The ES-BGK Model Equation with correct Prandtl number

Pierre Andries* and Benoit Perthame†

* INRIA, 78153 Le Chesnay, France and University of Kyoto, 606-8501, Japan
† INRIA, 78153 Le Chesnay, and Ecole Normale Superieure, 75005 Paris, France

Abstract. To avoid the complexity of the Boltzmann collision operator, the BGK Model Equation is widely used, but it is well known that one of its shortcomings is that it gives a Prandtl number of one in the fluid limit. The ES-BGK was introduced to obtain the correct Prandtl number, but the entropy property for this model was an open problem. In this talk we prove that this model actually verifies an H-stability theorem. Moreover, we show in a simple case that computations with this model are of the same order of complexity and cost as with the BGK model, so that it appears as a valid alternative of the BGK model.

INTRODUCTION

In rarefied regimes, a gas is best modeled by the Boltzmann equation,

$$\partial_t f + \mathbf{v} \cdot \nabla_x f = Q(f).$$

(1)

which governs the evolution of the density of particles $f$ in the phase i.e. in the monoatomic case $f = f(t, \mathbf{x}, \mathbf{v})$, $t \geq 0, (\mathbf{x}, \mathbf{v}) \in \mathbb{R}^3 \times \mathbb{R}^3$. Since the quadratic collision operator $Q(f)$ has a rather complex form, simpler models have been introduced and are commonly used. These models should respect the basic relaxation properties of the gas under study and should be easier to handle numerically. More precisely, we are looking for models whose hydrodynamic limits can be easily accessed and have the right transport coefficients. The simplest model is the BGK model based on relaxation towards local Maxwellians

$$Q(f) = A_c P(M[f] - f).$$

(2)

This model has the advantage of describing the right fluid limit. But in the Chapman-Enskog expansion, the transport coefficients, that is $\mu$ and $\kappa$ obtained at the Navier-Stokes level are not satisfactory, as their ratio, the Prandtl number, is equal to 1. For most gases, we have $Pr < 1$. In particular, the Maxwellian particles model in Boltzmann equation leads to a Prandtl number of 2/3.

A model was proposed by Holway [3] which gives non-negative distribution and a Prandtl number less than one, and various studies and numerical simulations have been conducted with results in good agreement with experimental data, see for example [2]. The actual form of the model, called Ellipsoidal Statistical (ES) model, involves non-convex quantities for $\frac{2}{3} \leq Pr \leq 1$. This fact made unlikely that the entropy inequality (a convex relation) might hold true and the problem of proving or disproving the H-Theorem was left open.

In this talk we solve this long standing question by showing that the model satisfies indeed the entropy inequality for the range $\frac{2}{3} \leq Pr \leq 1$. A second purpose of this talk is to verify that this model can be implemented practically, and that the implementation and computation is of the same order of complexity as the BGK model. In particular it is shown that the reduction of variables, a technique widely used for simple 1D problems and one of the main advantage of the BGK model - see [5] for example- can be extended to the ES-BGK model. Thus a finite difference scheme can be written and very precise results can be obtained at a small computational cost.
PRESENTATION OF THE MODEL

The collision operator

In the ES-BGK model the collision operator \( Q(f) \) is written as
\[
Q(f) = A_c \rho \mathcal{G}[f] - f, \tag{3}
\]
where \( G \) is a Gaussian with a quadratic form in the exponential term
\[
\mathcal{G}[f] = \frac{\rho}{\sqrt{\det(2\pi \mathcal{T})}} \exp \left( -\frac{1}{2} (u - u) \cdot \mathcal{T}^{-1} \cdot (u - u) \right). \tag{4}
\]
The choice of the matrix \( \mathcal{T} \) is the following
\[
\mathcal{T} = (1 - \nu)RTId + \nu \Theta, \tag{5}
\]
where \( \Theta \) is the pressure tensor associated to \( f \) and \( \nu \) is a parameter to be set afterwards.

