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Kinetic Model Solution for Axisymmetric Flow by the Method of Discrete Ordinates

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The method of discrete ordinates for the solution of the Boltzmann equation simplified by the BGK-model is extended to cylindrical coordinates. The curvature terms of the model equations are approximated by means of an ellipsoidal distribution function. The model equation is solved by means of finite-difference approximations. The rate of convergence of the iterative procedure employed is shown to be accelerated by introducing the deviation of the distribution function from a Maxwellian distribution into the model equation. To illustrate the applicability of the method, results are reported for the flow of an axisymmetric jet in a finite-pressure background gas of different species.

INTRODUCTION

Theoretical investigations of gaseous nonequilibrium flows commonly require the solution of the Boltzmann equation. One of the major difficulties in solving the Boltzmann equation is due to the complicated structure of the collision integral, which contains the details of the molecular interaction. Although significant advances have been made in numerical solutions for the Boltzmann equation in recent years (e.g., [1]), the solution of problems involving three-dimensional flow or two-dimensional flow of gas mixtures can, up to now, not be predicted in a reasonably short time with present available computers. For many a problem only certain macroscopic properties need to be determined. Consequently, instead of a detailed description of the molecular interaction by the collision integral, an approximate description is given by means of a simpler collision term ("collision model"), which retains only some qualitative and average properties of the collision integral. A most widely used collision model is given by the nonlinear Bhatnagar–Gross–Krook (BGK) model, which leaves two main properties of the collision integral unchanged: It involves the correct collisional invariants and expresses the tendency of the distribution function to a Maxwellian distribution in the limit $t \to \infty$, according to the H-theorem [2].

The model equation resulting from the replacement of the collision integral by the kinetic model is often solved by means of the method of discrete ordinates [3]. This method is built on the assumption, that the moments of the distribution function given by integrals over the molecular velocity space can be calculated by a numerical quadrature. Hence values of the distribution function are required only

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at certain discrete velocities ("discrete ordinates"). The solution of the model equation is then reduced to the solution of a system of partial differential equations, in which the molecular velocities appearing in the model equation are replaced by the discrete ordinates considered as fixed parameters. This system of differential equations can be solved by means of finite-difference approximations or by means of the method of characteristics. For the nonlinear BGK model equation the resulting equations have to be solved iteratively. This is done by taking all moments of the preceding iteration step. Convergence of the solution is assumed if the differences of the moments in two successive iteration steps are less than a prescribed error bound.

The solution sketched above was successfully applied to the calculation of plane flows (e.g., [4, 5]). By adapting the method to the calculation of flows, in which Coriolis and centrifugal accelerations are present, the analysis has been restricted to problems, which depend on the radial coordinate only [6–8]. This restriction was necessary because of the prohibitively large computational effort, if the curvature terms were to be included. In this paper the restriction is circumnavigated and the method of solution is extended to axisymmetric flow problems by means of prescribing the distribution function in a way similar to [6, 7].

The convergence of the iterative procedure is shown to be accelerated significantly by the use of a new form of the model equation, in which the deviation of the distribution function from a Maxwellian distribution is used as the dependent variable. Finally, for the problem of an axisymmetric jet issuing into a background gas of different species, some results of the calculation are presented to supplement the general considerations.

Model Equations

We consider the steady, two-dimensional, axisymmetric flow of a gas, assuming the distribution function $f(r, z, v_r, v_\varphi, v_z)$ to be governed by the BGK-model equation

$$v_z \frac{\partial f}{\partial z} + v_r \frac{\partial f}{\partial r} + \frac{v_\varphi^2}{r} \frac{\partial f}{\partial v_r} - \frac{v_r v_\varphi}{r} \frac{\partial f}{\partial v_\varphi} = \nu(F - f), \tag{1}$$

where

$$F = \frac{n}{(2\pi RT)^{3/2}} \exp\left\{ - \frac{(\mathbf{v} - \mathbf{U})^2}{2RT} \right\} \tag{2}$$

is a local Maxwellian distribution containing combinations of the moments

$$\begin{aligned} n &= \iiint_{-\infty}^{\infty} f \, d^3v, \\ n\mathbf{U} &= \iiint_{-\infty}^{\infty} \mathbf{v} f \, d^3v, \\ 3nRT &= \iiint_{-\infty}^{\infty} (\mathbf{v} - \mathbf{U})^2 f \, d^3v. \end{aligned} \tag{3}$$

The collision frequency ν in Eq. (1) is usually expressed by one of the transport coefficients derived from the Boltzmann equation for a given intermolecular potential by means of the Chapman–Enskog–method [3, 4]. In Eqs. (1)–(3), R denotes the gas constant, n the particle density, $\mathbf{U}$ the macroscopic flow velocity, and T the temperature.

To reduce the number of independent variables, the following reduced distribution functions are introduced:

$$g(z, r, v_z, v_r) = \int_{-\infty}^{\infty} f \, dv_\varphi, \qquad h(z, r, v_z, v_r) = \int_{-\infty}^{\infty} v_\varphi^2 f \, dv_\varphi. \tag{4}$$

The corresponding model equations for the reduced distribution functions are obtained from Eq. (1) by weighted integration with the weight function 1 and v_φ^2, respectively,

$$\begin{aligned} v_z \frac{\partial g}{\partial z} + v_r \frac{\partial g}{\partial r} + \frac{v_r}{r} g + \frac{1}{r} \frac{\partial h}{\partial v_r} &= \nu(G - g), \\ v_z \frac{\partial h}{\partial z} + v_r \frac{\partial h}{\partial r} + \frac{3v_r}{r} h + \frac{1}{r} \frac{\partial k}{\partial v_r} &= \nu(H - h), \end{aligned} \tag{5}$$

where

$$G = \frac{n}{2\pi RT} \exp\left\{ -\frac{(v_z - U_z)^2 + (v_r - U_r)^2}{2RT} \right\},$$

$$H = RTG,$$

are the corresponding reduced Maxwellian distributions. Because of the appearance of the reduced distribution function

$$k = \int_{-\infty}^{\infty} v_\varphi^4 f \, dv_\varphi,$$

the coupled set of Eqs. (5) is not closed. The closure can be achieved by assuming (similar to [6]) that, for the centrifugal terms in Eqs. (5), the dependence of the distribution function f on the velocity component v_φ can be approximated by

$$f \propto \left(\frac{\alpha}{\pi} \right)^{1/2} \exp\{ -\alpha v_\varphi^2 \}. \tag{6}$$

