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The strong shock wave structure in low density gas mixtures flows over cylinders and bands

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Abstract. This paper presents the results of direct Monte Carlo simulation of transversal hypersonic flow of gas mixture around a cylinder and band. The data for structure of disturbed flow, density, velocity, temperature distribution and energy distribution function of the heavy atoms colliding with the body are determined over a wide range of Knudsen numbers, temperatures of the body, absorption probabilities, and mixture composition. Deceleration of heavy atoms in the shock layer in front of the cylinder and band was the main objective of analysis.

Introduction

Development of modern vacuum technology brings out new problem statements for rarefied gas dynamics. For many years, the simulation techniques for gas supersonic flow around a body (for modes ranging from free-molecular to the continuum one) were developed for aerodynamic engineering of spaceships in earthly atmosphere [1,2]. A gas mixture flow around a vehicle flying in rarefied atmosphere has a more narrow interest, usually for analysis of processes in exotic atmospheres on some planets or for vehicle flights at very high velocity with possible gas dissociation and ionization [3]. Presently, many problems of rarefied gas aerodynamics have been solved successfully and became less urgent than in previous decades.

But in the framework of vacuum technology development, the gas dynamic problems very often arise for mixtures (including polyatomic gases) that flow around a solid body and undergo complex physical-chemical transformations. In some technologies of film deposition and generation of nanoparticles, more stress is made on the methods of acceleration of polyatomic molecules in a light gas with adiabatic expansion [4-6]. Heavy molecules that are separated in the rarefied disturbed zone near the body and yet approaching the target surface, may retain a considerable amount of kinetic energy (several eV) gained by acceleration in the light gas jet; this energy facilitates the film deposition process.

Supersonic flow around a body by a rarefied gaseous mixture with very disparate molecular masses and collision cross-sections is accompanied by several simultaneous nonequilibrium processes:

longitudinal and transversal gas separation, nonequilbrium in internal energies, and even anisotropy for translational temperatures. The study of those processes is of academic interest aimed to a search and description of new effects in gas separation, heat and momentum transfer, molecular beam deposition. Application of methods of nonequlibrium gas dynamics for production of new materials is an exciting perspective.

If one would try to make analysis of those processes using the solution for a system of Navier-Stokes equations for the case of no thermodynamic equilibrium, this approach is doomed to wrong results. But if the simulation is based on the Boltzmann equation for this kind of flow where phenomena of different scale take place (ranging from continuum conditions to the molecular mean free path), this approach will create a lot of difficulties in construction of algorithms and computations. The direct simulation Monte Carlo (DSMC) method becomes a universal and efficient tool for solution of this kind of problems [7].

The review is devoted to analysis of insufficiently explored phenomena occurring during gas mixture (with disparate molecular masses) flow around a infinite band or cylinder. Among unlimited variety of different problem statements, we focused on those satisfying the criterions simplicity, scientific novelty, informativeness and at least shed some light on features of most interesting and important technological processes. Computations were carried out for a binary mixture of monoatomic gases with helium and xenon as an example. The velocity range for the incident flow was narrowed to the vicinity of the Mach number (for helium) equal to 5. According to the energy conservation law, in the flow with this Mach number the most part of enthalpy in the stagnation chamber (more than 89% of enthalpy) is converted into a kinetic energy of ordered motion of the jet. This is close to reasonable conditions of heavy gas acceleration in deposition processes. To estimate the influence of temperature factor on the flow pattern, the ratio of the target temperature to the translational temperature of flow was varied in the range 3-30. The “condensation” coefficient of heavy particles on the target surface was varied from 0 to 1. Simulation covers the area of transient flow modes with the Knudsen number from 0.01 to 10.

For the considered conditions, the situation is far from formation of a separate shock wave zone. It is just merged with the compressed layer. The front part of this compressed layer may be considered as a shock wave with the more degree of convention the higher is a Knudsen number. That is why the disturbed zone upstream the body is called a shock layer in this text.

1. Problem statement and DSMC solution

Simulation for helium-xenon mixture flow is made within an orthogonal coordinate system (X,Y,Z). The X axis is directed along the undisturbed flow and the Y and Z axes are directed perpendicularly to the flow. The coordinate origin is on the symmetry axis of disturbed flow. In our modeling for cylinder, the Z axis coincides with the cylinder axis, and if we deal with a plate, the plate is infinite along Z.

Let us consider the undisturbed flow as a plane-parallel one. A flat source is situated in the cross-section $x=x_1< 0$. The gas particles are absorbed completely downstream at the distance $x=x_e$ is the supersonic area. In view of problem symmetry the plane y=0 is assumed to be mirror and the plane $y=y_e$ has the boundary conditions of undisturbed flow. The back flow of particles to the source plane is fully absorbed.

The following boundary conditions for gas mixture flow are given on the source plane: the translational temperature T_S, velocity V_S, number density n_S. The surface temperature of the cylinder or band is constant and equal to T_w.

