KINETIC DESCRIPTION OF A STRONG EXPLOSION IN A RAREFIED GAS

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A large number of studies have been dedicated to the investigation of the gasdynamic flows that develop upon an explosion within the gas. A self-similar solution has been obtained, and the effects related to the nonideal nature of the gas, finite counterpressure, etc., have been studied (see the bibliographies of [1, 2]).

The gasdynamic description is not applicable to explosions in a rarefied gas. If the kinetic effects are relatively weak, they may be considered by introducing viscosity and thermal conductivity into the system of gasdynamics equations [3, 4]. However, in a number of problems that stage of the explosion is of interest in which the dimensions of the region in motion is comparable to or not much larger than the free path length of gas particles or explosion products. An accurate description of this stage requires a kinetic approach.

In the present study the dynamics of a strong explosion in a rarefied gas will be studied by numerical solution of the system of Boltzmann equations for the distribution functions of media particles and explosion products. The applicability of the gasdynamic approximation for description of such explosions will be evaluated.

1. Formulation of the Problem. The system of Boltzmann equations describing the flow which develops in an explosion has the form

$$\frac{\partial F_\alpha}{\partial t} + \mathbf{v}\frac{\partial F_\alpha}{\partial \mathbf{r}} = \sum_{\beta=1,2} J_{\alpha\beta}(F_\alpha, F_\beta), \tag{1.1}$$

$$J_{\alpha\beta} = \int d\mathbf{v}_\beta \int d\sigma_{\alpha\beta} v_{\alpha\beta} (F'_\alpha F'_\beta - F_\alpha F_\beta),$$

where the subscript $\alpha = 1, 2$ distinguishes the distribuiton functions and parameters characterizing the state of the explosion products $\alpha = 1$) and the state of the surrounding medium ($\alpha = 2$); the primes denote velocity function after collisions; $v_{\alpha\beta}$ is the modulus of the relative velocity upon collision; $d\sigma_{\alpha\beta}$ is the differential elastic scattering section for type α particles on type β particles in the solid angle element $d\Omega$ in the system of the center of mass of the colliding particles. In order not to complicate the formulation, it will be assumed that the scattering sections do not depend on angle and that the total scattering sections for the particles of different types are equal, i.e., $d\sigma_{\alpha\beta} = (\sigma_0/4\pi)d\Omega$. Moreover, it is assumed that the total section σ_0 does not depend on the value of the relative velocity of the colliding particles. In the gasdynamic formulation of the problem of the strong explosion the pressure of the medium is neglected in comparison to the pressure in the shock front. This approximation in the kinetic formulation is equivalent to a choice of initial conditions for the medium particle distribution function in the form

(1.2)

where n_0 is the medium particle concentration; $\delta(\mathbf{v})$ is the Dirac delta-function. The initial explosion product distribution function, modeling point energy liberation, has the form

$$F_1(\mathbf{r}, \mathbf{v}, t = 0) = N\delta(\mathbf{r})F_0(\mathbf{v}), \tag{1.3}$$

where N is the total number of explosion product particles; $F_0(\mathbf{v})$ is the explosion product distribution function normalized to unity. The function $F_0(\mathbf{v})$ corresponds to the density distribution up to the moment at which inertial expansion of the explosion products into a void begins, the void being formed in the initial gasdynamic stage of the explosion. It is assumed that $F_0(\mathbf{v})$ has a form corresponding to isothermal expansion [5]:

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$$F_0(\mathbf{v}) = \frac{1}{\pi^{3/2} v_0^3} e^{-v^2/v_0^2}. \tag{1.4}$$

The character v_0 characterizes the expansion velocity of the explosion products.