Thus, we obtain

$$\begin{aligned} k &= \frac{3}{2\alpha} h, \\ h &= \frac{1}{2\alpha} g, \end{aligned} \tag{7}$$

where

$$\alpha^{-1}(z, r) = \frac{2}{n} \iint_{-\infty}^{\infty} h \, dv_z \, dv_r. \tag{8}$$

Under the assumption (6) the model equations for the reduced distribution functions take the form

$$\begin{aligned} v_z \frac{\partial g}{\partial z} + v_r \frac{\partial g}{\partial r} + \frac{1}{r}\left(v_r g + \frac{1}{2\alpha}\frac{\partial g}{\partial v_r}\right) &= \nu(G - g), \\ v_z \frac{\partial h}{\partial z} + v_r \frac{\partial h}{\partial r} + \frac{3}{r}\left(v_r h + \frac{1}{2\alpha}\frac{\partial h}{\partial v_r}\right) &= \nu(H - h). \end{aligned} \tag{9}$$

It should be noted that the relations (7) are not considered to be generally valid, but only as an approximation to the centrifugal terms. Sample calculations for the jet flow problem described further below indeed show, that the ratio h/g may still deviate from $(2\alpha)^{-1}$ (see Eqs. (7)) and slightly depend on the molecular velocity components.

With regard to the application of the method of discrete ordinates, a further approximation to the centrifugal terms seems to be useful by prescribing the v_r-dependence of the distribution function and carrying out the derivatives analytically. For the one-dimensional source flow in [6], the v_r-dependence of the distribution function was modelled by an exponential of a quadratic form with three adjustable parameters, which have to be determined during the calculation by local fitting in the velocity space. Similar to that procedure, we assume, that the centrifugal terms in Eqs. (9) can be described approximately with a v_r-dependence of the distribution function given by

$$f \propto \left(\frac{\beta}{\pi}\right)^{1/2} \exp\{-\beta(v_r - U_r)^2\}, \tag{10}$$

where the single parameter β can be determined by the equation

$$\beta^{-1}(z, r) = \frac{2}{n} \iint_{-\infty}^{\infty} (v_r - U_r)^2 \, g \, dv_z \, dv_r. \tag{11}$$

Thus, we finally obtain the model equations for the reduced distribution functions,

$$\begin{aligned} v_z \frac{\partial g}{\partial z} + v_r \frac{\partial g}{\partial r} + \frac{K}{r} g &= \nu(G - g), \\ v_z \frac{\partial h}{\partial z} + v_r \frac{\partial h}{\partial r} + \frac{3K}{r} h &= \nu(H - h), \end{aligned} \tag{12}$$

where the coefficient of the curvature terms is given by

$$K(z, r, v_r) = \left(1 - \frac{\beta}{\alpha}\right) v_r + \frac{\beta}{\alpha} U_r. \tag{13}$$

It should be noted, that the assumptions (6) and (10) do not restrict the solution to ellipsoidal distribution functions, since they represent an approximation to the curvature terms only. In sample calculations it could be verified, that the solution of the model equations (12) for the jet flow problem may deviate from the assumed v_r-dependence. Hence we conclude that the assumptions (6) and (10) lead to a sufficiently accurate representation of the curvature terms, if the flow field does not involve strong shock waves normal or inclined to the radial direction with a marked bimodal v_r-dependence of the distribution function.

An additional remark should be made about the influence of the approximations on the conservation of energy and angular momentum between molecular collisions, which follows from the characteristics of Eq. (1). (We are grateful to the reviewers for pointing out this question.) Equations (12) may be considered to be derived from a modified model equation, the centrifugal term of which has been approximated by means of relation (10). This modified model equation leads to characteristics that no longer coincide with molecular paths in case of free-molecular flow. Therefore, we cannot draw any conclusions about the molecular paths from the modified model equation only. The conservation of energy and angular momentum is, however, not affected by the approximations, if the solution of the modified model equation also satisfies Eq. (1). This we consider to be true, if the distribution function does not deviate too strongly from the ellipsoidal v_r- and v_φ-dependence.

Computational Procedure

Applying the method of discrete ordinates we substitute the integrals in Eqs. (3), (8), and (11) by the following quadratures:

$$\begin{aligned}
n &\simeq \sum_{\substack{\kappa=1,\ldots,m \\ \sigma=1,\ldots,n}} k_\kappa k_\sigma g_{\kappa\sigma}, \\
n(U_z, U_r) &\simeq \sum_{\substack{\kappa=1,\ldots,m \\ \sigma=1,\ldots,n}} k_\kappa k_\sigma (v_\kappa, v_\sigma)\, g_{\kappa\sigma}, \\
n\alpha^{-1} &\simeq 2 \sum_{\substack{\kappa=1,\ldots,m \\ \sigma=1,\ldots,n}} k_\kappa k_\sigma h_{\kappa\sigma}, \\
n\beta^{-1} &\simeq 2 \sum_{\substack{\kappa=1,\ldots,m \\ \sigma=1,\ldots,n}} k_\kappa k_\sigma (v_\sigma - U_r)^2\, g_{\kappa\sigma}, \\
3nRT &\simeq \sum_{\substack{\kappa=1,\ldots,m \\ \sigma=1,\ldots,n}} k_\kappa k_\sigma (v_\kappa - U_z)^2\, g_{\kappa\sigma} + \frac{n}{2}(\alpha^{-1} + \beta^{-1}),
\end{aligned} \tag{14}$$

where k_κ and k_σ are the weighting coefficients of the quadrature for the velocity components v_κ and v_σ, and $g_{\kappa\sigma}$ and $h_{\kappa\sigma}$ denote the spatial dependent functions $g(r, z, v_\kappa, v_\sigma)$ and $h(r, z, v_\kappa, v_\sigma)$, respectively. Since values of the reduced distribution functions are required only at discrete points in the velocity space, we replace the molecular velocities in the model equations (12) by the discrete velocities (v_κ, v_σ), so that the solution of the model equations is reduced to the solution of the following set of $2m \times n$ differential equations in physical space,