The present study was focused on features of binary gas flow (with strongly disparate molecular masses) around a cylinder or a band. In this simulation helium and xenon (mass ratio is 32.78) were used as the model of molecular particles. The law of particle interaction was described by the VSS model [7] with parameters corresponding to helium and xenon. The interaction between particles and cylinder surface was described by the diffusion model, corresponding to particle reflection at the surface temperature. It was assumed also that helium particles always underwent diffuse reflection from the surface, and xenon with probability α was absorbed by the cylinder surface and with probability (1-α) it underwent diffuse reflection. It was assumed also that helium and xenon had the same temperature and macroscopic velocity in the source plane. The concentrations in the mixture were described by the ratio of number densities $\Theta = n_S^{Xe} / n_S^{He}$. Hereafter, the superscripts Xe and He corresponded to the parameters for xenon and helium, respectively.

In reducing the problem to a non-dimensional form, one can use the temperature T_s, density n_s, the most probable thermal velocity at the temperature T_S, and the mean free path of molecules L. The value of L is calculated for parameters of undisturbed helium flow. After that, the problem has the following key parameters: the Mach number (for helium) in undisturbed flow M_S^{He}, temperature factor T_w/T_S, concentration Θ, probability of xenon absorption on the surface α, and the Knudsen number as a characteristic of rarefaction Kn=L/l, where l is the characteristic size for the body.

Obviously, the size of simulation zone (in particularly, the position of planes $x=x_e$ and $y=y_e$) may be significant for flow formation. Our analysis has demonstrated that starting from certain x_e and y_e the disturbed flow around a body is almost independent of the size of the simulation zone. These are the proper distances being used in our computations. The stationary solution of problem is of most interest.

In our simulation, we calculated the following macroparameters for each component of the mixture: density, the Mach number, temperature (velocities): along the flow - T_x (V_x), normal to flow - T_y (V_y) and T_z (V_z), total temperature $T=(T_x+T_y+T_z)/3)$, and also heat flux Q between the gas and target surface.

Numerical experiments have demonstrated that the accuracy in heat flux calculation depends strongly on grid mesh, time step, and number of particles in modeling. Therefore the requirements of a reasonable accuracy for every time step makes a demand for particle number from 1000 to 4000 thousand particles. The stationary solution has been built after many time steps. When we estimated the macroparameters of the light component flow, every cell included several million particles. The computation accuracy was controlled by varying the grid mesh and time intervals of DSMC algorithm. The solution was considered “accurate” if the further downsizing of grid mesh and time step did not produce any change of calculated parameters within the statistic error.

Flow around a cylinder

The gas rarefaction is characterized by the Knudsen number Kn=L/d, where d is the cylinder diameter. Computations have been carried out for values Θ = 0.01, 0.05, and 0.1. The Mach numbers for undisturbed flow at those concentrations were 5.73, 7.92, and 9.86, respectively. Streamlines and Mach number contours for pure helium (Θ = 0) at the Knudsen number of 0.01 are plotted in Fig. 1; it presents the general structure of the distribution zone almost equal to the condition of continuum gas flow around the cylinder. In all cases below, we give quantitative illustrations for parameter field only through the parameter profile along the symmetry axis. This is enough for justification of all important conclusions. Fig. 2 shows the parameter profiles on the flow axis for conditions of flow depicted in Fig. 1 (for more illustrative estimation of the effect of gas rarefaction and gas composition). The area of the cylinder in all figures is depicted by two vertical lines. The following features are notable on the profiles: a distinctive shock wave, almost isotropic behavior of translation temperatures near the stagnation point upstream the cylinder and significant temperature nonequilibrium behind the cylinder.

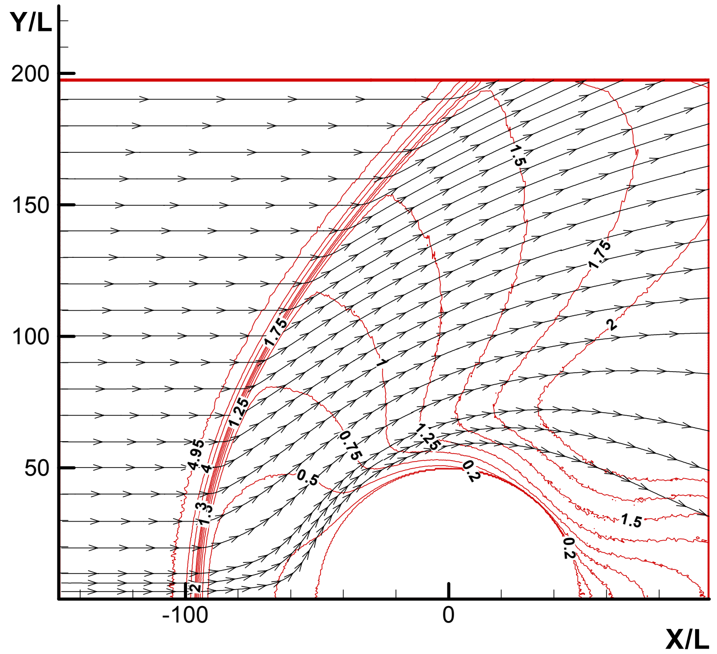


FIGURE 1. Streamlines and Mach number contours for pure helium (Θ = 0) at the Knudsen number of 0.01.