In the problem under consideration, Eqs. (1.1)-(1.4), it is convenient to transform to dimensionless variables $\mathbf{x}$, $\mathbf{u}$, τ, f_α, defined by the relationships

$$\mathbf{r} = R_0\mathbf{x}, \mathbf{v} = v_0\mathbf{u}, t = \frac{R_0}{v_0}\tau, F_\alpha = \frac{n_0}{v_0^3} f_\alpha, \tag{1.5}$$

where

$$R_0 = (3N/4\pi n_0)^{1/3}.$$

In these variables the system of Boltzmann equations has the form of Eq. (1.1) with new dimensionless section

$$\sigma = n_0 R_0 \sigma_0 = \mathrm{Kn}^{-1}.$$

Initial conditions (1.2)-(1.4) are rewritten as:

$$f_1(\mathbf{x}, \mathbf{u}, \tau = 0) = \frac{4\tau}{3} \frac{\delta(x)}{\pi^{3/2}} e^{-u^2}, \; f_2(\mathbf{x}, \mathbf{u}, \tau = 0) = \delta(\mathbf{u}).$$

The problem thus formulated is defined completely by two dimensionless parameters: the Knudsen number $\mathrm{Kn} = (n_0 R_0 \sigma_0)^{-1}$ and the ratio of the masses of particles of the explosion products and medium, m_1/m_2.

2. Method of Solution. Numerical solution of Eq. (1.1) is a very complex problem. The complexity is related mainly to the high dimensionality and nonlinearity of the Boltzmann equations describing the flow of a rarefied gas. Existing difference methods of solution of such equations require too large a volume of calculations, beyond the possibilities of present-day computers. Therefore, the problem was solved numerically by the Monte Carlo method. For a more accurate consideration of solution peculiarities, and also to increase the efficiency of the Monte Carlo method, an explicit separation of all unscattered particles, i.e., those not experiencing any collisions, was performed. It is quite simple to perform this separation, since the distributions of the unscattered particles over velocity are known — the velocities of unscattered explosion products at the point $\mathbf{x}$ at time τ is equal to $\mathbf{x}/\tau$, while for the medium, the velocity is equal to zero. Therefore, unscattered particles can be described by their densities and calculated by difference methods.

We will write the distribution function in the form

$$\begin{aligned} f_\alpha(\mathbf{x}, \mathbf{u}, \tau) &= n_\alpha(\mathbf{x}, \tau) p_\alpha(\mathbf{x}, \mathbf{u}, \tau) + \varphi_\alpha(\mathbf{x}, \mathbf{u}, \tau), \\ p_\alpha(\mathbf{x}, \mathbf{u}, \tau) &= \delta(\mathbf{u} - \mathbf{u}_\alpha), \; \mathbf{u}_1 = \mathbf{x}/\tau, \; \mathbf{u}_2 = 0, \end{aligned} \tag{2.1}$$

where n_α is the unscattered particle density; $\mathbf{u}_\alpha$, velocity of the unscattered particle; φ_α, scattered particle distribution function.

If we introduce the notation

$$J^-_{\alpha\beta}(\varphi, \psi) = \int d\mathbf{u}_\beta \int \varphi\psi u_{\alpha\beta} d\sigma_{\alpha\beta},$$
$$J^+_{\alpha\beta}(\varphi, \psi) = \int d\mathbf{u}_\beta \int \varphi'\psi' u_{\alpha\beta} d\sigma_{\alpha\beta}, \; J_{\alpha\beta}(\varphi, \psi) = J^+_{\alpha\beta}(\varphi, \psi) - J^-_{\alpha\beta}(\varphi, \psi),$$

then system (1.1) with consideration of Eq. (2.1) can be written as

$$\frac{\partial n_\alpha}{\partial \tau} + \frac{\partial}{\partial \mathbf{x}}(n_\alpha \mathbf{u}_\alpha) = -n_\alpha \int d\mathbf{u}_\alpha \sum_{\beta=1,2} [n_\beta J^-_{\alpha\beta}(p_\alpha, p_\beta) + J^-_{\alpha\beta}(p_\alpha, \varphi_\beta)];$$
$$\frac{\partial \varphi_\alpha}{\partial \tau} + \mathbf{u} \frac{\partial \varphi_\alpha}{\partial \mathbf{x}} = \sum_{\beta=1,2} J_{\alpha\beta}(\varphi_\alpha, \varphi_\beta) \tag{2.2}$$

$$+ \sum_{\beta=1,2} J^+_{\alpha\beta}(p_\alpha, p_\beta) n_\alpha n_\beta + \sum_{\beta=1,2} [J_{\alpha\beta}(\varphi_\alpha, p_\beta) n_\beta + J^+_{\alpha\beta}(p_\alpha, \varphi_\beta) n_\alpha]. \tag{2.3}$$