$$\begin{aligned} v_\kappa \frac{\partial g_{\kappa\sigma}}{\partial z} + v_\sigma \frac{\partial g_{\kappa\sigma}}{\partial r} + \frac{K_\sigma}{r} g_{\kappa\sigma} &= \nu(G_{\kappa\sigma} - g_{\kappa\sigma}), \\ v_\kappa \frac{\partial h_{\kappa\sigma}}{\partial z} + v_\sigma \frac{\partial h_{\kappa\sigma}}{\partial r} + \frac{3K_\sigma}{r} g_{\kappa\sigma} &= \nu(H_{\kappa\sigma} - h_{\kappa\sigma}) \qquad (\kappa = 1,..., m;\ \sigma = 1,..., n), \end{aligned} \tag{15}$$

where

$$K_\sigma = \left(1 - \frac{\beta}{\alpha}\right) v_\sigma + \frac{\beta}{\alpha} U_r.$$

Equations (15) are solved by employing finite-difference approximations in physical space. To reduce the computer time, forward and backward difference schemes have been used

$$\begin{aligned} \frac{\partial g_{\kappa\sigma}}{\partial z} &\simeq s \frac{g^{st}_{\kappa\sigma}(z, r) - g^{st}_{\kappa\sigma}(z - s\Delta z, r)}{\Delta z}, \\ \frac{\partial g_{\kappa\sigma}}{\partial r} &\simeq t \frac{g^{st}_{\kappa\sigma}(z, r) - g^{st}_{\kappa\sigma}(z, r - t\Delta r)}{\Delta r}, \end{aligned} \tag{16}$$

where

$$\begin{aligned} g^{st}_{\kappa\sigma} &= g_{\kappa\sigma}\Theta(sv_\kappa)\,\Theta(tv_\sigma), \\ s &= \operatorname{sign}(v_\kappa), \\ t &= \operatorname{sign}(v_\sigma) \end{aligned}$$

and

$$\begin{aligned} \Theta(x) &= 1, \qquad x \geqslant 0, \\ &\quad 0, \qquad x < 0 \end{aligned}$$

is the step function.

Taking equivalent expressions for h, we obtain the finite-difference approximation of Eqs. (15),

$$\left[\frac{|v_\kappa|}{\Delta z}+\frac{|v_\sigma|}{\Delta r}+\frac{K_\sigma}{r}+\nu\right] g^{st}_{\kappa\sigma}(z,r)$$
$$= \nu G^{st}_{\kappa\sigma}+\frac{|v_\kappa|}{\Delta z}\, g^{st}_{\kappa\sigma}(z-s\Delta z,r)+\frac{|v_\sigma|}{\Delta r}\, g^{st}_{\kappa\sigma}(z,r-t\Delta r),$$
$$\left[\frac{|v_\kappa|}{\Delta z}+\frac{|v_\sigma|}{\Delta r}+\frac{3K_\sigma}{r}+\nu\right] h^{st}_{\kappa\sigma}(z,r) \tag{17}$$
$$= \nu H^{st}_{\kappa\sigma}+\frac{|v_\kappa|}{\Delta z}\, h^{st}_{\kappa\sigma}(z-s\Delta z,r)+\frac{|v_\sigma|}{\Delta r}\, h^{st}_{\kappa\sigma}(z,r-t\Delta r).$$

The $(1/r)$-dependence of the curvature terms in Eqs. (17) requires a separate treatment of Eqs. (15) for the functions $g^{\pm -}$ and $h^{\pm -}$ on the symmetry axis, from which the functions $g^{\pm +}$ and $h^{\pm +}$ can be determined by the symmetry conditions,

$$r=0: \qquad g^{\pm +}=g^{\pm -},$$
$$h^{\pm +}=h^{\pm -}.$$

By means of the relations

$$r=0: \qquad \frac{\partial g^{\pm +}}{\partial r}+\frac{\partial g^{\pm -}}{\partial r}=0,$$
$$\frac{\partial h^{\pm +}}{\partial r}+\frac{\partial h^{\pm -}}{\partial r}=0,$$

which imply that $\partial n/\partial r=\partial T/\partial r=0$ on the axis, and l'Hospital's rule, the following finite-difference approximations to Eqs. (15) are deduced in the limit $r\to 0$,

$$\left[\frac{|v_\kappa|}{\Delta z}+\frac{U_r(z,\Delta r)-v_\sigma}{\Delta r}+\nu\right] g^{\pm -}_{\kappa\sigma}(z,0)$$
$$= \nu G^{\pm -}_{\kappa\sigma}+\frac{|v_\kappa|}{\Delta z}\, g^{\pm -}_{\kappa\sigma}(z-s\Delta z,0)+\frac{|v_\sigma|}{\Delta r}\, g^{\pm -}_{\kappa\sigma}(z,\Delta r),$$
$$\left[\frac{|v_\kappa|}{\Delta z}+\frac{3U_r(z,\Delta r)-v_\sigma}{\Delta r}+\nu\right] h^{\pm -}_{\kappa\sigma}(z,0) \tag{18}$$
$$= \nu H^{st}_{\kappa\sigma}+\frac{|v_\kappa|}{\Delta z}\, h^{\pm -}_{\kappa\sigma}(z-s\Delta z,0)+\frac{|v_\sigma|}{\Delta r}\, h^{\pm -}_{\kappa\sigma}(z,\Delta r).$$

The set of nonlinear finite-difference equations (17) and (18) have to be solved iteratively. The commonly used iterative procedure is defined by the following replacement in Eqs. (17) and (18) for the kth iteration step,

$$g, h \to g^{(K)}, h^{(K)},$$
$$\nu, U_r, G, H \to \nu^{(K-1)}, U_r^{(K-1)}, G^{(K-1)}, H^{(K-1)}.$$

Thus, in the iterative procedure, the resulting equations are linearized. (In the following, the iteration index will be omitted.) The iterative procedure is assumed to converge if the differences of the moments of two successive iteration steps fall short of a given bound.