Remark first that the choice \( \nu = 0 \) gives the classical BGK model and \( \nu = 1 \) gives the relaxation towards a Gaussian with the same pressure tensor as \( f \), the so-called 10 moments model (see \cite{4} ).
The model is valid when \( \mathcal{T} \) is invertible, so we have to check for which range of \( \nu \) this holds true.
When \( 0 \leq \nu \leq 1 \) it is easy to see that the matrix \( \mathcal{T} \) is strictly positive (and therefore invertible) when one considers \( \Theta \) in a diagonal base. In this base \( \mathcal{T} \) is also diagonal and its eigenvalues are a convex combination of \( RT \) and the eigenvalues of \( \Theta \). Since \( \Theta \) is a strictly positive matrix, the result follows.

In fact this idea can be extended to some (apparently) non-convex combinations of \( RTId \) and \( \Theta \). Let us denote by \( \lambda_1, \lambda_2, \lambda_3 \) the eigenvalues of \( \Theta \) and remember that \( 3RT = \lambda_1 + \lambda_2 + \lambda_3 \) (this is because the temperature is the trace of the pressure tensor), the eigenvalues of \( \mathcal{T} \) can be computed
\[
\mathcal{T}_i = \frac{1 - \nu}{3} \sum_j \lambda_j + \nu \lambda_i, \tag{6}
\]
\[
\mathcal{T}_i = \frac{1 + 2\nu}{3} \lambda_i + \frac{1 - \nu}{3} \sum_{j \neq i} \lambda_j. \tag{7}
\]
These are strictly positive when \( 1 + 2\nu \) and \( 1 - \nu \) are (simply) positive, so that the range of validity extends to \( -\frac{1}{2} \leq \nu \leq 1 \).

Introducing the matrices
\[
\Lambda_1 = \begin{pmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \end{pmatrix}, \quad \Lambda_2 = \begin{pmatrix} 0 & 0 & 0 \\ \lambda_2 & 0 & 0 \\ 0 & \lambda_3 & 0 \end{pmatrix}, \quad \Lambda_3 = \begin{pmatrix} \lambda_3 & 0 & 0 \\ 0 & \lambda_1 & 0 \\ 0 & 0 & \lambda_2 \end{pmatrix}, \tag{8}
\]

it follows from the computations above that, in a diagonal base for \( \Theta \)
\[
\mathcal{T} = \frac{1 + 2\nu}{3} \Lambda_1 + \frac{1 - \nu}{3} \Lambda_2 + \frac{1 - \nu}{3} \Lambda_3. \tag{9}
\]
This means that \( \mathcal{T} \) is a convex combination of three strictly positive matrices for the range of \( \nu \) we consider
(this will be one key point of the entropy proof).

Checking now the validity of this model from a physical point of view, it is essential to verify the conservation laws for the collision operator. In fact these are straightforward when one computes the three first moments of the Gaussian which are respectively \( \rho, \ u, \) and \( \text{trace}(\mathcal{T}) = 3RT \).
Another essential physical property (which is not verified in the Gaussian model proposed by Levermore in \cite{4}) is that the only equilibriums are Maxwellian distributions. In this model this is true for \( \nu < 1 \), since at equilibrium
\[
f = \mathcal{G}. \tag{10}
\]
Computing the pressure tensor (i.e. the integration over \( v_i v_j dv \)) of these two terms one obtain by definition \( \Theta \) on the left side and easily \( \mathcal{T} \) on the right side,
\[
\Theta = \mathcal{T} = (1 - \nu)RTId + \nu \Theta. \tag{11}
\]
When \( \nu \neq 1 \) one obtains \( \Theta = \mathcal{T} = RTId \), which means that the Gaussian is a Maxwellian, \( f = \mathcal{G} = \mathcal{M} \).

31
Chapmann-Enskogg expansion

Although this model verifies some basic mathematical and physical properties, we must keep in mind that it was introduced to obtain of Prandtl number different from one (else its usefulness as compared to BGK vanishes).

Here, without entering into the details and complexity of the Chapmann-Enskogg expansion we briefly recall how this result was obtained by Holway (see [3]).

For simplicity, we do not make the computations but simply stress the differences between the ES-BGK and BGK models.

