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Monte Carlo Simulation Method for Solving Gas Dynamics Kinetic Problems

N. Nurlibaev, V. Yanitskiy — USSR

New weighting schemes of the statistical method for a computer simulation of flows of neutral and chemically reacting gas mixtures are proposed. In what follows are given results of these calculations.

1. The direct statistical method for simulation of rarefied gas flows [1,2] is widely used in aerodynamics. There are different schemes of this method. Their common idea consists in a substitution of the real gas medium for an assembly of finite and comparatively not large number of model particles. Each particle is characterized by phase coordinates of its own and problem solution is realized by a computer simulation of particle motion, particle interactions and interactions between particles and the boundaries of the calculated domain.

Consider the algorithm structure as a numerically stochastic model of the Boltzmann equation. Suggest that physical space is divided into cells with small volume V while continuous time t is replaced for discrete time t_α, and, at any moment t_α, the cell with number j contains $N_{\alpha,j)}$ particles with velocities $\{C_1, \ldots C_{N(\alpha/j)}\}$.

The evolution calculation of this model, for a short time interval Δt, is realized in two stages:

Stage 1 — All cells of the physical space are succeedingly considered and particle collision simulation is carried out in each cell. However, particle spatial location within cells is not taken into account and particle velocities change only.

Stage 2 — Here particle motion, at a distance proportional to the time interval Δt and velocities C_i, is modelled as well as particle interaction with the physical boundaries.

When solving spatially homogeneous problems, Stage 2 is excluded from the algorithm and only Stage 1 is realized, the latter being repeatedly applied to the system as a whole.

The basic characteristics of various schemes are included in Stage 1 of the algorithm. The works refered to in this paper employ simulation schemes, regarding collisions of a series of $N(N$-$1)/2$ Bernouli trials [3,4]. New weighting schemes for the simulation of the kinetics of physical-chemical processes in multicomponent gas are built on such a basis. Gas mixtures are often characterized by a great difference between the component concentration, whereas the ratio between the latter can vary in time and/or space. The difference between component concentrations in weighting schemes is accounted for in such a manner that each particle A_l^i (here $l=1,\ldots,$ S — species of particles and $i=1, \ldots, N_l$ — particle number in species l) is given an additional phase characteristic η_l^i, i. e. a. "statistical weight" which represents the instantaneous portion of the real concentration for a given particle. However, the weight of each particle of a given species and in a neutral mixture is one and the same, proportional to real concentrations. Such weighting models are called "equipresented" — i. e. the quantity N_l of simulated particles A_l^i in all species are equal to one another (exactly or approximately) regardless of the ratio between real concentrations of

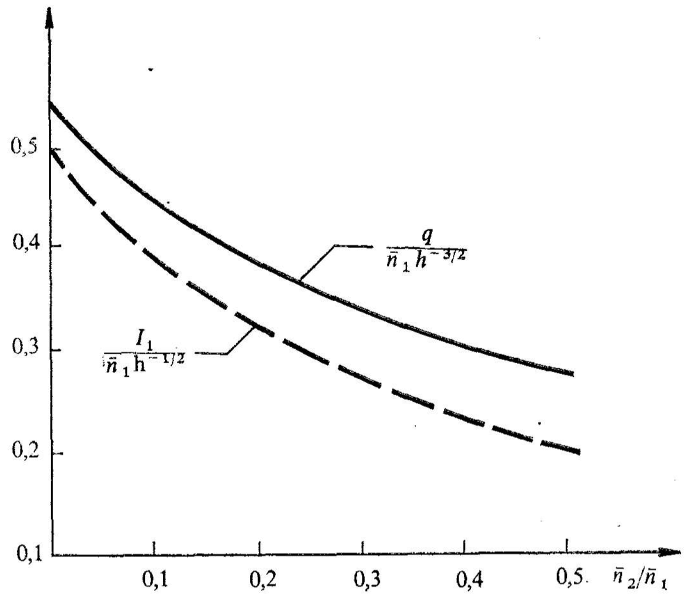

Fig. 1

the mixture components. Particle weights in the simulation scheme are included in the collision probability and in formulas for macroparameter calculation.

Bird [1] realized for the first time in practice the idea of "equipresentability" by including such a concept in his collision simulation scheme, but regarding only mixtures of chemically neutral gases. The weighting modification of the scheme was realized, employing Bernouli trials, for neutral [5—7], as well as for chemically active mixtures [8, 9].

2. An interesting set of problems arise when investigating nonequilibrium processes of evaporation-condensation. These processes often occur in practice in the presence of a neutral gas which molecules do not condense on the surface and do not evaporate from it. Moreover, such a mixture affects the velocity of evaporation, condensation and energy fluxes. Such a problem is analysed in [6], where a model problem of precondensation is solved, ragarding the presence of a neutral admixture. Neutral gas is present between two infinite parallel plates, whereas the gas average concentration $\bar{n}_2$ is less than the vapor concentration $\bar{n}_1$. Plates are with different temperatures, $T_b/T_0=4$, and hence a vapor flux is formed, which molecules collide with each other and with molecules of the neutral mixture. The relation between mass fluxes I_1 and energy fluxes q $(h_b=m/2kT_b)$, on one hand, and the ratio between concentrations of the neutral admixture and vapor $\bar{n}_2/\bar{n}_1$, on the other, is given in Fig. 1. The molecules of both mixture components are of one and the same masses and diameters. The effective Knudsen number is equal to 0,2 and parameter β, which controls the intensity of precondensation, is equal to 0, 1.