Stability Analysis

According to the Lax equivalence theorem [9], the finite-difference approximations (in the linearized form) are checked with regard to consistency and stability to assure that the solution of Eqs. (17) converges to the solution of the differential equations (15). Consistency may easily be verified by reducing Eqs. (17) to Eqs. (15) in the limit $\Delta r \to 0$, $\Delta z \to 0$. To ensure stability, the distribution functions were expanded into a Fourier series and conditions were imposed, according to which the Fourier coefficients remain bounded. With

$$\begin{pmatrix} g_{\kappa\sigma}^{st} \\ h_{\kappa\sigma}^{st} \end{pmatrix} = \sum_q \begin{pmatrix} g_q(z) \\ h_q(z) \end{pmatrix} e^{i\pi qr},$$

the stability conditions may be written in the form

$$\left| \frac{g_q(z)}{g_q(z - s\Delta z)} \right| \leqslant 1, \qquad \left| \frac{h_q(z)}{h_q(z - s\Delta z)} \right| \leqslant 1.$$

Inserting the Fourier expansion into Eqs. (17), we get

$$0 \leqslant \left(\nu + \varepsilon \frac{K_\sigma}{r} \right)^2 + 2 \frac{|v_\kappa|}{\Delta z} \left(\nu + \varepsilon \frac{K_\sigma}{r} \right) + 2 \frac{|v_\sigma|}{\Delta r} \left(\frac{|v_\kappa|}{\Delta z} + \frac{|v_\sigma|}{\Delta r} + \nu + \varepsilon \frac{K_\sigma}{r} \right) (1 - \cos(\pi r)), \tag{19}$$

where $\varepsilon = 1$ gives the stability condition for g, $\varepsilon = 3$ the corresponding condition for h. Since the collision frequency ν is always greater or equal to zero, the conditions (19) show, that the stepwidths Δr and Δz are restricted in axisymmetric geometry, since the curvature terms may take on negative values. (The corresponding stability conditions for plane flow are obtained from the conditions (19) by putting $\varepsilon = 0$ and regarding Δr and Δz as stepwidths in Cartesian coordinates; therefore, the choice of the stepwidths is not restricted in plane geometry.)

It should be noted that the source term instability occurring in cylindrical coordinates does not arise from a discrepancy between the physical and the numerical region of influence. As mentioned earlier, the approximations to the curvature terms, which lead to Eqs. (12), correspond to the solution of a modified model equation instead of Eq. (1). The characteristics of Eq. (1) are projected onto the (r, z) plane as hyperbolic curves, those of the modified model equation, however, as

straight lines. For the modified model equation, at any gridline $r = \text{const.}$ the region of influence is therefore defined by the sign of v_r only and independent of v_φ. Hence it follows that the values of the reduced distribution functions at the gridline r are influenced by the corresponding values at $r \pm \Delta r$.

From the stability conditions (19), we obtain the strongest restriction on the choice of the stepwidths in the case of free-molecular flow,

$$\Delta r \leqslant \min\left(\left|\frac{v_\sigma}{\varepsilon K_\sigma}\right| r\right), \qquad \frac{\Delta r}{\Delta z} \leqslant \frac{1}{2} \min\left|\frac{v_\sigma}{v_\kappa}\right|. \tag{20}$$

From conditions (20) it follows that the stepwidths can be determined only if the coefficients K_σ are known. Therefore, the stepwidths chosen at the beginning of the calculation must eventually be corrected in the course of the iterative procedure. In general, we started the procedure with the curvature terms set equal to zero. After a few iterations, the maximal value of K_σ was estimated, and the stepwidths were corrected according to the conditions (20). The procedure was then continued with the complete curvature terms.

Since in our sample calculations, the coefficients K_σ strongly decrease with increasing r, the number of radial gridlines could be reduced by the use of local estimates for the coefficients K_σ. For all results discussed further below a stable grid was found by means of the following simple relations:

$$r_n = r_{n-1}/\sin\chi_n, \qquad \chi_{n+1} = \chi_n - \Delta\chi \qquad (n = 1,\ldots, N),$$

where $r_0 = 0.076D$, $\chi_1 = 85°$ and $\Delta\chi = 2°$.

Rate of Convergence

In the iterative procedure described above the alteration of the distribution functions in the course of the procedure is driven by the moments of the preceding iteration step, i.e., only local macroscopic quantities appear as an iterative driving function. Thus, the iteration procedure does not properly describe the tendency to global equilibrium driven by spatial variations of the moments, but rather maintains some properties of the generally arbitrary initial guess of the moments over a large number of iterative steps. For this reason, the iteration procedure was changed to ensure a better rate of convergence by using the derivatives of the macroscopic quantities as the iterative driving functions. This can be done easily in the following way. It is not intended to give rigid proof here, but rather to show by means of a simple example, how the solution converges in the course of the iterations.

We consider a steady, one-dimensional flow assuming all external forces to vanish and the distribution function to be governed by the model equation

$$v_x \frac{\partial f}{\partial x} = \nu(F - f). \tag{21}$$

Equation (21) is rewritten as

$$v_\kappa \frac{\partial f_\kappa^{(K)}}{\partial x} + \nu^{(K-1)} f_\kappa^{(K)} = \nu^{(K-1)} F_\kappa^{(K-1)}, \tag{22}$$

where K denotes the iteration step and κ indicates one of the discrete ordinates. With the abbreviation $c(x, v_\kappa) = \nu(x)/v_\kappa$, the solution of Eq. (22) is given by

$$f(x) = \left[f(x_0) + \int_{x_0}^{x} cFe^{\int_{x_0}^{x'} c dx''} dx' \right] e^{-\int_{x_0}^{x} c dx'}. \tag{23}$$

The subscript κ and the iteration index K are omitted for the sake of simplicity. The value $f(x_0)$ is assumed to be previously determined or given as a boundary value. Defining a mean value by

$$\bar{\bar{F}} = \frac{\int_{x_0}^{x} cFe^{\int_{x_0}^{x'} c dx''} dx'}{\int_{x_0}^{x} ce^{\int_{x_0}^{x'} c dx''} dx'}, \tag{24}$$

we put Eq. (23) in the form

$$f(x) = f(x_0)\, e^{-\int_{x_0}^{x} c dx'} + \bar{\bar{F}}(1 - e^{-\int_{x_0}^{x} c dx'}). \tag{25}$$

