

## Kinetic Simulation of Air Flow Around Hollow Cylinder Flare Configuration

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### Abstract

Kinetic approach was used to study the shock wave/boundary layer interaction in diatomic gases and gas mixtures. The effect of non-equilibrium processes on the steady state solution was studied.

### Introduction

One of the most important aspects of the rarefied gas simulation is a high value of the Knudsen number  $Kn = \lambda/L$  in the flow and, consequently, the requirement of solution of the Boltzmann equation

$$\frac{\partial f_i}{\partial t} + \mathbf{v}_i \nabla f_i + \frac{\mathbf{a}_i}{m_i} \nabla_v f_i = \left( \frac{\delta f_i}{\delta t} \right)_{coll} \quad (1)$$

The situation is usually more complicated because most of the practical applications involve consideration of diatomic gases, which can be excited vibrationally and rotationally and for which ionization, dissociation and chemical transformations are possible. A need to model non-equilibrium hypersonic flows motivated the development<sup>1</sup> of numerical techniques to treat such problems. Nowadays the DSMC method<sup>2</sup> is *de facto* the standard method for rarefied gas dynamics, where the state of the rarefied gas flow, which is presented by an assembly of molecules, is determined by collisional dynamics of finite number of model particles and, hence, hold potential for providing information on flows where collisional rate is not sufficient to maintain equilibrium energy distribution.

This paper presents results of numerical study shock wave/boundary layer interaction and influents of relaxation of internal energy on the structure of gas flow.

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### Numerical Approach

The fundamental assumption of the Direct Simulation Monte Carlo method is the assumption of decoupling molecular collisions from translational motion. During a given time step, all model particles travel over computational domain and the neighboring particles which are residents of the same collisional cell are considered as prospective partners for collision. Such an approach result in correct description of collisional dynamics only when translational and collisional phases are separated by the time interval  $\Delta t \ll \min(\tau_m, \tau_c)$ , where  $\tau_m$  and  $\tau_c$  are corresponding characteristic times and require that the collisional cell be small that the spatial variation is negligible.

In the Monte Carlo simulations of rarefied flows, a realistic but sufficiently simple molecular model is required. Several models were proposed to model inverse power law

$$F = \kappa/r^\eta \quad (2)$$

as the potential for gas molecular interaction. It was shown<sup>6,7</sup> that the Variable Soft Sphere (VSS) model gives a better approximation of the viscosity coefficient and is more appropriate for the cases where viscosity is important. The model results in collisional a cross section which is a function on relative speed

$$d = d_{ref} \left( \frac{c_{r,ref}}{c_r} \right)^v \quad (3)$$

$$b = d \cos^\alpha \left( \frac{\chi}{2} \right) \quad (4)$$

$$\sigma_T = 2\pi \int b db = \pi d^2 \quad (5)$$

$$\sigma_\eta = \frac{2}{3} \frac{6\alpha}{(\alpha+1)(\alpha+2)} \pi d^2 \quad (6)$$

$$\sigma_D = \frac{2}{\alpha+1} \pi d^2 \quad (7)$$

where  $b$  is the impact parameter,  $d$  is an energy dependent “diameter” and  $\sigma_T$ ,  $\sigma_\eta$  and  $\sigma_D$  are total, viscosity and diffusion cross sections. The model’s constants can be obtained, for example, by fitting experimental viscosity and diffusion coefficients.

Various techniques have been proposed<sup>11,12,13,14,15</sup> for the evaluation of the elastic collision rate. Non-Time Counter method was used for modeling of elastic collisions in the current studies. For a small time step, the number of collision pairs is small relative to the total number of model particles. So, it is good to assume that each particle can collide only once during the time step, which considerably simplifies the numerical implementation of the computational procedure. A pair of model particles from the same cell is considered for possible collision irrespective of position. The probability of collision is defined in the form

$$P = g \sigma_t \frac{w \Delta t}{d_k} \quad (8)$$

where  $w$  is the particle’s “weight” and  $d_k$  is the collision’s cell measure. Transport cross section is used in DSMC to define the local value of collisional frequency, which could cause incorrect evaluation of collision rates for processes that has cross sections close to the transport one. A pair that is selected should also be tested for chemical reactions and internal energy exchange, whose probability is defined as a ratio to the elastic collision probability.