The expressions on the right sides of these equations have the following meanings: $J^=_{\alpha\beta}(p_\alpha, p_\beta)$ and $J_{\alpha\beta}(p^+_\alpha, p_\beta)$ are the loss of unscattered particles and gain in scattered particles due

to collisions of unscattered particles with each other. We note that since the relative velocities of one type of unscattered particle are equal to zero, then $J^-_{\alpha\alpha}(p_\alpha, p_\alpha) = J^+_{\alpha\alpha}(p_\alpha, p_\alpha) = 0$, while $J^-_{12}(p_1, p_2) = J^-_{21}(p_1, p_2) = \sigma\left|\frac{x}{\tau}\right|$, where $J^-_{\alpha\beta}(p_\alpha, \varphi_\beta)$ is the loss in unscattered particles due to collisions with scattered particles; $J^+_{\alpha\beta}(p_\alpha, \varphi_\alpha)$ is the gain in scattered particles due to collisions between unscattered and scattered; $J_{\alpha\beta}(\varphi_\alpha, p_\beta)$ is the collision integral describing collision of a scattered particle on an unscattered one; $J_{\alpha\beta}(\varphi_\alpha, \varphi_\beta)$ are the Boltzmann collision integrals for scattered particles.

System (2.2), (2.3) was solved by the splitting method. Each time step of the solution was divided into three partial steps. In the first partial step system (2.2), describing loss of unscattered particles in collisions with each other and with scattered particles, was solved. A second-order accuracy DS_N solution method with Wendorff modification [6] was used with iterations in the nonlinearity on the right side. The coefficients $J^-_{\alpha\beta}(p_\alpha, \varphi_\beta)$ were calculated in the preceding time step. In the second partial step the Monte Carlo method was used to solve the system

$$\frac{\partial \varphi_\alpha}{\partial \tau} + \mathbf{u}\frac{\partial \varphi_\alpha}{\partial \mathbf{x}} = \sum_{\beta=1,2}\left[n_\beta J_{\alpha\beta}(\varphi_\alpha, p_\beta) + n_\alpha J^+_{\alpha\beta}(p_\alpha, \varphi_\beta)\right] + S_\alpha \qquad (2.4)$$

with densities n_α and scattered particle sources $S_\alpha = n_\alpha \sum_{\beta=1,2} n_\beta J^+_{\alpha\beta}(p_\alpha,$ calculated in the first partial step. Thus, the change in φ_α due to transfer and interaction with unscattered particles was found. From the probability viewpoint Eq. (2.4) describes a branching process of scattered particle wandering over a background of unscattered particles, with which collision occur. With each such collision the scattered particle changes its velocity in accordance with the operator $J^+_{\alpha\beta}(\varphi_\alpha, p_\beta)n_\beta$ and a new scattered particle is created in accordance with the operator $J^+_{\alpha\beta}(p_\alpha, \varphi_\beta)n_\alpha$. Such a probability interpretation permits use of Standard Monte Carlo methods for solution of Eq. (2.4), as developed for solution of linear transfer processes [7]. In the process of modeling the wandering, the functionals $J^-_{\alpha\beta}(p_\alpha, \varphi_\beta)$ are estimated, these characterizing the rate of decrease of unscattered particles in collisions with scattered, and required for calculating the first partial step. The estimate chosen was one over path length.

Finally, in the third partial step the system of spatially homogeneous Boltzmann equations $\frac{\partial \varphi_\alpha}{\partial \tau} = \sum_{\beta=1,2} J_{\alpha\beta}(\varphi_\alpha, \varphi_\beta,)$ was solved. These equations describe the change in φ_α due to collisions of scattered particles with each other. A Monte Carlo method was used, analogous to the method of direct modeling of collisions of a set of particles, first proposed by Bird [8, 9]. The initial state of this set is the result of modeling in the previous step.

The essence of the method consists in picking paired particle collisions located in the same spatial cell. The colliding pair is selected with a probability proportional to the collision frequency. The co-lision time is chosen by an exponential law with exponent proportional to the total frequency.