Equation (25) shows, that during the iteration the distribution function is given by a mean value of the Maxwellian distribution of the preceding iteration step. A difference approximation of Eq. (25) is obtained by considering x and x_0 as two neighbouring grid points,

$$x_0 = x - \Delta x \operatorname{sign}(v_\kappa), \tag{26}$$

$$\Delta x = |x - x_0|, \tag{27}$$

where $\operatorname{sign}(v_\kappa)$ takes into account the region of influence according to the direction of the molecular flow. Defining another mean value by

$$\bar{c} = \frac{1}{\Delta x} \int_{x_0}^{x} c\, dx', \tag{28}$$

we obtain

$$f(x)\, e^{|\bar{c}|\Delta x} = f(x_0) + \bar{\bar{F}}(e^{|\bar{c}|\Delta x} - 1). \tag{29}$$

The expansion of the exponential function up to the order $O(\Delta x)$ yields

$$f(x)(1 + |\bar{c}|\, \Delta x) = f(x_0) + \bar{\bar{F}} |\bar{c}|\, \Delta x. \tag{30}$$

The first-order finite-difference approximation of Eq. (22) is given by

$$\operatorname{sign}(v_\kappa) \frac{f(x) - f(x_0)}{\Delta x} + c(x) f(x) = c(x) F(x)$$

or

$$f(x)(1+|c|\,\Delta x)=f(x_0)+F|c|\,\Delta x. \tag{31}$$

The comparison of Eqs. (30) and (31) shows, that in the first-order finite-difference approximation of Eq. (22), the mean values appearing in Eq. (30) are replaced by the local values at the point x. For the case of equilibrium flow, $f=F$, or, from Eq. (21), $\partial F/\partial x=0$ implies, that the moments and, consequently, the collision frequency have no spatial dependence [2], so that the mean values coincide with the local values. Generally, an arbitrary guess of the moments is made at the beginning of the iterative procedure, so that even for the equilibrium solution the condition $\partial F/\partial x=0$ is not satisfied during iterations. In Eq. (30) the spatial dependence of the moments is smoothed by the mean values and, therefore, the tendency to the equilibrium state is involved in the iteration. With the use of Eq. (31) the influence of the initial guess decreases only gradually, causing the rather low rate of convergence of the iterative procedure.

To avoid the somewhat cumbersome numerical treatment of mean values, we put the iterative procedure into another form, in which the gradients of Maxwellian distributions are considered as a physical "driving force" to the equilibrium state. By means of partial integration, Eq. (23) can be put into the form

$$\Delta f(x)=\left[\Delta f(x_0)-\int_{x_0}^{x}\frac{\partial F}{\partial x}e^{\int_{x_0}^{x'}c\,dx''}\,dx'\right]e^{-\int_{x_0}^{x}c\,dx'}, \tag{32}$$

where

$$\Delta f=f-F$$

denotes the deviation of the distribution function from the local Maxwellian distribution. Equation (32) is seen to be the solution of

$$\frac{\partial\,\Delta f}{\partial x}+c\,\Delta f=-\frac{\partial F}{\partial x}. \tag{33}$$

Carrying out the same derivation as above we obtain

$$\Delta f(x)\,e^{|\bar{c}|\Delta x}=\Delta f(x_0)-\overline{\overline{\frac{1}{c}\frac{\partial F}{\partial x}}}\,(e^{|\bar{c}|\Delta x}-1). \tag{34}$$

The first-order approximation to Eq. (34) is given by

$$\Delta f(x)(1+|\bar{c}|\,\Delta x)=\Delta f(x_0)-\overline{\overline{\frac{1}{c}\frac{\partial F}{\partial x}}}\,|\bar{c}|\,\Delta x. \tag{35}$$

Comparison of Eq. (35) with the first-order finite-difference approximation of Eq. (33)

$$\Delta f(x)(1+|c|\,\Delta x)=\Delta f(x_0)-\frac{\partial F}{\partial x}\operatorname{sign}(v_\kappa)\,\Delta x, \tag{36}$$

$$\frac{\partial F}{\partial x}=\operatorname{sign}(v_\kappa)\frac{F(x)-F(x_0)}{\Delta x} \tag{37}$$

again shows, that the mean values are replaced by local values in Eq. (36), but now the gradient of the Maxwellian distribution function appears as the "driving force" in the iteration. In the following we show, that the application of the iterative procedure to the difference Δf instead of the distribution function f leads to a greater rate of convergence. Consider the more general solutions, Eqs. (29) and (34), respectively, with the mean replaced by local values. This is permissible, since Eqs. (31) and (36), respectively, may be considered as having been derived from the former. We restrict our considerations to the equilibrium solution of Eq. (21) and assume that in the preceding iteration step the Maxwellian distribution has taken on the constant equilibrium value F_s at all grid points except x. Omitting the bars in Eq. (29) (resp. Eq. (34)) and taking into account, that under the assumption made above, $f(x_0)=F(x_0)=F_s$, we obtain from Eq. (29),

$$|f(x)-F_s|=|(F(x)-F_s)(1-e^{-z})| \tag{38}$$

and from Eq. (34), respectively,

$$|f(x)-F_s|_\Delta=\left|(F(x)-F_s)\left(1-\frac{1-c^{-z}}{z}\right)\right|, \tag{39}$$

where $z=|c|\,\Delta x$ and the subscript Δ on the left-hand side of Eq. (39) indicates the application of the iterative procedure to Δf. Thus, we have to show, that

$$|f(x)-F_s|_\Delta\leqslant|f(x)-F_s|$$

or, since $0\leqslant 1-e^{-z}\leqslant z$, and, consequently, the second factors on the right-hand sides of Eqs. (38) and (39) are positive semi-definite,

$$1-\frac{1-e^{-z}}{z}\leqslant 1-e^{-z}. \tag{40}$$

Condition (40) is easily seen to be satisfied for all values of z.

The better rate of convergence of the iterative procedure, if applied to the difference of the distribution function Δf, was also proved in numerical experiments, in which the decay of a perturbation with amplitudes up to 100% of the solution value was observed. For the model equation (1), convergence was reached after 4 instead of 15 iteration steps on average, if the iteration procedure was applied to

the difference Δf instead of the distribution function itself. For the sample calculations described in the following, the number of required iteration steps could be reduced up to 25%.

