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Evaluation of BGK-type Models of the Boltzmann Equation

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Abstract. A BGK-type model is a simplified model to the Boltzmann equation where the complicated collision integral is approximated using a simple relaxation term. In this paper, a generalized BGK-type model is proposed by combining the original BGK, Shakhov and ellipsoidal statistical models. To verify the new model, theoretical and numerical analysis is performed. The Chapman-Enskog expansion shows that the generalized model can recover the Navier-Stokes-Fourier and Burnett equations by choosing properly the introduced parameters. In addition, the collision term of the model is evaluated for several designed relaxation problems. Results show that the new model can match the results of third-order moments obtained with DSMC method by adjusting the free parameters.

Keywords: BGK-type model, Chapman-Enskog expansion, DSMC method, time relaxation
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INTRODUCTION

The Boltzmann equation [1] describes the fundamental and general behavior of a dilute gas which forms the basis of the kinetic theory. It is a nonlinear multi-dimensional integro-differential equation and difficult to solve. Hence it is not surprising that alternatives with simpler collision terms are proposed which is known as model equations. As pointed out by Cercignani, the idea behind model equations is that a large amount of detail of the two-body interaction in the collision term is not likely to influence significantly the values of many experimentally measured quantities.

In 1954, a kinetic model [2] was developed by Bhatnagar, Gross and Kook (BGK) where the complicated collision term of the Boltzmann equation is replaced by a simple relaxation term. It is assumed that the net effect of collisions makes the velocity distribution function relax towards a local equilibrium distribution over a characteristic time. Accompanied with the exciting simplification, a drawback is caused that the BGK model always produces a Prandtl number of unity rather than around 2/3 for monatomic gases. To fix the Prandtl number, many modified kinetic models are proposed in the past decades. The main idea is to introduce a new parameter in the reference relaxation state through which the correct Prandtl number can be recovered.

One example is the ellipsoidal statistical model (ES-model) proposed by Holway in 1966 [3]. In this model, the local equilibrium Maxwellian distribution is replaced by a local anisotropic Gaussian and non-equilibrium is introduced in the relaxation state by modifying the temperature scalar into an anisotropic temperature tensor. By introducing a weight parameter in the temperature tensor, correct Prandtl number can be obtained through Chapman-Enskog expansion. Unlike the BGK model, it is initially not obvious that the ES-model leads to the equilibrium state. However, Andries and co-workers proved that it obeys the H-theorem [4] and this arises in great interests of the model in the kinetic community.

Another very popular model is the Shakhov model (S-model) [5]. Direct modification is done by introducing an extra term on the local Maxwellian distribution. The term is constructed through Hermit polynomial expansion to make sure the heat flux is correct in the hydrodynamic limit and meanwhile the lower-order moments are the same with BGK. The rough modification in mathematics of this model make the velocity distribution function can be negative and the H-theorem is only proved in the near-equilibrium limit. But due to its fine property on the near-equilibrium flow and natural relation with the BGK model, the S-model is extensively used in the cross-flow-regime algorism development recently [6-9] and satisfying results are obtained especially on low-speed flow simulation [9].

The ES- and S-models both provide correct Prandtl number in the hydrodynamic limit. However, it is hard to validate them theoretically. Studies have been focused on numerical prediction of macroscopic quantities on test problems. Andries et al. [10] showed that the ES-model solutions agreed well with the DSMC results for planar Couette flow and for supersonic flow over a flat plate when the Knudsen (Kn) number is less than 0.01. For large Knudsen number flows, however, the accuracy of BGK models was found to be poor. Similar results are observed by Gallis and Torczynski [11] and they also found that the ES-model does not produce accurate values of the mass...
self-diffusion coefficient. Mieussens and Struchtrup [12] compared several BGK-type models for Couette flow and stationary shock wave problems. They concluded that all BGK models with proper Prandtl number were accurate in the continuum regime, qualitatively good in the transitional regime and inaccurate at large Knudsen numbers and for shock structures.

The molecular velocity distribution itself was also investigated. Garzó and Santos [13] studied the Boltzmann collision term, the BGK model, and the ES-model by comparing high-order moments of the velocity distribution function for uniform shear flow. They found that the BGK results were closer to the Boltzmann results than the ES-BGK results were in almost all cases. Sun et al. [14] evaluated the BGK collision term and found that the model-induced error in the BGK model depended greatly on the degree of non-equilibrium. When the flow is not far from Maxwellian, it predicted satisfactory history of velocity distribution function during relaxation but with the increase of the degree of non-equilibrium, the prediction deteriorated.

In the remaining sections, we will first analyze the BGK model, ES-model and S-model theoretically and base on this, a new generalized model will be proposed by combining the three models. The Chapman-Enskog expansion is then performed to restrain the free parameters in order to come back to the hydrodynamic limit. Following this, the models are evaluated numerically by comparing with DSMC results for several designed problems and a suggested choice of free parameters is given. The paper ends with our conclusion.