One of the most important advantages of the DSMC method is its ability to model gas flows in absence of thermodynamical equilibrium. For the considered problem, only the modeling of rotational relaxation process is important and the continuous distribution function (9) for rotational energy can be assumed. A number of models of internal energy relaxation were developed<sup>16</sup>, however, most of the models are phenomenological in nature. The Larsen-Borgnakke model was used to model rotational energy relaxation processes in the current studies.

$$f_{\varepsilon_i} \propto \varepsilon_i^{\zeta/2-1} \exp\left(-\frac{\varepsilon_i}{kT}\right) \quad (9)$$

In the case of linear molecules, which are used in the current simulation, the number of rotational degrees of freedom is  $\zeta = 2$ . Rotational collision number, i.e. the number of collisions that are required to equilibrate rotational and translational degrees of freedom, is taken to be  $Z_r = 5$ . Temperature dependent<sup>16,17</sup> rotational collision number (10)

$$Z_r(T) = \frac{Z_{r,\infty}}{1 + \frac{\pi^{3/2}}{2} \left(\frac{T^*}{T}\right)^{1/2} + \left(\frac{\pi^2}{4 + \pi}\right) \frac{T^*}{T}} \quad (10)$$

also can be used. Here  $Z_{r,\infty}$  and  $T^*$  are model constants which depends on the gas properties. It can be shown<sup>16</sup> that the probability of rotational-translational energy exchange  $\phi_r = 1/Z_r$  for the chosen molecular model is expressed in the form

$$\phi_r \frac{Z_{r,\infty}}{Z_r} = 1 + \frac{\Gamma(2-\omega)}{\Gamma(3/2-\omega)} \sqrt{\frac{2kT^*}{m_r g^2}} \frac{\pi^{3/2}}{2} + \frac{\Gamma(2-\omega)}{\Gamma(1-\omega)} \frac{2kT^*}{m_r g^2} \left(\pi + \frac{\pi^2}{4}\right)$$

An important feature of the algorithm is prohibiting multiple relaxation, which means that only one internal mode of only one collision partner can be relaxed during collision. Such an approach guarantees<sup>3</sup> that the rotational mode’s relaxation exactly matches Jean’s law. It is assumed that each mode is not very far from the equilibrium state. This allows us to use temperature description for relaxation processes.

In addition to colliding with others molecules, model particles can interact with the solid surface. Models of gas/surface interactions in the DSMC method can be described in terms of distribution function for reflected particles. Maxwell model of diffuse reflection with full accommodation was used in the current simulation, where the internal parameters of reflected particles are generated due to equilibrium distribution function with given temperature and zero bulk velocity. In reality, the particle/surface interaction should be described with accommodation coefficient (11) which lies somewhere between secular and diffusion reflection limit<sup>18</sup> and can be found experientially.

$$\alpha_e = \frac{T_r - T_g}{T_s - T_g} \quad (11)$$

Maxwell-Boltzmann distribution is used in the generation of internal parameters for particles entering the computational domain.

## Optimization techniques

The accuracy of the numerical results, which are obtained by the DSMC method, is very dependent on the size of sample and, finely, on the number of model particles per cell. So, in order to get effective use of computer resources, it is desirable to get the distribution of model particles over the domain close to uniform. This problem is especially important at the case of 2D axisymmetrical simulation. There are several methods<sup>19</sup> to control the distribution of particles: variation of time steps, grid manipulation and direct variation of particles weights. The last approach is the most widely used method in the case of axis symmetric computations: the model particle's weight is chosen proportionally to the distance from the symmetry axis, which decreases the variation of its distribution.