In the initial stage, with consideration of the spherical symmetry of the problem, the solution of Eq. (2.2) was carried out on a grid formed by the intersection of the characteristics $x/\tau = u_i$ of Eq. (2.2) with $\alpha = 1$ and the straight lines $\tau = \tau_n$. The same grid was used for modeling the wandering of particles in the second partial step. Since at small times the density of unscattered particles of the first sort is very high, direct modeling of the wandering requires calculation of a large number of collisions. But since the effect of collisions of scattered particles with unscattered is not great at this stage, this difficulty can be avoided, by taking at small $\tau < \tau_0$ ($\tau_0 = 10^{-3}$–10^{-1})

$$J_{\alpha 1}(\varphi_\alpha, p_1) = J^+_{\alpha 1}(p_1, \varphi_\alpha) = 0.$$

The independence of the solution from τ_0 was verified by calculations. In the computing process the grid was periodically readjusted so that its external radius would just encompass the range containing scattered particles. In the calculations 5000 particles were modeled at each time step. The grid contained 100 cells along the radius. At each step the moments of the distribution functions were calculated: ρ_α, density, $(\rho u)_\alpha$, mass flow, $p_{\alpha\parallel}$, $p_{\alpha\perp}$, radial

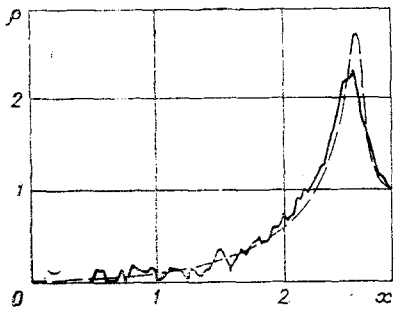

Fig. 1

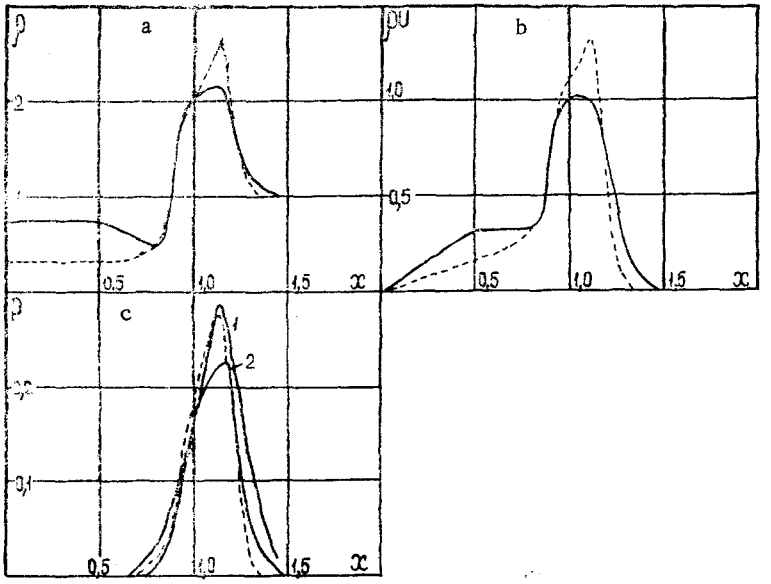

Fig. 2

and transverse components of the flow momentum tensor (radial and transverse pressure) of each component and their total values, ρ, ρu, $p_{\parallel}$, $p_{\perp}$.

The problem was also solved in the gasdynamic approximation, with consideration of viscosity and thermal conductivity. The coefficients of viscosity η and thermal conductivity $\varkappa$, corresponding to an isotropic velocity-independent elastic scattering section have the form

$$\eta = \frac{1}{\mathrm{Kn}} \frac{5\sqrt{\pi}}{16} \sqrt{T}, \varkappa = \frac{1}{\mathrm{Kn}} \frac{75\sqrt{\pi}}{64} \sqrt{T}.$$

in the dimensionless units chosen (Eq. (1.5)). At the initial moment of time the explosion products with a density and energy liberation homogeneous over radius are located within a sphere of radius $r_0 = 0.1$. Computation was performed by an implicit iterationless Lagrangian difference method, which is completely conservative [10]. Mathematical viscosity was not used. The calculations employed 50 Lagrangian cells for the explosion products and 200 for the surrounding medium.

