STUDY OF THE MAXWELLIZATION OF A GAS FLOW AND COUNTERFLOW BY THE MONTE CARLO METHOD

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Zhurnal Prikladnoi Mekhaniki i Tekhnicheskoi Fiziki, Vol. 8, No. 4, pp. 101-103, 1967

The theoretical study of relaxation processes occurring behind shock wave fronts in gases is of great interest for physical kinetics and the kinetics of chemical reactions. In particular, one of the basic processes is that of establishment of equilibrium with respect

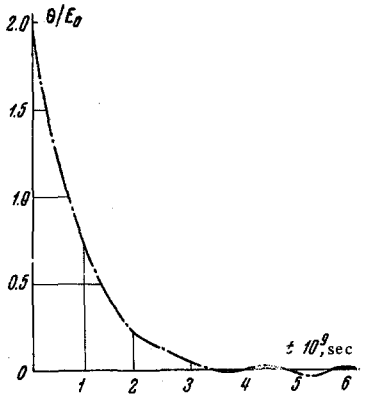

Fig. 1

to the translational degrees of freedom of the gas molecules. Solution of the system of nonlinear hydrodynamic equations (which can be solved only numerically) can yield only approximations of the macroscopic characteristics of the process; the relaxation kinetics remain inaccessible. An extremely promising approach to these problems is the Monte Carlo method; this method makes it possible to avoid solving the equations and to treat the processes on the molecular level. In conjunction with the method of "periodic boundary conditions" [1] the Monte Carlo method has been successfully used to solve equilibrium and nonequilibrium problems in statistical physics and physical kinetics [1, 2]. In this paper we use the Monte Carlo method to investigate the kinetics of energy dissipation in ordered motion; we use a spatially homogeneous model of a system of neutral particles which belong to a flow and counterflow. A physical example of this type of problem is the process of "Maxwellization" which occurs behind shock wave fronts.

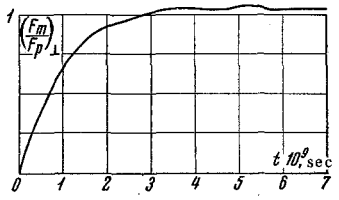

Fig. 2

Two groups of particles, 54 in each flow, formed a closed system. The particle density was 10^{18} cm^{-3}. Each of the flows was homogeneous in composition; the mass ratio for particles in different flows was approximately 2000. The initial kinetic energy of each particle corresponded to $3 \cdot 10^{4}$° K.

We will introduce the laboratory coordinate system. Assume that $V_{\parallel} = V_z$ and $V_{\perp} = (V_x^2 + V_y^2)^{1/2}$ are, respectively, the longitudinal and transverse components of the velocity. All particles had only longitudinal velocity components at the initial instant of time. The quantities $T_{\parallel} = mV_{\parallel}^2$ and $T_{\perp} = mV_{\perp}^2/2$ are arbitrarily called the "longitudinal" and "transverse" components of the temperature. Particle collisions were assumed to be completely elastic, while the particles themselves were regarded as noninteracting solid spheres. The coordinates of the particles were not included in the calculation procedure [2]; the kinetics of diffusion were considered in the velocity space for scattering of fast light particles by slow heavy ones. It is known that this process is characterized by three relaxation times with respect to the translational degrees of freedom. In our case the solution was terminated when a Maxwellian distribution was established within the group of light particles. The calculation procedure employed an algorithm for solving the problem of Maxwellization of a nonequilibrium mixture of two gases whose initial temperatures are different [2]. In effect the solution amounts to computer implementation of a Markov chain with nonzero transition probabilities. The results of calculating one chain are probabilistic and depend on the choice of the initial pseudorandom number.