Introduction of a heavy component into helium flow causes flow restructuring and qualitative change in the parameter distributions in the flow due to inertial gas separation and slow inter-gas collisional relaxation. This is illustrated by Fig.3 for distributions of helium/xenon parameters at the Knudsen number equal to 0.1 and 5, for xenon concentration 10%, temperature factor 9.33, and zero absorption for the heavy gas. At the Knudsen number of 0.1, in the shock layer upstream the cylinder a high-temperature zone with strong nonequilibrium is formed. The maximum value of xenon average temperature may be 75 times higher than in the undisturbed flow; the longitudinal temperature T_x increases by a factor of 180. This is quite understandable: at prominent slippage of the heavy gas under high rarefaction, this gas is retarded by itself in the shock layer. The stagnation temperature of the accelerated gas exceeds the flow temperature by 274 times. Some part of stagnation energy is transferred to helium; its temperature upstream the cylinder is by 2.5 times higher than the stagnation temperature. As a consequence of the above, the gas density is also lower than the equilibrium one.

In general, these nonequilibrium features are also typical for the flow with the Knudsen number equal to 5, with the only difference that the shock layer is deprived on a hint for the gas dynamic compressed layer at thermodynamic equilibrium. The cylinder is surrounded by a scattered gas with almost free-molecular flow.

Another flow peculiarity is the longitudinal gas separation: it is seen in the form of a zone with high xenon concentration near the cylinder surface (due to inertial slippage of the heavy gas).

These charts also present the gas parameter distributions downstream the cylinder. These data are interesting from the point of view of the nonequilibrium analysis in this zone and significant for accurate calculation of force and heat impact of the flow on the cylinder.

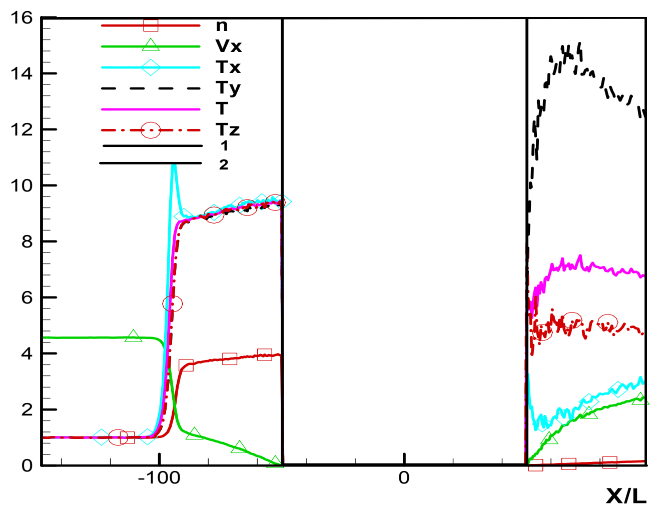


FIGURE 2. Distribution of density n, velocity V_x, temperature in directions T_x, T_y, T_z, and average temperature T along the plane of symmetry for Kn = 0.01 at T_w/T_S=9.33 for flow of pure helium. Lines 1 and 2 show the size of the cylinder.