Writing the collision operator in the following way,

$$\partial_t f + v \cdot \nabla_x f = \frac{1}{\epsilon} (\tilde{G}[f] - f),$$

we want to write $f$ as a power expansion of $\epsilon$. From

$$f = \tilde{G}[f] - \epsilon (\partial_t f + v \cdot \nabla_x f),$$

it is clear that the first order term is the equilibrium distribution which is a Maxwellian distribution (from now on we consider $\nu < 1$); including this in the first order development, one obtains

$$f^e = \tilde{G}[f^e] - \epsilon (\partial_t M[f^e] + v \cdot \nabla_x M[f^e]) + O(\epsilon^2).$$

It is completely evident that the BGK development is exactly the same, taking a Maxwellian instead of the Gaussian as the first term on the right.

To obtain a system based on macroscopic quantities, one has to compute the moments of $f^e$ which will also be considered as power expansions of $\epsilon$. The difference between the ES-BGK and BGK expansions will appear only from the difference of the moments of $M$ and $G$.

The third moment of both $M$ and $G$ (the integration over $(v_i - u_i)^2(v_i - u_i)dv$) is null by simple parity considerations. It is then clear that the BGK and ES-BGK equation will lead to the same development for the heat flux equation.

For the second order moment (the integration over $(v_i - u_i)(v_j - u_j)dv$) it is easy to obtain that the Gaussian gives $T_{ij}$, recalling the definition of $T_{ij}$ we obtain from 14

$$\Theta = (1 - \nu)RTIId + \nu \Theta + O(\epsilon)$$

$$\Theta = RTIId + \frac{1}{1 - \nu} O(\epsilon).$$

Because the BGK equation (directly, or taking $\nu = 0$ above) gives $\Theta = RTIId + O(\epsilon)$, we conclude that the correction given by the ES-BGK model is that the first order term of the development of the stress tensor is divided by $1 - \nu$.

It is a classical result that the BGK equation leads in the first order to the Navier Stokes system with a Prandtl number of one. Combining this with the results above, the ES-BGK model will lead to the same system except that the viscosity coefficient is divided by $1 - \nu$, the heat conductivity being unchanged. Taking the ratio of these two coefficients, we obtain

$$Pr_{ES-BGK} = \frac{1}{1 - \nu}Pr_{BGK} = \frac{1}{1 - \nu}.$$

Remark that the physically relevant Prandtl number of $\frac{2}{3}$ (which is exactly derived from the Boltzmann equation for maxwellian particles) is obtained from the lower range of $\nu = -\frac{1}{2}$. 

32
We prove here the entropy inequality
\[ \partial_t \int H(f) dv + \text{div} \int vH(f) dv \leq 0, \quad (18) \]

where
\[ H(f) = f \ln f. \]

First, using the definition of the ES-BGK collision operator and the convexity of the function \( H \)
\begin{align*}
\partial_t \int_{\mathbb{R}^3} H(f) dv + \nabla_x \cdot \int_{\mathbb{R}^3} vH(f) dv &= A_c \rho \int_{\mathbb{R}^3} H'(f)(\tilde{g} - f) dv \\
&\leq A_c \rho \int_{\mathbb{R}^3} (H(\tilde{g}) - H(f)) dv.
\end{align*}

It is thus sufficient to prove
\[ \int H(\tilde{g}) dv \leq \int H(f) dv. \quad (19) \]

A classical result is that this inequality holds if the gaussian is taken over the pression tensor of \( f \), that is in the case \( \nu = 1 \). This can be easily obtained from the 10 moment problem (see \cite{4}): given a pression tensor, a mean velocity and a density, the distribution with the lowest entropy is the gaussian distribution (with the imposed pression tensor). Denoting by \( \mathcal{G}_\theta \) this gaussian distribution and \( S \) the entropy, we have in other words
\[ S(\mathcal{M}) \leq S(\mathcal{G}_\theta) \leq S(f). \quad (20) \]

It is thus sufficient to prove that the Gaussian of the ES-BGK model as a lower entropy that the Gaussian of the 10 moments problem, that is
\[ S(\tilde{g}) \leq S(\mathcal{G}_\theta) \quad (21) \]
for \( -\frac{1}{2} \leq \nu < 1 \).

