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The nonlinear BGK model—a derivation and two applications

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Abstract. Employing a single well defined approximation, a derivation is given of the nonlinear BGK model. The model is applied to the formulation of equations governing the temporal and spatial variation of macroscopic parameters in the regime where changes in these parameters within a mean free path cannot be neglected. Using the model, an extension is given of earlier results concerning the sign of successive time derivatives of the entropy.

1. Derivation of the nonlinear BGK model

The rate of change due to intermolecular collisions of the distribution function $f(v)$ for a system of gas molecules can be expressed in the form

$$\left(\frac{\partial f}{\partial t}\right)_c = \int \int \int P(f_2 f_3 - f f_1) \, dv_1 \, dv_2 \, dv_3 \quad (1)$$

where $P(v, v_1, v_2, v_3)$ is a known function of the velocities and $f_n \equiv f(v_n)$ ($n = 1, 2, 3$). The well known BGK model (see, for example, Cercignani 1969) replaces the correct form (1) by the model operator

$$\left(\frac{\partial f}{\partial t}\right)_c^m = \nu(F(v) - f(v)) \quad (2)$$

where ν is a collision frequency and $F(v)$ is a Maxwell equilibrium distribution, given by

$$F = n \left(\frac{m}{2\pi kT}\right)^{3/2} \exp\left(-\frac{m}{2kT}(v - V)^2\right). \quad (3)$$

The latter contains five parameters σ_p ($= n, T, V_1, V_2, V_3$) corresponding to the five quantities γ_p (number, energy and three components of momentum) conserved in collisions and the values of these parameters are then determined by the equations

$$\int \nu \gamma_p (F - f) \, dv = 0 \quad (1 \leq p \leq 5) \quad (4)$$

which correspond to the requirement that the model operator should conserve overall the five γ_p which are conserved by the true operator $\partial f / \partial t$.

When all f are close to an equilibrium distribution the connection between the corresponding linearized forms for $\partial f / \partial t$ and $\partial f / \partial t$ has been clarified by Cercignani (1966). However, for the nonlinear forms it would appear that this has not yet been done. In particular an explicit form for ν as a function of v and the state of the gas has not been given and generally ν has been treated as an *ad hoc* parameter. It is the purpose of the

present section to remedy this, and this we shall do by making use of a single well defined approximation.

We begin by noting that in expression (1) an integration is performed over the variables v_1, v_2, v_3 on which f_1, f_2, f_3 depend and it is therefore reasonable to replace each of the f_1, f_2, f_3 (as distinct from f) by some average form involving parameters which can then be chosen to satisfy the condition

$$\int \gamma_p \left(\frac{\partial f}{\partial t} \right)_c d\mathbf{v} = 0 \quad (5)$$

which is satisfied by the true collision operator. We choose for this average form equilibrium distributions F_1, F_2, F_3 involving undetermined parameters σ_p and note that the number of such parameters is equal to the number of equations (5). This gives

$$\left(\frac{\partial f}{\partial t} \right)_c^m = \int P(F_2 F_3 - f F_1) d\mathbf{v}_1 d\mathbf{v}_2 d\mathbf{v}_3. \quad (6)$$

Now since F is an equilibrium distribution, it is known that

$$\int P(F_2 F_3 - F F_1) d\mathbf{v}_1 d\mathbf{v}_2 d\mathbf{v}_3 = 0 \quad (7)$$

and hence on eliminating $F_2 F_3$ between equations (6) and (7) we obtain equation (2) with

$$v = \int P F_1 d\mathbf{v}_1 d\mathbf{v}_2 d\mathbf{v}_3. \quad (8)$$

It is clear from this that v will depend on v (since P does) and also on all the σ_p since F_1 involves them; the precise dependence on these variables is given by equation (8). The detailed evaluation of v is considered by Cercignani (1969) for the cases of hard-sphere molecules and power-law intermolecular potentials with angular cut-off. In all these cases v depends on v , except for the case of Maxwell molecules where v turns out to be constant. For hard-sphere molecules the variation of v with v for v in the region of \bar{v} is also quite slow, since v only changes by a factor of about two as v varies between $0.25 \bar{v}$ and $2 \bar{v}$.