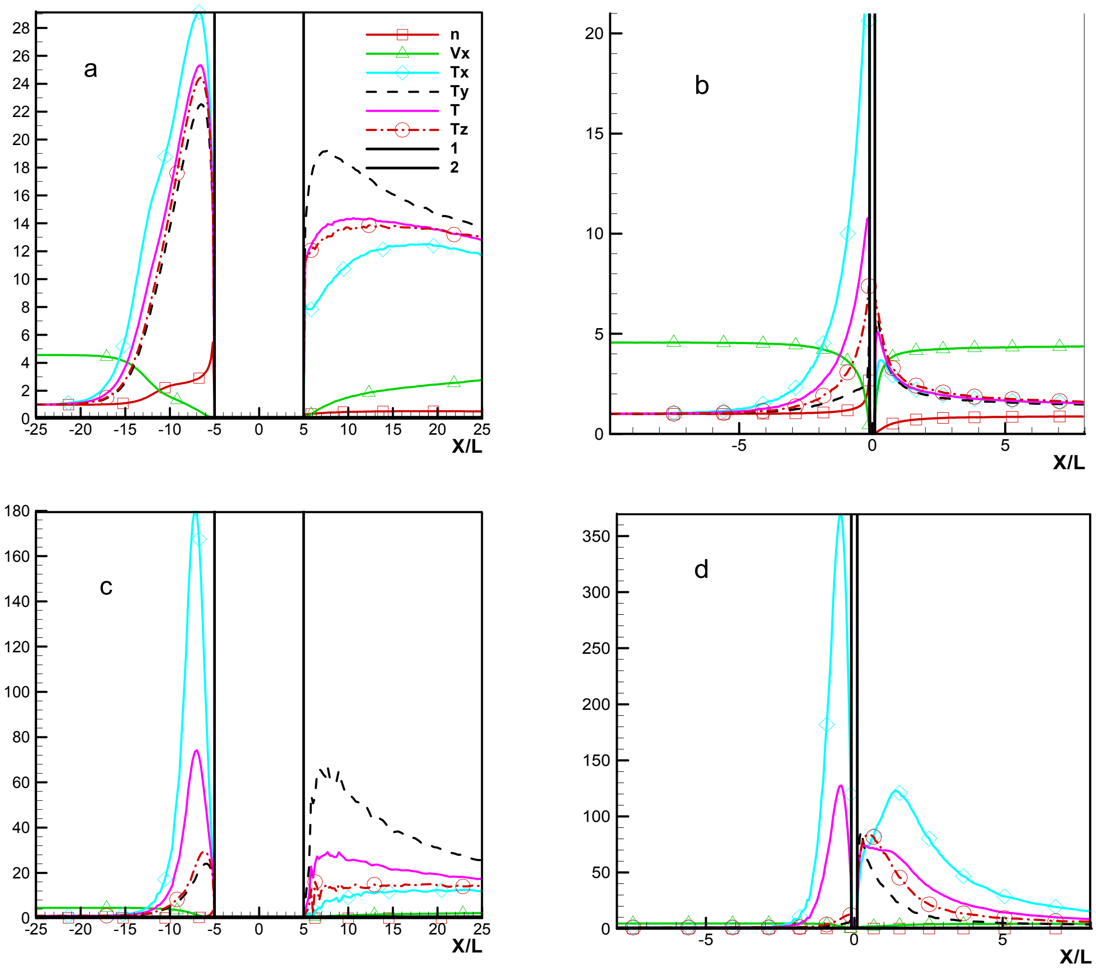


FIGURE 3. Distribution for He (a,b) and Xe (c,d) of density n, velocity V_x, temperature in directions T_x, T_y, T_z, and average temperature T along the plane of symmetry for Kn = 0.1 (left) and 5 (right) at T_w/T_S=9.33 , α=0 for the flow of gas mixture Θ=0.1. Lines 1 and 2 show the size of the cylinder.

The heat transfer peculiarities were studied for different Knudsen numbers at the xenon concentration of 1% and 10%. Fig.4 shows the heat flux (for xenon and helium) for the cases of xenon full absorption or total rebound. The unexpected phenomenon is a decline in heat flux for helium at increasing Knudsen number. This fact can be explained only by a lower helium temperature near the cylinder surface due to a smaller number of xenon-helium collisions.

The detailed information about the heavy particle energy at the target surface is very interesting for choice of optimal operation modes of devices for gas-jet film deposition. The DSCM simulation gives the essential qualitative ideas about the translation energy of xenon atoms colliding with the cylinder surface at the concentration Θ =0.1 (Fig.5). This figure presents the distribution function for xenon atoms interacting with the cylindrical surface for the Knudsen number ranging from 0.1 to 5 and two values of concentration α. For α = 0 one can observe the transition of atomic energy from almost unimodal distribution at Kn = 5 to bimodal distribution at Kn = 1 and again to unimodal distribution at Kn = 0.1 with a peak at the zero velocity. For α=1 we do not observe any bimodal distribution for xenon atom energy. The maximum energy in distribution peaks may be so high that this initiates collisional ionization.