These quantities can be computed and one obtains
\[ S(\tilde{g}) = \rho \ln \left( \frac{\rho}{\sqrt{\det(2\pi T)}} \right) - \frac{5}{2} \rho, \quad (22) \]
yielding
\begin{align*}
S(\tilde{g}) - S(\mathcal{G}_\theta) &= \rho \ln \left( \frac{\rho}{\sqrt{\det(2\pi T)}} \right) - \rho \ln \left( \frac{\rho}{\sqrt{\det(2\pi \Theta)}} \right) \\
&= \frac{1}{2} \rho \ln \frac{\det \Theta}{\det T},
\end{align*}

Thus, we just have to prove that
\[ \det T \geq \det \Theta. \quad (23) \]

This is obtained as a lemma of matrix theory.
Lemma of matrix theory

We prove here from a mathematical point of view

\[ \det \mathcal{T} \geq \det \Theta. \] (24)

Here \( \mathcal{T} \) is related to \( \Theta \) by \( \nu \). This is not a convex combination when \( -\frac{1}{2} \leq \nu < 0 \) so that we write as in \( 9 \)

\[ \mathcal{T} = \frac{1 + 2\nu}{3} \Lambda_1 + \frac{1 - \nu}{3} \Lambda_2 + \frac{1 - \nu}{3} \Lambda_3 \] (25)

where

\[ \Lambda_1 = \begin{pmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \end{pmatrix}, \quad \Lambda_2 = \begin{pmatrix} \lambda_2 & 0 & 0 \\ 0 & \lambda_3 & 0 \\ 0 & 0 & \lambda_1 \end{pmatrix}, \quad \Lambda_3 = \begin{pmatrix} \lambda_3 & 0 & 0 \\ 0 & \lambda_1 & 0 \\ 0 & 0 & \lambda_2 \end{pmatrix}. \] (26)

Now \( \det \mathcal{T} \) can be seen as the determinant of a convex combination of matrices.

In this case a mathematical inequality (called Brunn-Minkowsky inequality) holds

\[ \det(aA + (1 - a)B) \geq (\det A)^a (\det B)^{1-a} \] (27)

for \( 0 \leq a \leq 1 \) and \( A, B \) positive symmetric matrices. This inequality can be evidently extended to a general convex combination of matrices.

**Proof.**

To prove this inequality, we can chose \( A = \text{Id} \) without any loss of generality. This is consequence of the strict positivity of one of the two matrices, for example \( A \), so that \( A \) is invertible, and

\[ \det(aA + (1 - a)B) = \det(A) \det(a\text{Id} + (1 - a)A^{-1}B). \]

Changing the the matrices names, we have only to prove

\[ \det(a\text{Id} + (1 - a)C) \geq (\det C)^{1-a}. \]

Here \( C = A^{-1}B \) is still diagonalisable and we denote by \( c_i \) its eigenvalues. Computing the determinants in a diagonal basis for \( C \),

\[ \Pi(a + (1 - a)c_i) > (\Pi c_i)^{1-a}. \]

Taking the logarithm, we have to prove that

\[ \Sigma \ln(a + (1 - a)c_i) > (1 - a)\Sigma \ln c_i. \]

This is now a direct consequence of the concavity of the logarithm between 1 and \( c_i \)

\[ \ln(a + (1 - a)c_i) > (1 - a)\ln c_i. \]

\[ \square \]

In our case, applying this inequality to \( \mathcal{T} \)

\[ \det \mathcal{T} \geq (\det \Lambda_1)^{\frac{1 + 2\nu}{3}} (\det \Lambda_2)^{\frac{1 - \nu}{3}} (\det \Lambda_3)^{\frac{1 - \nu}{3}} \] (28)

the result follows immediatly from

\[ \det \Lambda_1 = \det \Lambda_2 = \det \Lambda_3 = \lambda_1 \lambda_2 \lambda_3 = \det \Theta. \] (29)
We must now recall that model equations (like the BGK or ES-BGK equations) were introduced as simplifications of the Boltzmann collision operator in order to compute more easily rarefied flows. Thus it is essential to check that the ES-BGK model can be actually used for computations in much the same way as the BGK model.