The values of the σ_p are now obtained from equation (4), but the explicit dependence of v on the σ_p now makes the application of this equation more complicated. If the f are all close to an equilibrium distribution it is readily shown that the above analysis reduces to that of Cercignani (1966) for the linearized case with the values of σ_p to be used with v corresponding to those of the equilibrium distribution. However, in general the values of σ_p will *not* equal those of an equilibrium distribution with the same total γ_p as the given nonequilibrium distribution, since this latter condition would correspond to

$$\int \gamma_p (F - f) d\mathbf{v} = 0 \quad (9)$$

which in general differs from equation (4). The two equations are only identical if v is independent of v .

2. Application of the BGK model to general spatial and temporal variations of the macroscopic parameters σ_p

We proceed to derive in this section general partial differential equations governing the spatial and temporal variation of the parameters σ_p when the collision operator is represented by the BGK model (2) with ν given by equation (8). Our approach will lead to the familiar Navier–Stokes equations in the first approximation and corrections to them in higher approximations.

We begin by considering the general Boltzmann equation for the system which takes the form

$$\left(\frac{\partial f}{\partial t}\right)_c = \frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla f \tag{10}$$

where $f \equiv f(\mathbf{v}, \mathbf{r}, t)$. On using the model (2) equation (10) becomes

$$(1 + \tau L)f = F \tag{11}$$

where $\tau = \nu^{-1}$ and $L \equiv (\partial/\partial t) + \mathbf{v} \cdot \nabla$. Subject to convergence criteria we may expand $(1 + \tau L)^{-1}$ as a power series in τL to yield the solution of equation (11) as

$$f = (1 - \tau L + \tau L \tau L - \dots)F \tag{12}$$

where it must be borne in mind that τ and L do not in general commute since τ involves the σ_p which are themselves dependent on \mathbf{r} and t . We now apply the condition (4) to the solution (12) and this yields

$$\int \gamma_p L F \, d\mathbf{v} - \int \gamma_p L \tau L F \, d\mathbf{v} + \dots = 0 \quad (1 \leq p \leq 5) \tag{13}$$

which on substituting for F from equation (3), gives the basic set of five partial differential equations governing the σ_p . It is clear that the ratio of successive terms in this expansion is of the order of $\Delta F/F$ where ΔF is the change in F in a mean free path or a relaxation time and thus if $\Delta F/F$ is not too large, a sufficiently accurate result may be obtained by curtailing the series (13) after the required number of terms.

Before developing equation (13) further, we must emphasize that in general, as discussed in § 1, the values of the σ_p given by the solution of equations (13) will not be the physical values of these parameters as would be given, for example, by measuring the temperature (or other parameter) at a point. The physical value (in which we are principally interested) σ_p^* is obtained by equating the total value of γ_p for the given nonequilibrium distribution f to that of an equilibrium distribution with parameter values σ_p^* . This corresponds to

$$\begin{aligned} \int \gamma_p F(\sigma_1^*, \dots) \, d\mathbf{v} &= \int \gamma_p f \, d\mathbf{v} \\ &= \int \gamma_p F(\sigma_1, \dots) \, d\mathbf{v} - \int \gamma_p \tau L F(\sigma_1, \dots) \, d\mathbf{v} + \dots \end{aligned} \quad (1 \leq p \leq 5) \tag{14}$$

on using the solution (12). This gives a set of five equations in each of which a certain function of the σ_p^* (as obtained by integrating the left hand side of equation (14)) is equated to specific functions of the σ_p . Thus if equations (12) together with appropriate boundary conditions have been solved for the σ_p as a function of \mathbf{r} and t , equations (14)

may then be used to obtain the corresponding σ_p^* . We may note that if τ is independent of v it follows from equation (13) that, apart from the first term, the right hand side of equation (14) is zero, and therefore $\sigma_p^* = \sigma_p$. This is in agreement with the point made in § 1 that the σ_p correspond to the ‘physical value’ of the parameter only if τ is independent of v .

We now return to equation (13) whose first term is readily shown to be equivalent to the Navier–Stokes equations, bearing in mind that in this approximation $\sigma_p^* = \sigma_p$ as only the first term of equation (14) is significant.