ANALYSIS OF BGK-TYPE MODELS

BGK-type Models

The Boltzmann equation describes the evolution of the velocity distribution function of gas molecules and provides a complete description of a dilute monatomic gas at the molecular level:

\[ \frac{\partial f}{\partial t} + c_i \frac{\partial f}{\partial x_i} = Q(f, f'), \]

where \( t \) is the time, \( f(t, x, c_i) \) is the velocity distribution function, \( x_i \) and \( c_i \) are the position and molecular velocity respectively, \( Q(f, f') \) is the collision integral. Macroscopic quantities such as the density \( \rho \), the average velocity \( \bar{c} \), temperature \( T \) and pressure \( p \) can be found in terms of moments of \( f \).

The BGK approximation to the Boltzmann equation is

\[ \frac{\partial f}{\partial t} + c_i \frac{\partial f}{\partial x_i} = \frac{f_m - f}{\tau_g}, \]

where \( f_m = (2\pi RT)^{-3/2} \exp(-C^2/2RT) \) is the local Maxwellian distribution, \( R \) is the gas constant, \( C_i = c_i - \bar{c} \) is the thermal velocity and \( \tau_g \) is the relaxation time of the BGK model. The BGK model reproduces the correct Maxwellian distribution at equilibrium, preserves conservation of mass, momentum and energy, satisfies the H-theorem and leads to Navier-Stokes-Fourier equations (N-S-F equation) when Chapman-Enskog expansion is applied. It is a pity that the elegant BGK model does not produce the correct Prandtl number.

The Chapman-Enskog expansion of the BGK model relates the viscosity coefficient \( \mu \) and thermal conductivity \( \kappa \) to the relaxation time:

\[ \mu = \tau_g p, \quad \kappa = \frac{5}{2} R \tau_g p. \]

A Prandtl number of unity rather than around 2/3 for monatomic gases can be obtained: \( Pr = \mu C_p / \kappa = 1 \) (where \( C_p = 5R/2 \)). The viscosity coefficient and thermal conductivity can also be obtained from the first order expansion of the Boltzmann equation:

\[ \mu = 0.499 \rho \bar{c}^2 \tau, \quad \kappa = \frac{15}{4} R \left( 0.499 \rho \bar{c}^2 \tau \right). \]

The consistency of \( \mu \) with the Boltzmann equation demands \( \tau_g = (3.992/\pi) \left( \lambda / \bar{c} \right) \) and when \( \kappa \) is captured, \( \tau_g = (5.998/\pi) \left( \lambda / \bar{c} \right) \) is required. It is clear that \( \mu \) and \( \kappa \) can not be correct at the same time.
To ensure the model has the correct momentum and energy transport simultaneously, more information needs to be included in the relaxation term. Take the S-model and ES-model as examples, the relaxation state is reconstructed by introducing a new parameter followed by an implicit adaptation of the relaxation time. Hence the generalized form of the modified BGK equation can be expressed as

$$\frac{\partial f_r}{\partial t} + c_i \frac{\partial f_r}{\partial x_i} = \frac{f_r - f}{\tau_r},$$  \hspace{1cm} (5)

where $f_r$ is the modified relaxation state which is called the reference distribution and $\tau_r$ is the corresponding relaxation time.

The S-model is constructed directly from the BGK model through Hermit polynomial expansion. To make sure the heat flux $q_i = \frac{1}{2} \int C_i C f \, dc$ is correct in the N-S-F limit, an extra term is added to the equilibrium distribution in the relaxation state:

$$f_r = f_s = f_M \left[ 1 + (1 - C_s) \left( \frac{C_i}{RT} - 5 \right) \right],$$  \hspace{1cm} (6)

in which $C_s = Pr$ is required. It is obvious that the even order moments remains the same with BGK and only odd order moments are modified. A worry is that the pure mathematical consideration in the construction of S-model may lead to negative distribution function for relatively large velocities. Although it is not a problem for continuum flow on which the hydrodynamic variables interested are not influenced, impact of this negative distribution on non-equilibrium flow still remains to be investigated.

The ES-model is proposed in a different way. The relaxation state is assumed to be a functional restricted by conservation of the mass, momentum and energy. By use of the maximum entropy theory, the relaxation state is derived as:

$$f_r = f_{ES} = \frac{1}{\sqrt{\det(2 \pi \lambda)}} \exp \left( -\sum_{i,j=1}^{3} \frac{1}{2} C_i \lambda_{ij} C_j \right),$$  \hspace{1cm} (7)

in which an anisotropic temperature tensor $\lambda_{ij} = (1 - C_{ES}) RT \delta_{ij} + C_{ES} \int f C_i C_j \, dc$ is introduced in replace of the Maxwellian distribution in BGK and the anisotropy is controlled by the parameter $C_{ES}$. To recover the correct Prandtl number, $C_{ES} = 1 - 1/Pr$ is required and when $C_{ES} = 0$, it returns to the BGK model.