Application of the Method of Solution

To illustrate the application of the method of solution, some results are reported here for axisymmetric jet flow in a finite-pressure background gas of different species [10]. The distribution functions f_i of jet and background gas are assumed to be governed by the extended model equations for binary gas mixtures [11, 12],

$$v_z \frac{\partial f_i}{\partial z} + v_r \frac{\partial f_i}{\partial r} + \frac{v_\varphi^2}{r} \frac{\partial f_i}{\partial v_r} - \frac{v_r v_\varphi}{r} \frac{\partial f_i}{\partial v_\varphi} = \nu_{ii}(F_i - f_i) + \nu_{ij}(F_{ij} - f_i), \tag{41}$$

where ν_{ii} and ν_{ij}, respectively, are the self- and cross-collision frequencies, F_i are the Maxwellian distributions of species i and F_{ij} Maxwellian distributions containing parameters n_{ij}, $\mathbf{U}_{ij}$, and T_{ij}, which, following the line given in [12], can be determined by comparing the conservation and relaxation equations of the model and the Boltzmann equations for binary gas mixtures. Similar to the case of a homogeneous gas, the collision frequencies may be expressed by a corresponding number of transport coefficients derived from the Boltzmann equations for a given intermolecular potential. For that purpose, we have chosen the diffusion coefficients, and, for the sake of simplicity, the hard-sphere model was applied. Thus, we obtain

$$\begin{aligned}
\nu_{ii} &= \frac{8(2\pi)^{1/2}}{3} n_i (2R_i T_M)^{1/2} d_i^2, \\
\nu_{ij} &= \frac{8(2\pi)^{1/2}}{3} n_j \left(\left(1 + \frac{m_i}{m_j} \right) R_i T_M \right)^{1/2} \left(\frac{d_i + d_j}{2} \right)^2, \\
T_M &= T_i + \frac{n_j}{n_i + n_j} (T_j - T_i) + \frac{n_i n_j m_j (\mathbf{U}_j - \mathbf{U}_i)^2}{3R_i (n_i + u_j)(n_i m_i + n_j m_j)}, \\
n_{ij} &= n_i, \\
\mathbf{U}_{ij} &= \mathbf{U}_i + \frac{m_j}{m_i + m_j} (\mathbf{U}_j - \mathbf{U}_i), \\
T_{ij} &= T_i + \frac{m_i m_j}{(m_i + m_j)^2} \left[2(T_j - T_i) + \frac{(\mathbf{U}_j - \mathbf{U}_i)^2}{\mathrm{R} R_j} \right],
\end{aligned} \tag{42}$$

where m_i and m_j are the molecular masses and d_i and d_j the molecular diameters.

For the formulation of the boundary conditions we consider the half-space $z \geqslant 0$ and assume, that the nozzle exit lies in the plane $z = 0$. Because of the hyperbolic type of Eqs. (41) in physical space, values of the distribution functions must be

prescribed at the entire boundary for molecules, the velocity vectors of which are directed into the integration domain. At infinity, we assume that the pressure is due to the background component only, which is supposed to be in the equilibrium state of a quiescent gas with given density $n_{B,\infty}$ and temperature T_∞,

$$\begin{aligned} z\to\infty,\quad 0\leqslant r\leqslant\infty: &\qquad f_{\mathrm{B}}^{-\pm}=F_{\mathrm{B}}^{-\pm}(n_{\mathrm{B},\infty},\mathbf{U}_{\mathrm{B}}=0,T_\infty;\mathbf{v}),\\ &\qquad f_{\mathrm{J}}^{-\pm}=0,\\ 0\leqslant z\leqslant\infty,\quad r\to\infty: &\qquad f_{\mathrm{B}}^{\pm-}=F_{\mathrm{B}}^{\pm-}(n_{\mathrm{B},\infty},\mathbf{U}_{\mathrm{B}}=0,T_\infty;\mathbf{v}),\\ &\qquad f_{\mathrm{J}}^{\pm-}=0, \end{aligned} \tag{43}$$

where the signs are chosen as in Eqs. (16) and the subscripts J and B denote the jet and background component. At the wall, diffuse reflexion is assumed for a given temperature T_{W},

$$z=0,\quad D/2\leqslant r\leqslant\infty: \qquad f_i^{+\pm}=F_i^{+\pm}(n_{i,\mathrm{W}},\mathbf{U}_i=0,T_{\mathrm{W}j}\,\mathbf{v}). \tag{44}$$

The wall densities $n_{i,\mathrm{W}}$ are not known a priori and must be determined by means of a further condition. For an impermeable wall, the particle fluxes normal to the wall vanish. Inserting Eqs. (44) into this condition, we get

$$n_{i,\mathrm{W}}=-\left(\frac{2\pi}{R_iT_{\mathrm{W}}}\right)^{1/2}\iint_{-\infty}^{\infty}\int_{-\infty}^{0}v_z(f_i^{-+}+f_i^{--})\,dv_z\,dv_\varphi\,dv_r\Big|_{z=0}. \tag{45}$$

For the nozzle exit, we assume that all background molecules with negative v_z-components are back-scattered in the inside of the nozzle by collisions with jet molecules, and that they have adapted the mean velocity $\mathbf{U}_D$ and the temperature T_D of the jet component when re-entering the domain of integration:

$$z=0,\quad 0\leqslant r<D/2: \qquad f_i^{+\pm}=F_i^{+\pm}(n_{i,\mathrm{D}},\mathbf{U}_{\mathrm{D}},T_{\mathrm{D}};\mathbf{v}). \tag{46}$$