Considering now the first two terms on the left hand side of equation (13), it is readily shown that this equation takes the form

$$\begin{aligned} & \left(\frac{\partial}{\partial t}\right) \int \gamma_p F \, d\mathbf{v} + \left(\frac{\partial}{\partial x_q}\right) \int \gamma_p v_q F \, d\mathbf{v} + \left(\frac{\partial^2}{\partial t^2}\right) \int \gamma_p \tau F \, d\mathbf{v} \\ & + 2\left(\frac{\partial^2}{\partial x_s \partial t}\right) \int v_s \gamma_p \tau F \, d\mathbf{v} + \left(\frac{\partial^2}{\partial x_s \partial x_q}\right) \int v_s v_q \gamma_p \tau F \, d\mathbf{v} \\ & - \left\{ \frac{\partial}{\partial t} \left(\frac{\partial \sigma_r}{\partial t} \int \gamma_p F \frac{\partial \tau}{\partial \sigma_r} \, d\mathbf{v} + \frac{\partial \sigma_r}{\partial x_q} \int \gamma_p v_q F \frac{\partial \tau}{\partial \sigma_r} \, d\mathbf{v} \right) \right. \\ & \left. + \frac{\partial}{\partial x_s} \left(\frac{\partial \sigma_r}{\partial t} \int \gamma_p v_s F \frac{\partial \tau}{\partial \sigma_r} \, d\mathbf{v} + \frac{\partial \sigma_r}{\partial x_q} \int \gamma_p v_q v_s F \frac{\partial \tau}{\partial \sigma_r} \, d\mathbf{v} \right) \right\} = 0 \end{aligned} \tag{15}$$

and if τ can be taken as independent of the σ_p , then the term inside the large braces in equation (15) is zero. On substituting for F from equation (3), together with the five forms for γ_p , equation (15) will yield a set of five second order differential equations for the σ_p . The relation between σ_p^* and σ_p is given by equation (14) and retaining the first two terms on the right hand side gives

$$S_p(\sigma_1^*, \dots, \sigma_5^*) = S_p(\sigma_1, \dots, \sigma_5) - T_p(\sigma_1, \dots, \sigma_5) \quad (1 \leq p \leq 5) \tag{16}$$

where

$$S_p = \int \gamma_p F \, d\mathbf{v}$$

and

$$T_p = \left(\frac{\partial}{\partial t}\right) \int \gamma_p \tau F \, d\mathbf{v} + \left(\frac{\partial}{\partial x_q}\right) \int v_q \gamma_p \tau F \, d\mathbf{v} - \frac{\partial \sigma_r}{\partial t} \int \gamma_p F \frac{\partial \tau}{\partial \sigma_r} \, d\mathbf{v} - \frac{\partial \sigma_r}{\partial x_q} \int \gamma_p v_q F \frac{\partial \tau}{\partial \sigma_r} \, d\mathbf{v}. \tag{17}$$

Thus $\sigma_p^*(\mathbf{r}, t)$ can be found if $\sigma_p(\mathbf{r}, t)$ is known. Equations (15) and (16) are the analogue in the present treatment of the Burnett equations in the conventional approach. Equation (15) simplifies if τ is independent of v , as all terms involving τ can then be taken outside the relevant integrals and if, in addition τ is independent of the σ_p , equations (15) become

$$\begin{aligned} & \left(\frac{\partial}{\partial t}\right) \int \gamma_p F \, d\mathbf{v} + \left(\frac{\partial}{\partial x_q}\right) \int \gamma_p v_q F \, d\mathbf{v} \\ & + \tau \left\{ \left(\frac{\partial^2}{\partial t^2}\right) \int \gamma_p F \, d\mathbf{v} + 2\left(\frac{\partial^2}{\partial x_s \partial t}\right) \int v_s \gamma_p F \, d\mathbf{v} + \left(\frac{\partial^2}{\partial x_s \partial x_q}\right) \int v_s v_q \gamma_p F \, d\mathbf{v} \right\} = 0 \end{aligned} \tag{18}$$

with $\sigma_p^* = \sigma_p$. The derivation of this equation and equation (15) shows them to be valid when the proportional effect of the terms after the first two terms is small. This suggests that an iterative technique could be employed for the solution: we first solve equation (15) retaining only the first two terms and then substitute this solution for σ_p into the neglected terms in order to obtain second and subsequent iterates of σ_p .