We will concentrate on 1D problems where the BGK model has been widely used, and proved to be quite successful (see [1] for example), especially in comparison with DSMC. Although these may seem to be oversimplified problems, they are the basic problems one has to solve for boundary layer problems. In that case, after rescaling, the problem is that of a flow over an infinite flat plate. In these cases one is more interested by jump coefficients than by the exact velocity profiles, and computations show that the jump coefficients are quite independent of the molecular model considered in the Boltzmann kernel and can be obtained with very good accuracy from the BGK model.

Moreover, using the symmetry of the BGK collision operator, 1D (in position space) and 3D (in velocity space) problems can be reduced to a 1D velocity problem which can then be very easily solved by a finite difference scheme (see [6]). Recently, this method has been successfully used by Aoki and al. ([5]) in the important case of evaporation-condensation boundary conditions.

Basically, the method consists of integrating the BGK equation over $dv_2 dv_3$. The new unknown becomes $F = \int f dv_2 dv_3$ which depends only on $v_1$. The system is not closed because some moments in the Maxwellian (the temperature and the tangential velocity) cannot be computed from $F$. Therefore one introduces the unknowns $G = \int f v_2 dv_2 dv_3$ and $H = \int f(v^2_2 + v^2_3) dv_2 dv_3$. All the moments can be computed from these three functions, and it is easy to see that by integrating the BGK equation one obtains a closed system of three equations over $F$, $G$, $H$ which are dependent on only one velocity variable.

For the ES-BGK model, one has to introduce one more function: $I = \int f v_2^2 dv_2 dv_3$, and we will note $H = \int f v_2^2 dv_2 dv_3$. The pressure tensor of $f$ can be computed from these quantities: integrating $F$ over $v_1^2 dv_1$ and $H$ and $I$ over $dv_1$ gives the diagonal coefficients, integrating $G$ over $v_1 dv_1$ gives two more coefficients. The other coefficients are null since $f$ is expected to have a parity over $v_3$.

The matrix $T$ can then be computed from these quantities, as well as the Gaussian. Using the notations of [5], it is a simple computation to obtain the closed system of four equations

\begin{align}
\partial_t F + v \partial_x F &= \frac{2}{\sqrt{\pi}} \rho \left( \frac{1}{\sqrt{\pi}} \rho T_{11}^{\frac{1}{2}} \exp \left( \frac{(v_2-v_1)^2}{2T_{11}} \right) - G \right) \tag{30} \\
\partial_t G + v \partial_x G &= \frac{2}{\sqrt{\pi}} \rho \left( \frac{1}{\sqrt{\pi}} \rho T_{11}^{\frac{1}{2}} \omega \exp \left( \frac{(v_2-v_1)^2}{2T_{11}} \right) - G \right) \tag{31} \\
\partial_t H + v \partial_x H &= \frac{2}{\sqrt{\pi}} \rho \left( \frac{1}{\sqrt{\pi}} \rho T_{11}^{\frac{1}{2}} (\omega^2 + \frac{1}{2} \lambda) \exp \left( \frac{(v_2-v_1)^2}{2T_{11}} \right) - H \right) \tag{32} \\
\partial_t I + v \partial_x I &= \frac{2}{\sqrt{\pi}} \rho \left( \frac{1}{\sqrt{\pi}} \rho T_{11}^{\frac{1}{2}} \frac{1}{2} T_{33} \exp \left( \frac{(v_2-v_1)^2}{2T_{11}} \right) - I \right) . \tag{33}
\end{align}

where

\[ \omega = u_2 + \frac{T_{12}}{T_{11}} (v_1 - u) \]

\[ \lambda = T_{22} - \frac{T_{12}^2}{T_{11}} . \]

It is easy from this system to compute by a finite difference scheme 1D flows. An example of results is given for an evaporation-condensation problem with normal incidence, for a given Mach number and temperature ratio (taken as unity) one obtains an unique pressure ratio giving an equilibrium solution (see [5]).
**FIGURE 1.** Pression ratio curve for subsonic normal velocities at a temperature ratio of one.

**REFERENCES**