Of particular importance in studies of this type are factors relating to the details of the resultant distribution functions. Therefore these functions must be obtained with a high degree of accuracy, and this is not provided for by a single calculation of the chain using 54 particles of one kind. Therefore to increase the accuracy to one percent and better, each particular variant (or chain) was repeated statistically independently about 60 times and the results were then averaged at certain instants. This procedure is equivalent to increasing the effec-

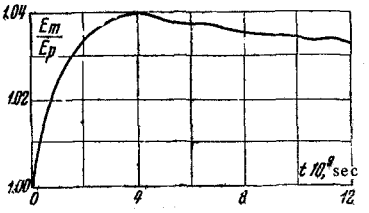

Fig. 3

tive number of particles by a factor of approximately 1.5 and results in increased accuracy without substantially increasing the machine time. The resultant statistical error was $\leq \mp 2\%$. Therefore all anomalies in the distribution functions and in their behavior as functions of time which exceeded these error limits were taken to reflect the physical behavior of the system. The results are shown in Figs. 1-7.

The difference between the temperature components $\theta = T_{\parallel} - T_{\perp}$ can provide a measure of the deviation of the system from equilibrium. In an equilibrium system this difference should be close to zero. Figure 1 shows $\theta = \theta(t)$ as a function of time; $T_{\parallel}$ and $T_{\perp}$ relate to light particles and E_0 is the initial energy of the particles. The curve intersects the abscissa axis at $3.5 \cdot 10^{-9}$ sec (or about 4.2 collisions per particle) and subsequently fluctuates weakly around the zero level; this indicates that the equilibrium in the light particle group is relatively stable. The equilibrium value of the average transverse energy component $(E_m)_{\perp}$ for light particles, as obtained from the solution, is approximately 4.5% greater than the corresponding thermodynamic-equilibrium energy component $(E_p)_{\perp}$. Figure 2 shows how the ratio of these components changes with time.

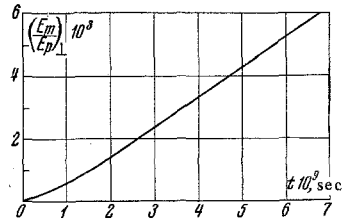

Fig. 4

Figure 3 shows the time behavior of the average total energy of light particles. The increase in the average energy for light particles at the initial instants is due to the fact that collisions between light and heavy particles predominate. This causes transfer of energy from

heavy to light particles, since the initial momenta of heavy particles are substantially greater than those of the light ones. The increase in energy for light particles ceases around $4 \cdot 10^{-9}$ sec (approximately 5.0 collisions per particle) and subsequently E_m gradually decreases. When complete equilibrium is established in the system the average energies of light and heavy particles should be the same. A similar situation arises when a beam of charged particles interacts with a plasma [3]. In the general case, the energy exchange between the beam and the plasma does not cease when the temperatures of both components are equal. Of course, this equilibrium is not total equilibrium. Figure 4 shows the time behavior of the average transverse energy component $(E_M)_\perp$ for heavy particles. The energy increases monotonically with time and at the instant when equilibrium is established within the group of light particles the value of $(E_M)_\perp$ is a fraction of a percent of the equilibrium value of $(E_p)_\perp$.

Figure 5 shows the distribution functions for light particles over their velocity moduli. The time step $\Delta\tau = 0.476 \cdot 10^{-9}$ sec is the parameter; curves 1, 2, and 3 correspond to $t = 2\Delta\tau$, $4\Delta\tau$, and $6\Delta\tau$.