Finally we consider the situation when the parameters σ_p depart by only a small amount from a spatially and temporally constant value σ_p^0 ; this corresponds to the linearized problem where the distribution function is always close to a constant equilibrium distribution. We therefore let

$$\sigma_p = \sigma_p^0 + \sigma'_p \tag{19}$$

with $|\sigma'_p| \ll |\sigma_p^0|$, and in terms $B(\sigma_1, \dots, \sigma_5)$ occurring in integrands of equation (15), we put

$$B(\sigma_1, \dots, \sigma_5) = B(\sigma_1^0, \dots, \sigma_5^0) + \left. \frac{\partial B}{\partial \sigma_r} \right|_{\sigma = \sigma^0} \sigma'_r. \tag{20}$$

Equations (15) then become

$$A_{pr} \frac{\partial \sigma'_r}{\partial t} + B_{pqr} \frac{\partial \sigma'_r}{\partial x_q} + C_{pr} \frac{\partial^2 \sigma'_r}{\partial t^2} + D_{prs} \frac{\partial^2 \sigma'_r}{\partial x_s \partial t} + E_{pqsr} \frac{\partial^2 \sigma'_r}{\partial x_q \partial x_s} = 0 \tag{21a}$$

where

$$\begin{aligned} A_{pr} &= \int \gamma_p \frac{\partial F}{\partial \sigma_r} \Big|_0 \, dv & B_{pqr} &= \int \gamma_p v_q \frac{\partial F}{\partial \sigma_r} \Big|_0 \, dv \\ C_{pr} &= \int \gamma_p \tau \frac{\partial F}{\partial \sigma_r} \Big|_0 \, dv & D_{prs} &= 2 \int \gamma_p v_s \tau \frac{\partial F}{\partial \sigma_r} \Big|_0 \, dv \\ E_{pqsr} &= \int \gamma_p v_s v_q \tau \frac{\partial F}{\partial \sigma_r} \Big|_0 \, dv. \end{aligned} \tag{21b}$$

Letting $\sigma_p^* = \sigma_p^0 + \mu_p$, it readily follows from equations (16) and (17) that:

$$\mu_p = \sigma'_p - F_{pr} \frac{\partial \sigma'_r}{\partial t} - G_{pqr} \frac{\partial \sigma'_r}{\partial x_q} \tag{22a}$$

where

$$F_{pr} = \frac{\int \gamma_p \tau \frac{\partial F}{\partial \sigma_r} \Big|_0 \, dv}{\int \gamma_p \frac{\partial F}{\partial \sigma_r} \Big|_0 \, dv} \quad G_{pqr} = \frac{\int \gamma_p v_q \tau \frac{\partial F}{\partial \sigma_r} \Big|_0 \, dv}{\int \gamma_p \frac{\partial F}{\partial \sigma_r} \Big|_0 \, dv} \tag{22b}$$

and substituting from equation (22) into (21) gives the following second order equation for μ_p :

$$\begin{aligned} A_{pr} \frac{\partial \mu_r}{\partial t} + B_{pqr} \frac{\partial \mu_r}{\partial x_q} + (C_{pr} + A_{ps} F_{sr}) \frac{\partial^2 \mu_r}{\partial t^2} \\ + (D_{prs} + A_{pq} G_{qsr} + B_{psq} F_{qr}) \frac{\partial^2 \mu_r}{\partial x_s \partial t} + (E_{pqrs} + B_{pqt} G_{istr}) \frac{\partial^2 \mu_r}{\partial x_q \partial x_s} = 0. \end{aligned} \tag{23}$$

As mentioned earlier, $\mu = \sigma'$ if τ is independent of v . Again, as in the nonlinear case, an iterative approach to the solution with given boundary conditions is indicated. Finally we may make the point that in many linearized problems the equilibrium value

$v^0 = 0$. This means that $\partial F/\partial T)_0$ and $\partial F/\partial n)_0$ will be even functions of v while $\partial F/\partial v_p)_0$ will be odd. This in turn implies that many of the integrals appearing in equations (21b) and (22b) will be zero.