The number densities $n_{i,\mathrm{D}}$ were determined from the condition of constant particle flux. Similar to Eqs. (45) this yields,

$$n_{i,\mathrm{D}}=\left(\frac{2\pi}{R_iT_{\mathrm{D}}}\right)^{1/2}S_i^{-1}\left[\Phi_{i,\mathrm{D}}-\iint_{-\infty}^{\infty}\int_{-\infty}^{0}v_z(f_i^{-+}+f_i^{--})\,dv_z\,dv_\varphi\,dv_r\Big|_{z=0}\right], \tag{47}$$

where the function S_i are given by

$$S_i=\exp\left\{-\frac{\mathbf{U}_{\mathrm{D}}^2}{2R_iT_{\mathrm{D}}}\right\}+\frac{|\mathbf{U}_{\mathrm{D}}|}{(2R_iT_{\mathrm{D}})^{1/2}}\operatorname{erfc}\left\{-\frac{|\mathbf{U}_{\mathrm{D}}|}{(2R_iT_{\mathrm{D}})^{1/2}}\right\},$$

and $\Phi_{i,\mathrm{D}}$ are the values of the chosen particle fluxes (erfc is the complementary error function). Finally, along the symmetry axis, we have

$$0\leqslant z\leqslant\infty,\quad r=0: \qquad f_i^{\pm+}(v_r)=f_i^{\pm-}(-v_r). \tag{48}$$

Introducing the transformation

$$\xi = 1 - \exp\{-\alpha_1 z/\mathrm{D}\}, \qquad \eta = 1 - \exp\{-\alpha_2 r/\mathrm{D}\}, \tag{49}$$

which ensures a correct representation of the boundary conditions at infinity, we obtain the approximated model equations for the reduced distribution functions,

$$\begin{aligned} v_z \frac{\alpha_1}{\mathrm{D}}(1-\xi)\frac{\partial g_i}{\partial \xi} + v_r \frac{\alpha_2}{\mathrm{D}}(1-\eta)\frac{\partial g_i}{\partial \eta} - \frac{\alpha_2 K_i g_i}{\mathrm{D}\ln(1-\eta)} \\ = A_{ii} v_{ii}(G_i - g_i) + A_{ij} \cdot v_{ij}(G_{ij} - g_i), \\ v_z \frac{\alpha_1}{\mathrm{D}}(1-\xi)\frac{\partial h_i}{\partial \xi} + v_r \frac{\alpha_2}{\mathrm{D}}(1-\eta)\frac{\partial h_i}{\partial \eta} - \frac{3\alpha_2 K_i g_i}{\mathrm{D}\ln(1-\eta)} \\ = A_{ii} v_{ii}(H_i - h_i) + A_{ij} v_{ij}(H_{ij} - h_i). \end{aligned} \tag{50}$$

In Eqs. (50) all variables were made dimensionless with the nozzle diameter D, the densities $n_{\mathrm{J,D}}$ and $n_{\mathrm{B},\infty}$ for the jet and the background component, respectively, the velocity $(2B_{\mathrm{B}}T_\infty)^{1/2}$ and the temperature T_∞ as reference quantities. The dimensionless quantities A_{ii} and A_{ij} may be expressed by the Knudsen numbers

$$\mathrm{Kn}_{\mathrm{J,D}} = (2^{1/2}\pi\, d_{\mathrm{J}}^2 n_{\mathrm{J,D}}\, \mathrm{D})^{-1}, \qquad \mathrm{Kn}_{\mathrm{B},\infty} = (2^{1/2}\pi\, d_{\mathrm{B}}^2 n_{\mathrm{B},\infty}\, \mathrm{D})^{-1},$$

and the ratios of molecular masses $M = m_{\mathrm{B}}/m_{\mathrm{J}}$ and diameters $\Delta = d_{\mathrm{B}}/d_{\mathrm{J}}$ as

$$\begin{aligned} A_{\mathrm{JJ}} &= \frac{8}{3}\left(\frac{M}{\pi}\right)^{1/2} \mathrm{Kn}_{\mathrm{J,D}}^{-1}, \\ A_{\mathrm{BB}} &= \frac{8}{3}\left(\frac{1}{\pi}\right)^{1/2} \mathrm{Kn}_{\mathrm{B},\infty}^{-1}, \\ A_{\mathrm{JB}} &= \frac{8}{3}\left(\frac{1+M}{2\pi}\right)^{1/2}\left(\frac{1+\Delta}{2\Delta}\right)^2 \mathrm{Kn}_{\mathrm{B},\infty}^{-1}, \\ A_{\mathrm{BJ}} &= \frac{8}{3}\left(\frac{1+M}{2\pi}\right)^{1/2}\left(\frac{1+\Delta}{2}\right)^2 \mathrm{Kn}_{\mathrm{J,D}}^{-1}. \end{aligned} \tag{51}$$

Introducing the new dependent variables Δg_i and Δh_i, the corresponding model equations are obtained from Eqs. (50) by substracting equivalent terms for the Maxwellians G_i and H_i. The boundary conditions, Eqs. (43)–(46), can be written in the simple form $\Delta g_i = 0$ and $\Delta h_i = 0$, respectively; the symmetry condition Eq. (48) is reduced to $\Delta f_i^{+\,+}(v_r) = \Delta f_i^{+\,-}(-v_r)$.

The model equations where discretized in the (ξ, η)-plane with constant stepwidths in the ξ direction and increasing stepwidths in the η direction; this choice was discussed in the stability analysis. According to Eqs. (16), in the computational procedure each quadrant of the velocity space requires a separate treatment. Since, for the boundary conditions at $\xi = 0$ and $\eta = 0$, the distribution

functions for the incoming molecules must be known, the sequence of the quadrants within the calculation is fixed. In each iteration step, the calculation starts at the point $(1-\Delta\xi, 1-\Delta\eta)$ for a chosen pair of discrete ordinates $v_\kappa < 0$, $v_\sigma < 0$ (Fig. 1). For this pair of discrete ordinates, the values of the distribution functions are then determined along the gridline $1-\Delta\xi$ until the axis $\eta = 0$ is reached. Applying the symmetry condition, the values of the distribution functions for the pair $(v_\kappa, -v_\sigma)$ can be calculated marching along the same gridline. This procedure is repeated for all gridlines $\xi = \text{const.}$ and for all discrete ordinates with $v_\kappa < 0$. After arriving at the line $\xi = 0$, the wall and nozzle densities may be determined from the boundary conditions. Then, for $v_\kappa > 0$ an analogous procedure is carried out until $\xi = 1-\Delta\xi$ is reached again. Thus, for all quadrants of the velocity space the distribution functions are determined and the moments may be calculated by means of a proper quadrature formula (Eqs. (14)). The iterative procedure was stopped when the differences of all moments in two successive iteration steps was less than 10^{-3}.