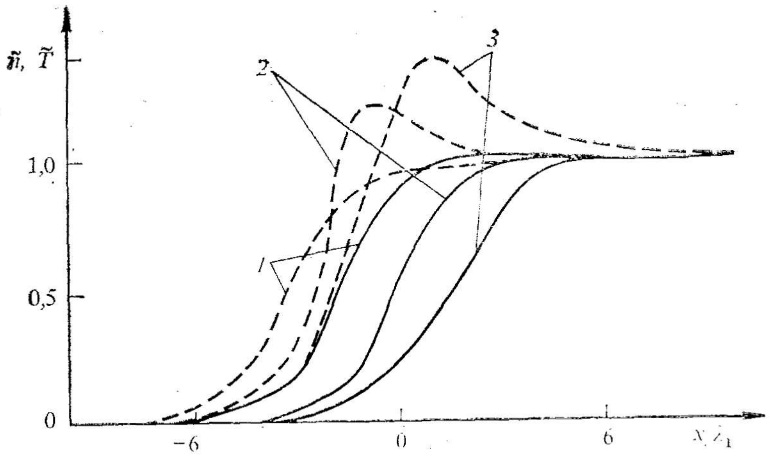

Fig. 2. ——— Temperatures $\tilde{T} = \frac{T - T_{\infty}}{T_{+\infty} - T_{-\infty}}$

——— Densities $\tilde{n} = \frac{n - n_{-\infty}}{n_{+\infty} - n_{-\infty}}$

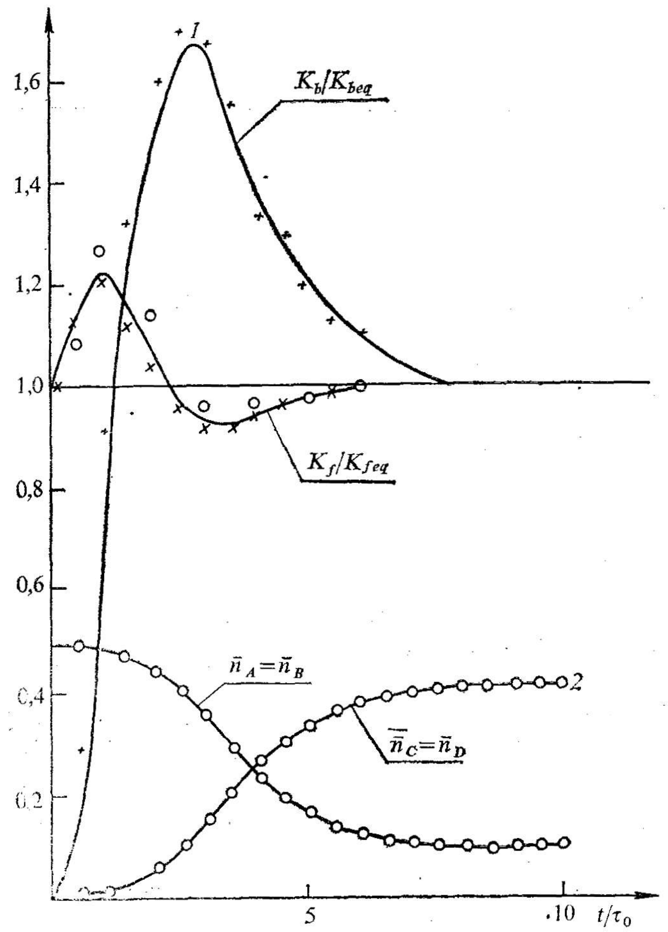

Fig. 3. ○ ○ ○ — results of [8]
× × × — results of [9]

One of the classical problems of gas kinetics, important for practice, is that of the shock wave structure. The results of the shock wave model, considering a 3-component gas [7], are given in Fig. 2, where the Mach number in the upstream flux is $M_\infty = 5$. Two heavy admixtures are present in the initially light gas. The prejump concentration ratio is $n_1{:}n_2{:}n_3 = 100{:}2{:}1$, the molecule mass ratio is $m_1{:}m_2{:}m_3 = 1:5:10$, while the molecule diameters are taken to be one and the same. It is interesting to note that the full temperatures of the heavy admixtures have a definitely expressed maximum. Similar temperature effects are also observed in two-component mixtures.

Among the problems of chemical kinetics, "exchange" reactions that occur in significantly nonequilibrium conditions are of definite interest. The results of the calculation of homogeneous relaxation in gas mixtures are given in Fig. 3 [8,9]. However, the mixture components react as $A+B \rightleftarrows C+D$ and a simulation scheme with variable weighting factors is adopted. The initial products $\bar{n}_A = \bar{n}_B = 0{,}5$, $\bar{n}_C = \bar{n}_D = 0$ exist at zero time only. The tresholds for direct and inverse reactions are equal to $\varepsilon_f = 3_k T_o$ and $\varepsilon_b = 53_k T_o$ respectively. The direct reaction velocity is normalizet with respect to its equilibrium value $K_{feq}(T)$ for a current temperature T of the components A and B. The difference between $K_{feq}(T)$ and the unit value characterizes the reaction non equilibrium state.

3. Hence, the direct simulation scheme, being effective when solving problems of aerodynamics, can be successfully employed for other problems. The new scheme realizations given in this paper, as well as the numerical results became the basis of new analyses where real and more complex problems were solved. An extension of [7,8] is [10], where the effect of the translation nonequilibrium within the shock wave region of]"exchange" reactions is studied. The direct simulation schemes [2—4] are applied in [11 for the study of material evaporation from an axisymmetric crater and into vacuum.

A number of new papers appeared recently [9,12—15] which study the method presented, as well as similar approaches. A new weighting scheme is proposed in [9] where dispersion estimations, significantly lower than in [8], are given. Crosses in Fig. 3 show the results of [9]; the employment of the methods presented in [8] did not provide stable results with respect to velocity K_b of the inverse reaction. Interesting approaches to the solution of kinetic equations when employing the Monte Carlo method are given in [12—15].

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