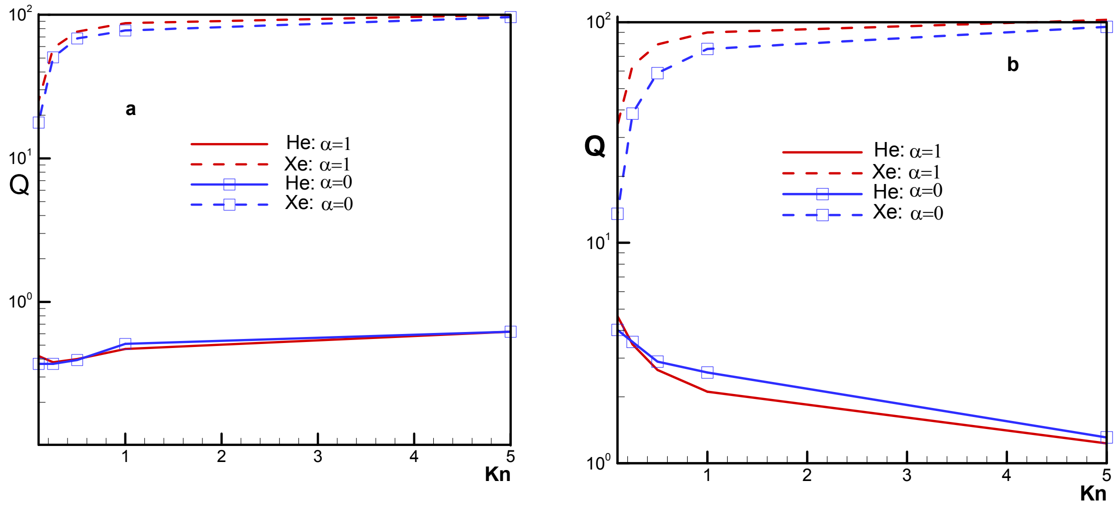


FIGURE 4. Dependences of heat flux on the Knudsen number Kn for Xe (dashed line) and He (solid line). Θ=0.01 (a) and Θ=0.1 (b). T_w/T_S=9.33

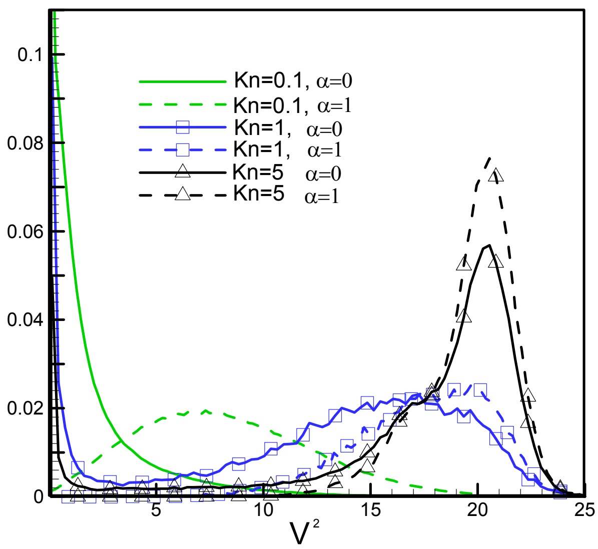


FIGURE 5. Distribution function of V^2 xenon atoms colliding with the cylinder for different Knudsen numbers and absorption probabilities α. Θ=0.1.

These data not only illustrate the impressing effect of nonequilibrium hypersonic binary gas flow around a cylinder but also demonstrates the high efficiency of mathematical apparatus of direct statistic simulation.

Transversal flow around an infinite band

The rarefaction for gas flow around an infinite band is characterized by the Knudsen number Kn = L/h, where h is the band width.

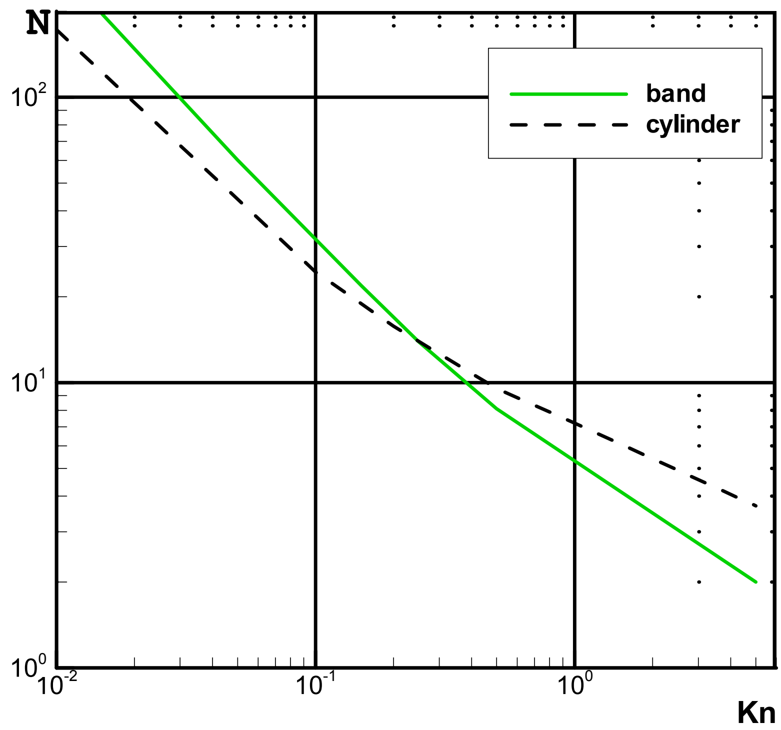


FIGURE 6. Helium mean free path number in the shock wave and the compressed layer at T_W/T_S = 9.33.