In the following some of the results calculated by means of the described method are reported. As a proper quadrature formula, the modified Gauss–Hermite half-range quadrature [13] with 8×8 discrete ordinates per quadrant of velocity space has been used. The (ξ, η) plane was covered by 26×31 grid points. In all cases the wall temperature was chosen to be $T_W = T_\infty$. To illustrate the influence of the centrifugal and the Coriolis force on the particle densities, Figs. 2 and 3 show the lines of constant density in plane and axisymmetric geometry for a sonic jet with $\mathrm{Kn}_{J,D} = 2.6 \times 10^{-2}$ and a background gas of equal species with $\mathrm{Kn}_{B,\infty} = 1.54 \times 10^{-1}$, respectively.

Both in plane and in axisymmetric geometry, Fig. 2 suggests that three flow regions can be distinguished with respect to the density of the jet near the symmetry plane or axis, respectively. Due to the very low number of background molecules near the nozzle exit (Fig. 3), there is a free expansion of the jet component, which is stopped at approximately two nozzle diameters by the onset of the jet-background interaction. This leads to a slight increase of the jet density farther downstream, which is steeper in plane geometry because of the steeper increase of the background density. This increase of the jet density corresponds to the onset of a normal shock, which in axisymmetric flow is known as Mach disk. After about four

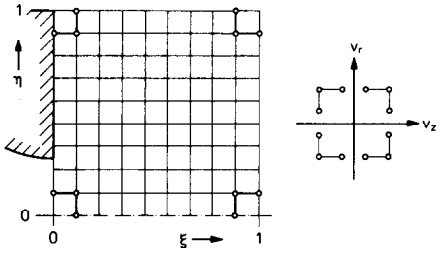

FIG. 1. Arrangemet of the difference schemes in the computational grid.

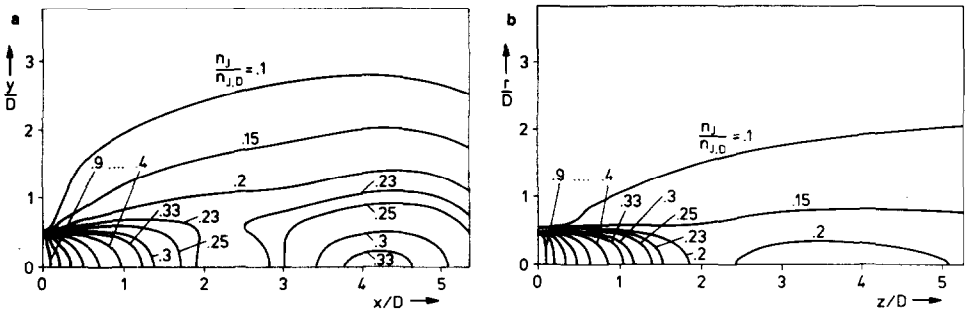

FIG. 2. Density distribution of the jet component in (a) plane and (b) axisymmetric flow.

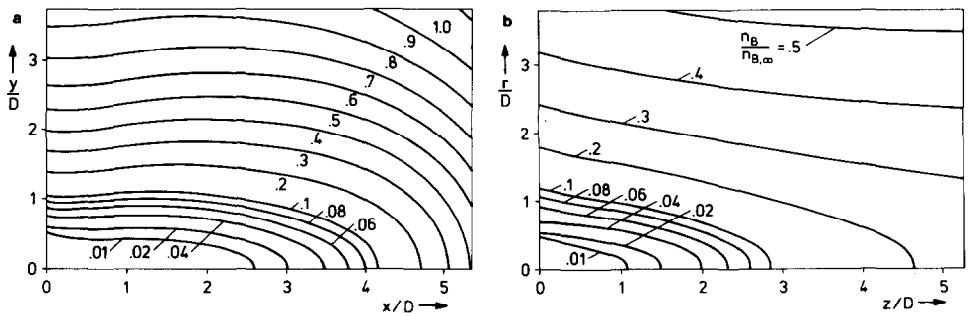

FIG. 3. Density distribution of the background component in (a) plane and (b) axisymmetric flow.

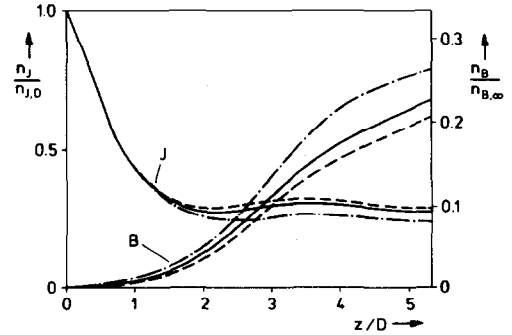

FIG. 4. Axial density distribution for different background species; $Kn_{J,D} = 2.60 \times 10^{-2}$, $Kn_{B,\infty} = 1.54 \times 10^{-1}$; (———), $M = 1$, $\Delta = 1$; (– – –), $M = 1.4266$, $\Delta = 0.9707$; (– · –), $M = 0.5725$, $\Delta = 1.1040$.

nozzle diameters, where the jet–background interaction is dominant, the jet density falls off again because of the increasing number of back-scattered jet molecules.

In Fig. 4 both jet and background density are plotted against the distance from the nozzle exit along the symmetry axis for different background species. For the case of a two-component background mixture, the different penetration behaviour of background components with different molecular masses, which is clearly seen in Fig. 4, leads to an enrichment of the light background component in the inner part of the jet structure ("jet membrane", e.g., [14]).

The sample calculations showed, that the additional computational effort, being due to the curvature terms, can be kept within reasonable bounds, if the v_φ- and v_r-dependence of the distribution function are prescribed approximately by ellipsoidal-type distribution functions in the curvature terms with the derivatives evaluated analytically. This approximation proved to be sufficiently accurate in the absence of strong shock waves normal or inclined to the radial direction. Furthermore, the sample calculations showed, that the improvement of the rate of convergence by using the deviation of the distribution function from the Maxwellian distribution, which was considered only for the equilibrium case, proved to be valid also for nonequilibrium flows.

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