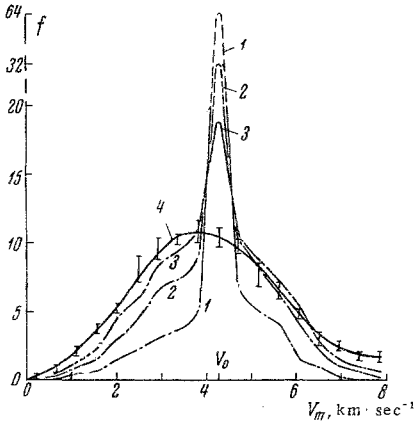

Fig. 5

The vertical bars indicate the mean-square deviation of the functions from the equilibrium distribution function. A total of 15 functions were obtained, but Fig. 5 shows only typical ones which indicate the general pattern in the behavior of the distribution functions. At the initial instants (below $3.5-4 \cdot 10^{-9}$ sec) the functions have an absolute maximum at $V_0 = 4.27$ km · sec^{-1} (the initial velocity). As equilibrium is approached the peak decreases. At the same time the dispersion of the distribution functions increases. Fluctuations around the equilibrium distribution function are observed after $4 \cdot 10^{-9}$ sec (approximately 5.0 collisions per particle). It is significant that these fluctuations are clearly not involved in the statistical error. At each given instant the distributions depart substantially from the equilibrium distribution, but after approximately $4 \cdot 10^{-9}$ sec the average over the set of functions is a Maxwellian distribution function with respect to the velocities; it is indicated in Fig. 5 by the heavy line. The "lifetime" of the individual fluctuation maxima and minima is less than $0.5-1.0 \cdot 10^{-9}$ sec (0.55–1.10 collisions per particle). The distribution functions for light particles with respect to the longitudinal (Fig. 6) and transverse (Fig. 7) velocity components behave similarly. Curves 1, 2, and 3 in Fig. 6 correspond to $t = \Delta\tau$, $4\Delta\tau$, and $6\Delta\tau$, while curves 1, 2, 3, and 4 in Fig. 7 correspond to $t = \Delta\tau$, $3\Delta\tau$, $5\Delta\tau$, and $6\Delta\tau$. The heavy lines indicate the equilibrium functions. An interesting feature of the curves in Fig. 7 is the appearance of relative maxima at $(V_m)_\perp = V_0 = 4.27$ km · sec^{-1}. This is explained by the fact that the particle scattering probability for elastic collision in an element of solid angle is given by $d(\cos\theta)d\varphi$, and therefore the probability of scattering at an angle θ in the scattering plane is determined by $\sin\theta$ and hence is at maximum at $\pi/2$. For collisions at the initial instants of time, this causes the velocity vector for light particles to shift by $\pi/2$.

For a system of particles with initial ordered velocities, we have considered the kinetics of the process of relaxation to a Max-

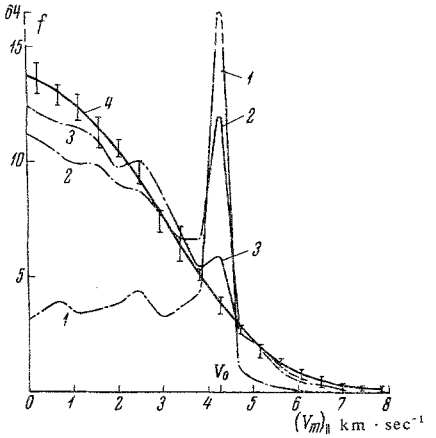

Fig. 6

wellian equilibrium within a group of light particles. The equilibrium is relatively stable. At the instant that the Maxwellian distribution is established for light particles their average energy is higher than that of the heavy particles. We have shown that, when equilibrium with respect to $T_\parallel$ and $T_\perp$ is attained, the distribution functions over the velocities differ from the Maxwellian distributions at each given instant; it is the time average of the set of distribution functions which is in equilibrium, provided that the time interval used in

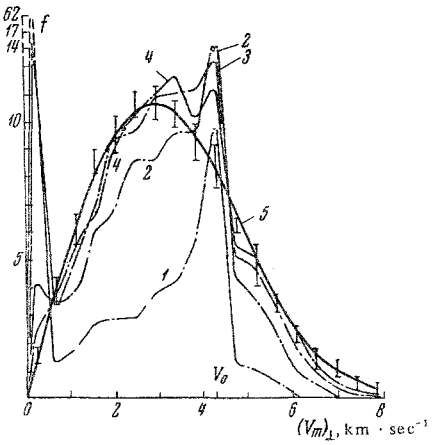

Fig. 7

averaging is not too large (around $4 \cdot 10^{-9}$ sec). We have obtained the characteristic times of the relaxation process and the number of collisions per particle.

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13 March 1967 Moscow