Several techniques could be used to decrease total computational cost of steady state simulation. Due to methodology of the DSMC method, a steady state solution can be obtained as the limit of unsteady flow simulation, which is a considerable part of the computation time. To get faster convergence, it is possible, starting with low accuracy, to improve it gradually as the current solution converges to the final result. One of the possible implementations<sup>5</sup> of the strategy is to gradually increase total number of model particles as the flow pattern converges to the steady state. Another scheme was developed and implemented in the current work. The simulation is conducted on a set of meshes with different level of refinement, starting with a coarse grid at the very beginning and maintaining the number of model particles per cell in desired limits. As the number of collisional cells and particles employed increase, the resolution of the computational procedure improves both in terms of flow macroparameters distribution and captured physical processes. Such a technique decreases the actual time of the simulation dramatically.

Use of parallel computers can significantly increase the range of application of the DSMC method. Effective use<sup>4</sup> of such computational systems can be achieved only with careful load balancing. The procedure of static load balancing, which was implemented in the current implementation, ensures equal number of model

particles among all processors used in the simulation. Such a method doesn't take into account geometry or symmetry considerations and results in a crude work balancing. But taking into account the simplicity of the method and the fact that the initial condition, usually, is very far from the steady state, this is a good choice to balance the load at the beginning of the simulation. As the solution converges to the steady state, some corrections in the load balancing are required. A dynamic load balancing procedure is used to correct the processor load.

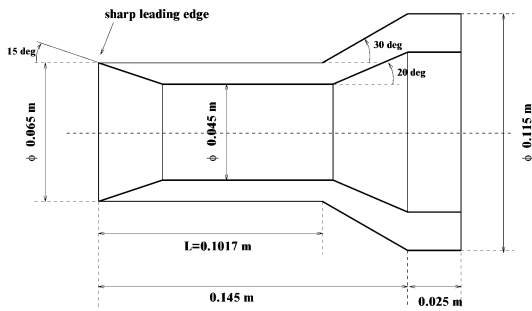
## Results and Discussions

Supersonic gas expansion into a vacuum results in a rapid decrease of the gas temperature and density. The decrease of the collision frequency results in a violation of equilibrium between internal and translational degrees of freedom. For low temperatures, vibrational degrees of freedom are not excited, and the energy exchange occurs only between rotational and translational degrees of freedom.

The freestream conditions are presented in Table 1. The geometry configuration of the hollow cylinder flare is presented in Fig. 1. As the problem is axis-symmetric, only half of physical domain is considered. In order to get correct a description of the collision dynamics, the cell's size was adapted to the local mean free path value. Unstructured meshes are the most natural way to capture the effect of complex geometry on the gas flow pattern. In the current simulation triangle/tetrahedral unstructured meshes<sup>8</sup> were used. In order to investigate influence of the grid resolution of the numerical solution, the simulation was repeated on a set of meshes with different level of resolution. The problem was solved on meshes with  $(4 \div 16) \times 10^5$  collisional cells employing  $(10 \div 45) \times 10^6$  model particles.

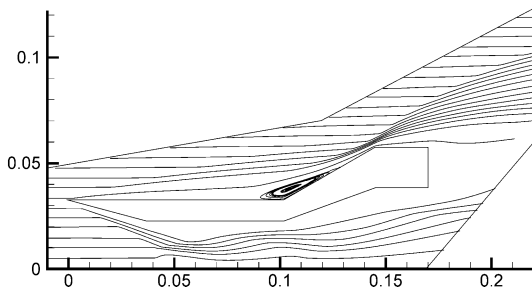
$p_\infty, Pa$	$T_w, K$	$M_\infty$	$T_\infty, K$
6.3	51	9.91	293