3. Results. Calculations were carried out for dimensionless parameter values Kn = 0.1 and $m_1/m_2 = 1$. The results are illustrated by Figs. 1-3, where the solid lines denote profiles obtained in the kinetic calculations, while dashes are for the gasdynamic approximation. In Figs. 2 and 3 the results of the kinetic calculations are presented as smoothed curves. The scale of the fluctuations which appear when the kinetic equations are solved by the method described above is illustrated by Fig. 1, where the unsmoothed density profile obtained at time $\tau = 4.5$ is shown. The profiles of Fig. 2 correspond to times $\tau = 1$ in Fig. 2c curve 1 is radial, curve 2, transverse pressure.

As is evident from Figs. 1 and 2, the interaction of explosion products with the surrounding medium leads to the appearance in the medium of shock-wave type perturbations. We

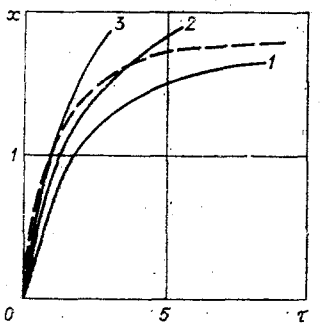

Fig. 3

note that the profiles obtained in the kinetic and gasdynamic calculations agree well with each other in the main part of the flow. Characteristic features of the kinetic profiles are the smoother variation of all quantities in the region of their maxima and somewhat lower values of the maxima themselves. The effect of kinetic processes on the wave front causes situations in which the maximum density compression $(\gamma + 1)/(\gamma - 1)$, equal in the given case to 4, is not reached over the course of a lengthy time. This is true because the characteristic width of the density profile in the front region is much less than the dimensions of the entire region undergoing motion. For example, at time $\tau = 4.5$ the flow region encompasses ~30 path lengths, while the characteristic width of the density profile comprises only 3-4 path lengths. For the same reason, in the front region at one or two path lengths the radial pressure is higher than the transverse, which agrees with conclusions made in a study of the structure of planar shock fronts [11].

The marked divergence between the density and mass flow profiles obtained in the kinetic and gasdynamic calculations near the explosion point is explained by the fact that in this region there exist freely expanding explosion products which have not collided with particles of the medium. Particles of the medium are "swept" from this region as a result of interaction with more rapid explosion product particles at earlier times. The density and mass flow profiles in this region are determined by the form of Eq. (1.4), the initial explosion product distribution. The dimensions of this region decrease with time at $\tau > 1$.

The explosion product distributions differ significantly in the kinetic and gasdynamic calculations. In the gasdynamic calculation the explosion products are located within a region bounded by a contact discontinuity, the position of which as a function of time is shown by the dashed line of Fig. 3. At the same time, the mass of explosion products located within this region decreases with time in the kinetic calculation. Figure 3 shows the time dependence of radii encompassing a region in which a definite fraction ν of the combustion product mass is enclosed ($\nu = 0.2$; 0.5 and 0.9, curves 1-3, respectively). It is evident that even at $\tau = 3.5$, within the region bounded by the contact discontinuity only half the explosion products are present. Motion of the explosion products through the contact discontinuity has the character of diffusion, so that the total mass of the material concentrated in the region limited by the contact discontinuity coincides to an accuracy of 10-20% with the mass of the explosion products at all times.

The calculations performed reveal that at Kn = 0.1 the stage of significant interaction of explosion products with the medium at distances of ~R_0 (~1 in dimensionless variables) and development of a perturbation in the surrounding medium at larger scales is described to an accuracy of 10-20% by the gas dynamics equations with viscosity and thermal conductivity. At the same time, such a gasdynamic model does not describe the space–time distribution of combustion products.

In conclusion, we note that similar studies of rarefied gas flows were performed in [12-14], where in contrast to the present study a simplified kinetic equation with S-model collision integral was used. In [4] the problem of a planar strong explosion in a rarefied gas was studied. Results were presented for Knudsen numbers Kn = 0.1, 0.5. There was no detailed comparison to the gasdynamic solution, although it was shown (Fig. 3 of [14]) that the position of the maximum of medium density agreed well with the position of the shock wave front in the gasdynamic problem.

Detailed comparisons of gasdynamic solutions considering viscosity and thermal conductivity with kinetic solutions for reflection of a plane shock wave from a rigid wall [12] and

convergence of a spherical wave to the center of symmetry [13] were performed in [15]. As in the present study, in [15] there was satisfactory qualitative and even quantitative agreement between the corresponding kinetic and gasdynamic solutions.

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