One of the search-tasks was the simulation of conditions for heavy particles transportation towards the plate surface. In this framework, the key significance belongs to deceleration of heavy particles in a shock wave and in a compressed layer (which are merged at a low density). A simple and comprehensive characteristic for "permeability" of this combined shock layer is the "optical thickness" of the layer given as the number N of atom free paths per thickness layer. For definition sake, the front boundary of this combined shock layer is accepted as a point where the helium velocity decreases by 10%. For example, Fig.6 shows the dependence of N in pure helium at M_S = 5 for the

Knudsen number ranging from 0.01 to 10. This plotting allows us to estimate the deceleration of xenon atoms (at low concentration) in the shock layer. On other hand, this dependence demonstrates that even at Kn=10 the thickness of shock structure is determined by more than one free path of the helium atom. The figure also presents the similar data for a flow around a cylinder.

The processes in mixtures like He + Xe, the gases with very disparate atomic masses, illustrate the peculiarities of the nonequilibrium processes in the gas mixture flow. Herein we present the simulation results for xenon concentrations $\Theta^{Xe} = n_S^{Xe}/(n_S^{He} + n_S^{Xe})$ 0.01 and 0.03. The Mach number for those mixtures was 5.7 and 7, respectively. Numerical experiments were carried out for the Knudsen numbers equal to 1.0, 0.3, and 0.1.

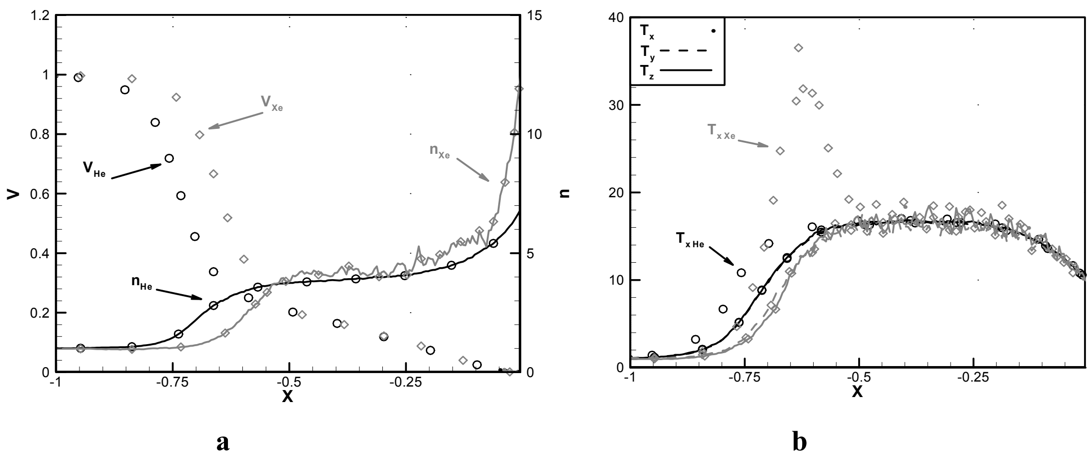


FIGURE 7. Density (a) and temperature (b) profiles for small Knudsen number. Kn=0.01; T_W/T_S=9.33; Θ^{Xe} = 0.03.

The exception was the simulation of a shock layer structure at a low Knudsen number (Kn = 0.01). The simulation objective was to see how gas separation occurred for the conditions when the carrier gas (helium) had almost continuum flow (Fig.7 a, b). For this simulation, the xenon concentration was 3% with the condition of full reflection from the surface. The strong enrichment in Xe for the compressed layer near the band testified to a strong effect of gas separation in the vicinity of stagnation point. The illustrative manifestation of nonequilibrium was a high difference in the gas temperatures T_x in the front of the compressed layer.

Quite a specific flow pattern is formed near the band at high rarefaction conditions. Fig. 8 a,b shows the simulation for velocity, density and temperatures for the gases inside the shock wave at Kn = 0.1, T_w/T_S = 10, xenon concentration equal to 3% (full reflection from the surface). In this case, the shock wave exhibits complete merging with the compressed layer. The longitudinal gas separation is well marked. This is obvious for density profiles for helium and xenon. The temperature separation of gases (Fig. 8b) is accompanied by a strong temperature anisotropy for both gases. The similar nonequilibrium effects take place also for other conditions of transient flow modes.