**Table 1 Freestream condition and the wall temperature**

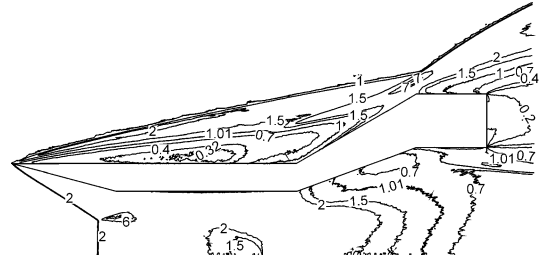


**Fig. 1 Hollow-cylinder flare configuration**

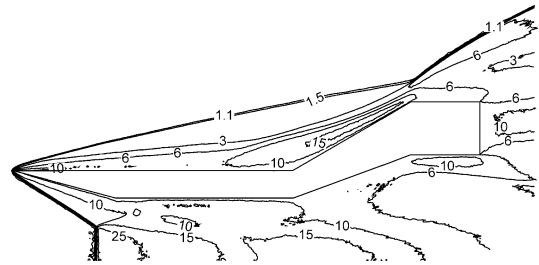
In order to study influence of the non-equilibrium processes on the numerical solution, two sets of models were considered: with and without rotational degrees of freedom. To validate the model, nitrogen flow was considered and the obtained solutions were compared with numerical results<sup>9,10,12,20</sup>. The computational domain and the streamlines of the gas flow are presented on Fig. 2. The isolines of gas macroparameters are presented on the Figs. 3,4. In addition to the simulation in the nitrogen environment, the problem was solved for the oxygen/nitrogen mixture (78%  $N_2$ , 22%  $O_2$ ), which is our model the air flow. Results of the simulation are given on Fig. 5-9. The main difference in the solutions is the displacement of the front of Mach reflection.



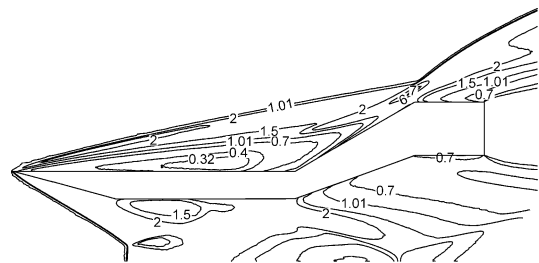
**Fig. 2 Streamlines**



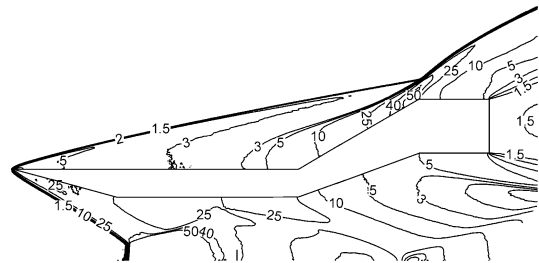
**Fig. 3  $N_2$  density number isolines. Model without RT relaxation.**



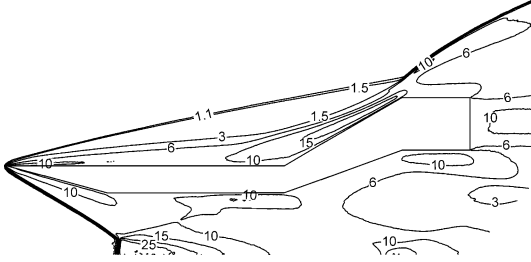
**Fig. 4  $N_2$  temperature isolines. Model without RT relaxation.**



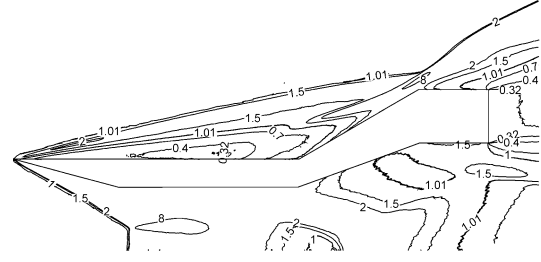
**Fig. 5 density number for the air flow. Model without RT relaxation.**



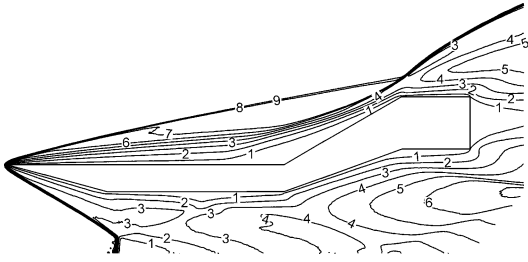
**Fig. 6 pressure isolines for the air flow. Model without RT relaxation.**