3. Application to entropy production

It is known that the approach to equilibrium for an isolated system is characterized by the time variation of the entropy being such that

$$ds/dt \geq 0. \quad (24)$$

It has been pointed out previously (Simons 1969, 1971a, 1971b) that for certain systems the result (24) may be generalized to the form

$$(-1)^n d^n s/dt^n \leq 0 \quad (25)$$

for $1 \leq n \leq N$ where in some cases N is finite and in others $N = \infty$. These earlier discussions were, however, restricted to systems in which the physical quantities varied by only a small amount from local equilibrium values, and it is therefore clearly of interest to examine whether the inequality (25) is true for any systems in which large variations in these quantities can occur. In the present section we employ the BGK model to discuss the case of a spatially homogeneous gas relaxing to equilibrium with arbitrary initial values of the distribution function $f(v, t)$. For simplicity we shall deal with the case of Maxwell molecules where, as mentioned in § 1, ν is independent of v , and proceed to show that inequality (25) holds for $1 \leq n \leq 10$.

We begin with the general expression

$$s = -k \int f \ln f \, dv \quad (26)$$

for the entropy density of the gas, and differentiating with respect to time we obtain

$$\frac{ds}{dt} = -k \int (1 + \ln f) \frac{\partial f}{\partial t} \, dv. \quad (27)$$

Now if F is a Maxwell equilibrium distribution, $\ln F$ is a linear combination of the five quantities γ_p conserved in collisions, and so

$$\int \frac{\partial f}{\partial t} \ln F \, dv = 0 = \int \frac{\partial f}{\partial t} \, dv$$

from which equation (27) may be expressed in the form

$$\frac{ds}{dt} = k \int \frac{\partial f}{\partial t} \ln \left(\frac{F}{f} \right) \, dv. \quad (28)$$

Substituting for $\partial f/\partial t$ from the model operator (2), it follows that:

$$\frac{ds}{dt} = kv \int (F - f) \ln \left(\frac{F}{f} \right) \, dv = kv \int fu \ln(u + 1) \, dv \quad (29)$$

where

$$u = (F/f) - 1. \quad (30)$$

In order to differentiate equation (29) repeatedly we first note that, as pointed out at the end of § 1, the relevant σ_p for both F and v will equal those of an equilibrium distribution with the same total γ_p as the given nonequilibrium distribution, since v is assumed independent of v . Since this total γ_p is unaltered throughout the evolution of the system with time, it follows that σ_p and hence F and v will be independent of the time. Now, it is readily seen from equation (2) and (30) that

$$\frac{\partial u}{\partial t} = -vu(u+1) \quad \text{and} \quad \frac{\partial(fu)}{\partial t} = -vfu \tag{31}$$

and it therefore follows from equation (29) that :

$$\frac{d^2s}{dt^2} = -kv^2 \int fu\{\ln(u+1)+u\} dv. \tag{32}$$

Further differentiation of this equation, combined with induction, readily leads to the result that

$$\frac{d^n s}{dt^n} = (-1)^{n-1} kv^n \int fu\{\ln(u+1)+H_n(u)\} dv \tag{33}$$

where $H_n(u)$ is a polynomial in u of degree $n-1$ given by the recurrence relation

$$H_{n+1}(u) = u + H_n(u) + u(u+1) dH_n(u)/du \tag{34}$$

with $H_1(u) = 0$. Now, since f and F are both positive it follows from equation (30) that $-1 \leq u \leq \infty$, and the required result (25) will therefore hold for those values of n for which the integrand z in equation (33) is positive for the above range of values of u . We consider separately the ranges $0 \leq u \leq \infty$ and $-1 \leq u \leq 0$. To deal with the former range, we note that $H_n(u)$ is a polynomial with all coefficients positive (by induction from relation (34)) and hence for positive u , z is positive for all n . For the latter range, that is, $-1 \leq u \leq 0$, it is clear that z will be positive if the function

$$J_n(u) = \ln(1+u) + H_n(u) \tag{35}$$

is negative. To examine the range of values of n for which this holds, the polynomials $H_n(u)$ were generated on a computer for values of $n = 1, 2, \dots$ and the corresponding values of $J_n(u)$ were computed at intervals of 0.01 for the range $0 \geq u \geq -0.99$. As a result it was found that throughout this range $J_n(u)$ remains negative for $1 \leq n \leq 10$ but becomes positive over part of the range for $n = 11$. We therefore conclude that equation (25) holds for the system with $1 \leq n \leq 10$. This means that $S - S_{eq}$ and its first nine derivatives tend monotonically to zero as $t \rightarrow \infty$. Although this result has only been proved here for Maxwell molecules where v is constant, it may be possible to generalize it, at least for some range of n , to other intermolecular potentials such as hard-sphere molecules where, as mentioned in § 1, the variation of v with v can be quite slow.

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