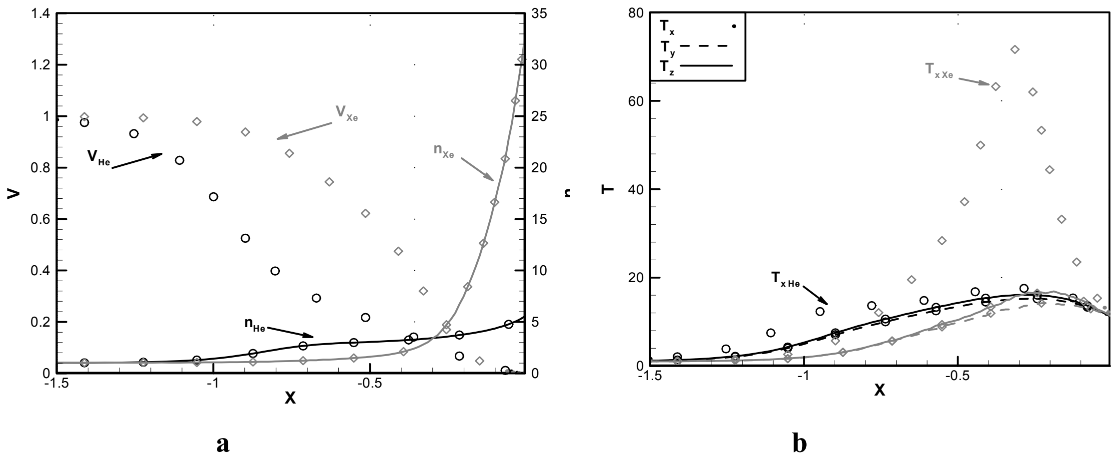
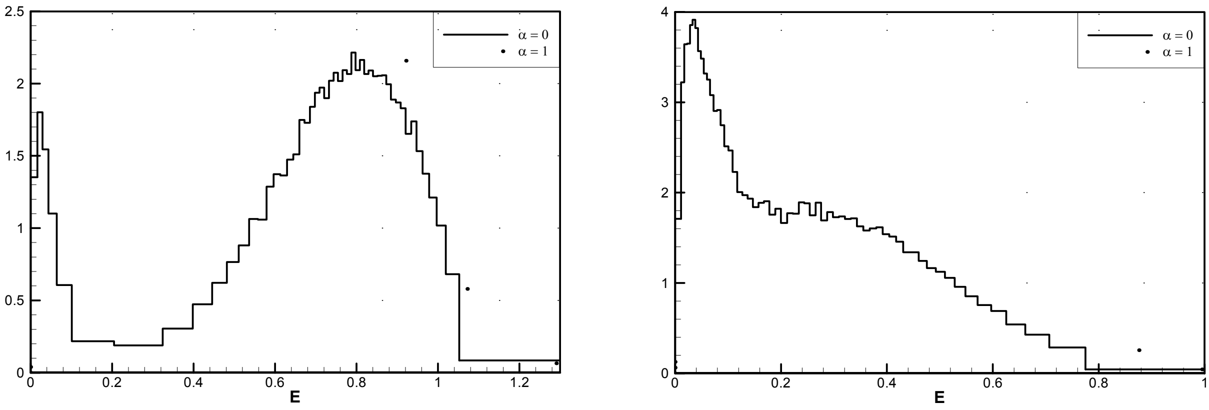


FIGURE 8. The changing of velocities and densities (a) and temperatures (b) in the front of the band at Kn=0.1; T_W/T_S=10; Θ^{Xe} = 0.03 without xenon absorption.

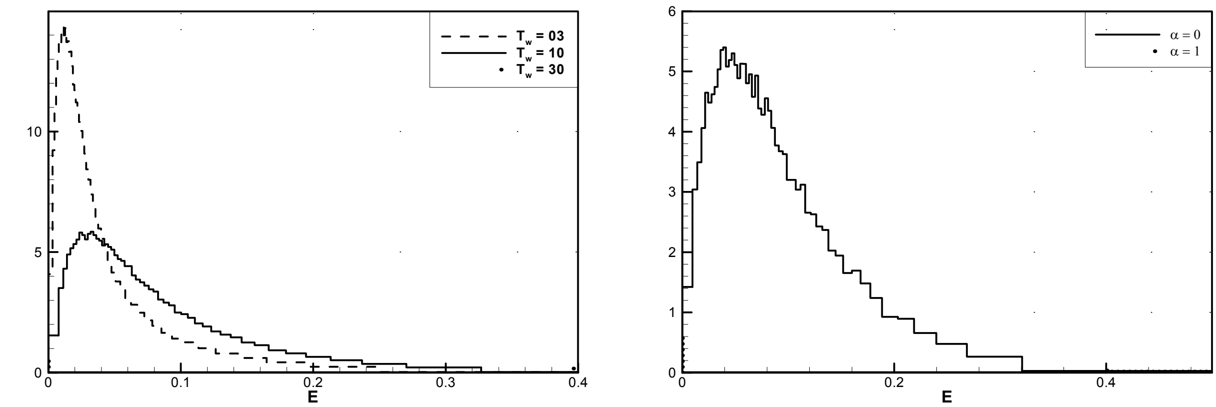
Analysis of the calculation results for macroparameters is not so informative for an understanding of energy interaction of heavy atoms with the target surface. Fortunately, the DSCM method has the feature of direct calculation of the energy distribution function for atoms colliding with the surface (this has also been demonstrated for a flow around the cylinder). In turn, this opens an easy way to optimization of gas-jet inertial deposition of heavy particles on the target surface.