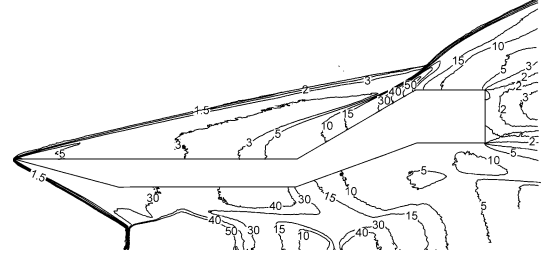
**Fig. 7 Temperature isolines of the air flow. Model without RT relaxation.**



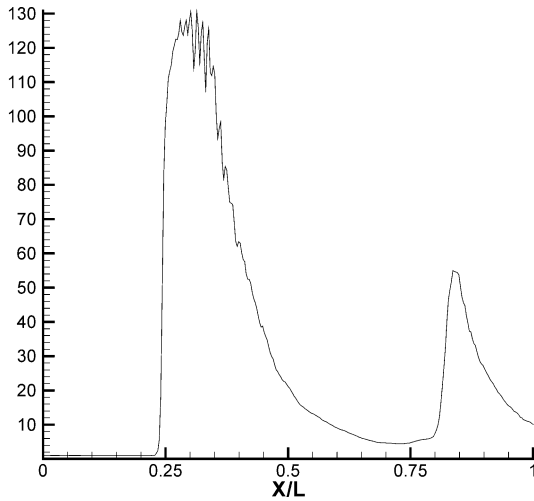
**Fig. 10 Density number isolines for nitrogen flow with modeling RT transitions**



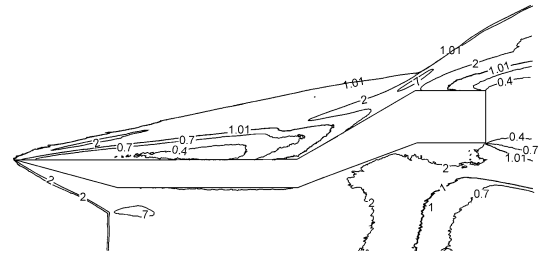
**Fig. 8 The Mach number isolines in the air flow. Model without RT relaxation.**



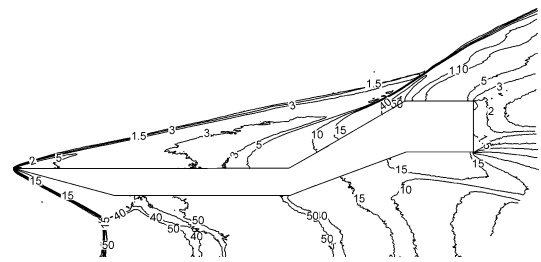
**Fig. 11 Pressure isolines for nitrogen flow with modeling RT transitions**



**Fig. 9 Pressure distribution along the center line. Air flow simulation without RT relaxation.**

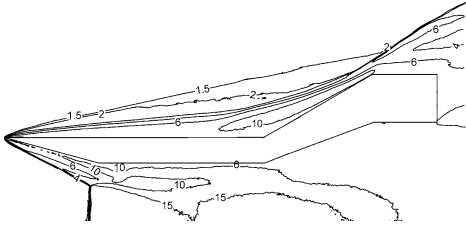


**Fig. 12 Density number isolines for air flow with modeling RT transitions**



**Fig. 13 Pressure isolines for air flow with modeling RT transitions**

Analogous simulations were performed with modeling of the rotational-translational transitions. Because initial temperature is much higher than the characteristic rotational temperature, classical Borgnakke-Larsen model with equilibrium distribution function for internal (9) energy was used. The results of simulation of the problem for nitrogen environment and for the case of air are presented on Figs 10-14.



**Fig. 14** Temperature isolines for nitrogen flow with modeling RT transitions

## Conclusion

The problem of simulation of the shock wave/boundary layer interaction for the hollow cylinder configuration was considered. The problem was solved for nitrogen and air environments. It was shown that the change of gas flow composition result in considerable change in the gas macroparameters distribution and especially on the position of the front of Mach reflection. Influence of the rotational-translational relaxation was studied. It was found that assumption of frozen rotations degrees of freedom result in considerable changes in the number density distribution for the both cases.

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