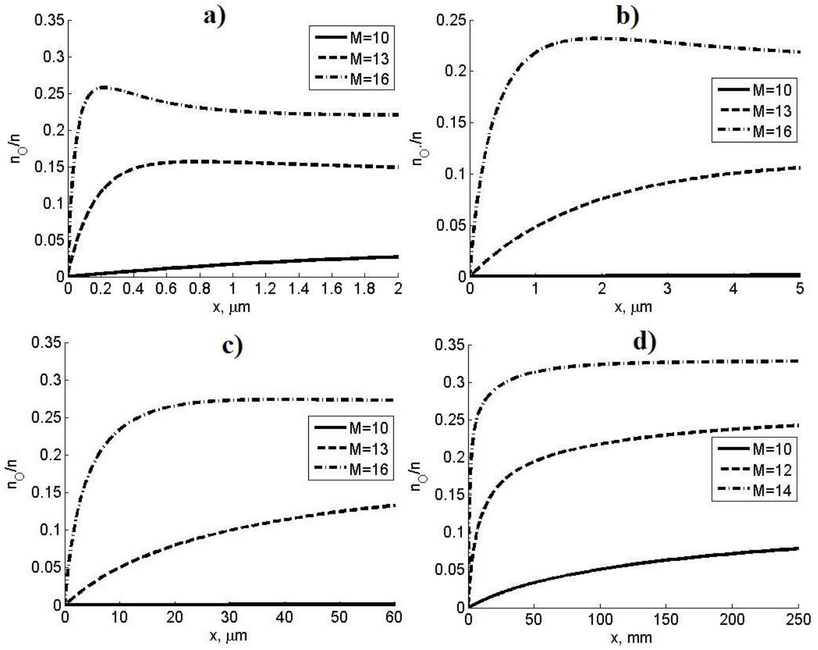

Figure 6: The dependence of the O concentration on the distance behind the shock wave front for altitudes h=0 km (a), h=10 km (b), h=24 km (c), h=60 km (d)

Figure 7 shows the change in the numerical density of NO component depending on the distance from the shock wave. The numerical density of the molecules increases as they move away from the front. The numerical density also increases as the Mach number increases. As the altitude increases, the concentration of nitric oxide molecules decreases. It is possible to note a non-monotonic change in the numerical density of nitrogen oxide molecules with parameters before the shock wave equal to the parameters of the atmosphere at an altitude of 60 km.

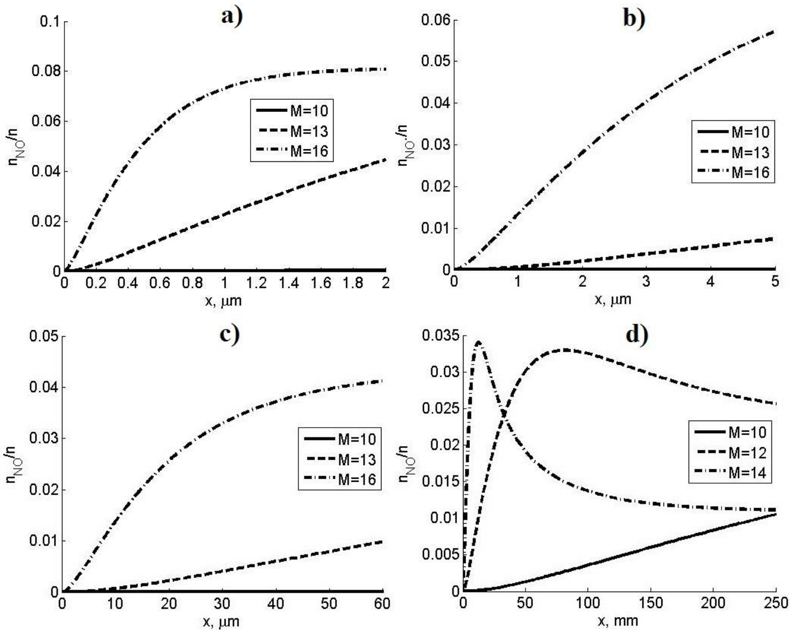

Figure 7: The dependence of the NO concentration on the distance behind the shock wave front for altitudes *h*=0 km (a), *h*=10 km (b), *h*=24 km (c), *h*=60 km (d)

4. Conclusion

Distributions in the flow parameters of the air flow behind shock waves at different altitudes from the Earth's surface at various Mach numbers of the incoming flow are numerically computed and investigated.

The study has shown that when moving away from the shock wave front, the concentrations of the components of the air mixture N_2 and O_2 decrease, and the concentrations of N, O and NO increase. As the velocity of the incoming flow increases, the temperature and velocity behind the shock wave increase, the concentrations of N_2 and O_2 molecules decrease, and the concentrations of N, O and NO increase. At low pressures, there is a non-monotonic change in the numerical density of nitrogen oxide NO molecules.

A comparison is made of the lengths of the zones of variation of the flow parameters behind the shock waves. Studies have shown that the length of the zone of change in the concentration of the mixture components can exceed the length of the zone of change in the flow macro-parameters behind the shock wave. In cases where there is no need to obtain the results of changes in the concentration of mixture components, the zone of numerical calculations of the flow can be reduced to the length of the zone of change in gas dynamic variables.

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