Fig.9 a,b illustrates the xenon atom energy distribution that heat the surface with velocity T_W/T_S = 30, Θ^{Xe} = 0.03, different Knudsen numbers (Kn = 1.0 and 0.3) and different variants of coefficient for heavy particles absorption α. Herein the energy E is normalized to the kinetic energy of xenon in undisturbed flow. For a shock layer, the equilibrium (Maxwell) distribution of translation motion of xenon atoms (corresponding to undisturbed flow) is transformed into the distribution depicted in Fig. 9 a,b. The general feature of these distributions as shifting of maximum of distribution to lower energies is pronounced even at high rarefaction (Kn = 1.0) and becomes significant at the Knudsen number Kn = 0.3 (maximum of the equilibrium distribution of energy in undisturbed flow which is normalized to one). For the full absorption (α = 1) we obtain a unimodal distribution, but for full reflection the distribution becomes bimodal one, with a cloud of xenon atoms with low energy. Obviously, the stagnation effect is stronger at low Knudsen numbers.



a b

FIGURE 9. Energy distribution of Xe atoms colliding with the band at different absorption coefficient α
a) Kn=1.0; T_W/T_S=30; Θ^{Xe} = 0.03
b) Kn=0.3; T_W/T_S=30; Θ^{Xe} = 0.03



a b

FIGURE 10. Energy distribution of Xe atoms colliding with the band at Kn=0.1; Θ^{Xe} = 0.03
a) at full sorption and different band temperature,
b) at T_W/T_S=30 and different sorption.

For a denser flow and Kn=0.1 (Fig.10 a,b) and any condition of the temperature factor (the xenon concentration is the same) the plot exhibits only unimodal distributions with a maximum shifted to lower energies. This is a manifestation of strong stagnation for heavy atoms in a rather rarefied gas flow. The quantitative features of the energy distribution are obvious from the plot and easy for the understanding.

The simulation data were the basis for more general and comprehensive information in the form of the most probable energy of xenon atoms colliding with the surface E_{mp} vs. the Knudsen number (Fig.11). We also plotted this dependence for the case of full reflection of xenon atoms from the surface at different temperature factors. One qualitative feature of this dependence is the fact of stronger deceleration at a lower temperature due to the formation of a denser cloud of xenon atoms. The more important observation is the task to retain the energy of accelerated atoms for successful deposition requires to conduct the process with flow at the Knudsen number higher than 1. Even at Kn = 1.0 the value of E_{mp} decreases by almost 20%. This figure also presents the data for flow around the cylinder.

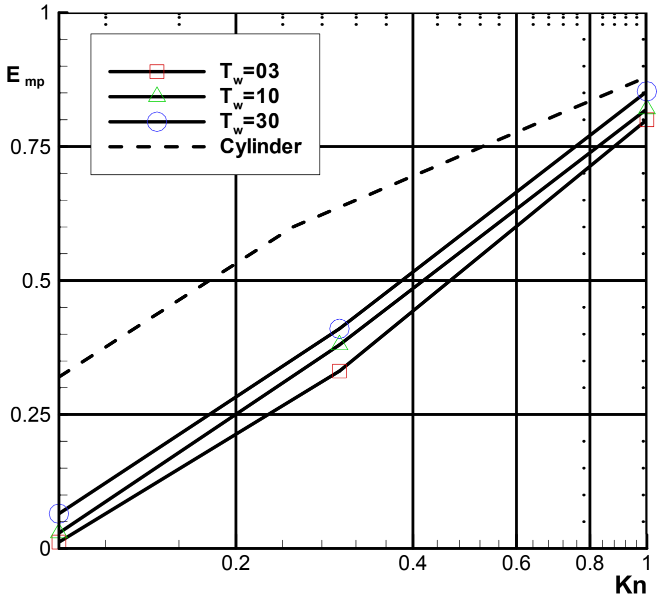


FIGURE 11. Dependence of most probable Xe energy E_{mp} on Knudsen number at different band temperatures (Θ^{Xe} = 0.03)(solid lines) and cylinder (Θ = 0.1, T_w/T_S=9.33) (dashed line) .

Conclusion

The direct simulation Monte Carlo method provides excellent possibilities to study supersonic gas mixture flows around bodies with full information on molecular kinetics in the range of transition regime from continuum flow to free molecular one.

The results of modeling transversal hypersonic flow around the cylinder and band have shown that the nonequilibrium effects in front of bodies are essential in all conditions at Kn > 0.01.

The striking effect of temperature boom in front of bodies deserves special attention for different practical applications. It has been shown that heavy gas deceleration is meaningful even at Knudsen number of the order of 1.

Acknowledgements

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