It is natural and reasonable that the collision operator of the Boltzmann equation describes a process that the velocity distribution function relaxes to the equilibrium state. This is what the BGK model does. But unfortunately it produces a wrong Prandtl number in the N-S-F limit. To fix the Prandtl number, the equilibrium state to be relaxed is modified by adding some locally non-equilibrium information which is controlled by the parameter introduced. It is to say that the modified model compromises to the continuum limit by relaxing to equilibrium in an indirect way. On this condition however, it appears to be a difficult task to achieve good performance on flow far from continuum at the same time. Hence it seems to be helpful to introduce more parameters into the model to give more freedom to cover more properties. This is similar to the situation of the S-model and ES-model in which a parameter is introduced to cover the correct Prandtl number.

### A Generalized BGK Model

As an attempt, a generalized BGK-type model (G-model) is proposed in this paper. In this model, the relaxation state is constructed by linearly combining the relaxation state of the ES-model, S-model and BGK model:

$$f_r = f_G = \alpha f_{ES} + \beta f_S + \gamma f_M,$$  \hspace{1cm} (8)

where $\alpha$, $\beta$ and $\gamma$ are weights of the corresponding model. The equilibrium condition demands $\alpha + \beta + \gamma = 1$ and after some manipulations, the relaxation state can be expressed as

$$f_G = \alpha f_{ES} + \beta f_S + (1 - \alpha) f_M,$$  \hspace{1cm} (9)

in which $\beta' = \beta (1 - C_s)$ is the coefficient of $f_S = f_M \left( \frac{C_i}{5pRT} \left( \frac{C_i^2}{RT} - 5 \right) \right)$, which is the corresponding extra term in the relaxation state of the S-model with the coefficient $1-C_s$ removed.
There are four parameters appearing in the G-model: $\alpha$, $\beta'$, $C_{ES}$ and the implicit relaxation time $\tau_G$. In the next section, we try to determine these parameters in the hydrodynamic limit using the Chapman-Enskog expansion.

**Chapman-Enskog Expansion**

The Chapman-Enskog expansion is a perturbation method. Its main assumption is that the Knudsen number is much smaller than 1 or the characteristic time of the flow is much larger than the physical mean collision time.

Non-dimensional form of the generalized model is used here

$$\frac{\partial f}{\partial t} + \sum_i \frac{\partial f}{\partial x_i} = -\frac{1}{Kn} f_{\tau} - f.$$  \hspace{1cm} (10)

The distribution function is expanded as powers of $Kn$

$$f = \sum_{n=0}^{\infty} Kn^n f^{(n)}.$$  \hspace{1cm} (11)

As moments of $f$, the trace-free pressure tensor and heat flux can be expressed as

$$\sigma_i = \sum_{n=0}^{\infty} Kn^n \sigma_i^{(n)} = \sum_{n=0}^{\infty} Kn^n \rho \int \left( C_i C_j - \frac{1}{3} C^2 \delta_{ij} \right) f^{(n)} \, df,$$

$$q_i = \sum_{n=0}^{\infty} Kn^n q_i^{(n)} = \sum_{n=0}^{\infty} Kn^n \frac{p}{2} \left( C_i C_j f^{(n)} \right) \, df,$$

where $\delta_{ij}$ is the unit tensor and hence the pressure tensor is $p_{\tau} = p \delta_{ij} + \sigma_{ij}$.

The relaxation state is also expanded as powers of $Kn$

$$f_{\tau} = \sum_{n=0}^{\infty} Kn^n f^{(n)}_{\tau},$$  \hspace{1cm} (13)

in which the coefficients of the first three terms are derived as:

$$f_{\tau}^{(0)} = f_M, \quad f_{\tau}^{(1)} = f_M \left( \frac{C_{ES}}{2RT} \sigma_i^{(1)} C_i \right),$$

$$f_{\tau}^{(2)} = f_M \left[ \alpha \left( \frac{C_{ES}^{(2)}}{2p} \sigma_i^{(2)} \sigma_i^{(1)} - \frac{1}{RT} \right) \sigma_j^{(3)} C_i C_j + \frac{C_{ES}}{4p(2RT)} \sigma_i^{(3)} (C_i \sigma_i^{(1)} C_j C_k C_l) \right]$$

$$+ \frac{\beta'}{5pRT} C_i Q_i^{(2)} \left( \frac{C_i^2}{RT} - 5 \right).$$  \hspace{1cm} (14)

The derivation follows the work of Zheng & Struchtrup on the ES-model [15]. Another assumption in their literature is that the distribution function depends on position $x_i$ and time $t$ only through hydrodynamic variables ($\rho, \tau, T$) and their derivatives. Below results of the expansion are demonstrated.

The zeroth-order expansion produces the Euler equation. The distribution function; stress tensor and heat flux is

$$f^{(0)} = f_M, \quad p_{\tau}^{(0)} = p \delta_{ij}, \quad \sigma_{ij}^{(0)} = 0, \quad q_i^{(0)} = 0.$$  \hspace{1cm} (15)

The first-order expansion leads to the N-S-F equations. The corresponding velocity distribution function is:

$$f^{(1)} = f^{(0)} \left[ \alpha \left( \frac{C_{ES}}{2pRT} \sigma_i^{(1)} C_i \right) + \frac{\beta'}{5pRT} C_i Q_i^{(1)} \left( \frac{C_i^2}{RT} - 5 \right) \right] - f^{(0)} \tau_G \left[ C_i C_j \frac{\partial f}{\partial x_j} + C_i \left( \frac{C_i^2}{2RT} - \frac{5}{2} \right) \frac{\partial}{\partial x_i} \left( \ln T \right) \right],$$  \hspace{1cm} (16)

from which the stress tensor and heat flux can be obtained and the corresponding viscosity coefficient and thermal conductivity are

$$\mu = \frac{2\tau_G p}{1 - aC_{ES}}, \quad \kappa = \frac{5R\tau_G p}{2(1 - \beta')}. $$  \hspace{1cm} (17)

In (17), $f^{(1)}$ can be rewritten as

$$f^{(1)} = f^{(0)} \left[ \alpha \left( \frac{1}{2pRT} C_i C_j + \frac{\beta'}{5pRT} C_i Q_i^{(1)} \left( \frac{C_i^2}{RT} - 5 \right) \right) \right].$$

This is the same as with the Boltzmann equation.
From (17), the Prandtl number and the relaxation time can be expressed as

\begin{equation}
Pr = \frac{\mu C_p}{\kappa} = \frac{1 - \beta^2}{1 - \alpha C_{Es}};
\end{equation}

and

\begin{equation}
\tau_\rho = \frac{(1 - \alpha C_{Es}) \mu}{\rho}.
\end{equation}

It is then obvious that (18) and (19) are the two conditions on which the G-model can recover the N-S-F equations.

Burnett level equations can be obtained from the second-order expansion. The velocity distribution function is derived as

\begin{equation}
f^{(2)} = f^{(2)}_G + \tau_\rho f_m \Theta,
\end{equation}

where

\begin{equation}
f^{(2)}_G = \frac{C_j C_j}{(1 - \alpha C_{Es}) \rho} \frac{\partial^2 u_i}{\partial x_i \partial x_j} + 4 - 5 \alpha C_{Es} \frac{C_j}{(1 - \alpha C_{Es})} \frac{\partial u_j}{\partial x_j} + \frac{C_j C_j}{1 - \alpha C_{Es}} \frac{\partial^2 u_i}{\partial x_i \partial x_j} + \frac{C_j C_j}{RT (1 - \alpha C_{Es})} \frac{\partial^2 u_i}{\partial x_i \partial x_j} \frac{\partial^2 u_i}{\partial x_i \partial x_j},
\end{equation}

It seems to be a little lengthy and from this the corresponding heat flux is obtained below:

\begin{equation}
q^{(2)} = \frac{\tau_\rho^2 \rho^2}{(1 - \alpha C_{Es})^2} Pr (4 - 9 \beta^2) \left( \frac{2 \partial u_i}{\partial x_i} \frac{\partial^2 u_i}{\partial x_i \partial x_j} + 2 \frac{\partial^2 u_i}{\partial x_i \partial x_j} + 2 \frac{\partial^2 u_i}{\partial x_i \partial x_j} + 5 \frac{\partial^2 u_i}{\partial x_i \partial x_j} + 6 \frac{\partial^2 u_i}{\partial x_i \partial x_j} + 10 \frac{\partial^2 u_i}{\partial x_i \partial x_j} \right).
\end{equation}

A comparison of (2) with the Boltzmann equation for monatomic gases and Maxwell molecules. An interesting result is that the Burnett level heat flux of the G-model is consistent with the Boltzmann equation if and only if (18), (19) and

\begin{equation}
\beta = 0 \quad \text{(that is } \alpha C_{Es} = -1/2),
\end{equation}

are satisfied. Insert (22) into (20), \( f^{(2)} \) can be simplified and is the same with that of the ES-model in. A conclusion is then drawn that on condition (22) is satisfied, an N-S-F level model can recover the Burnett equations.

**EVALUATION OF BGK-TYPE MODELS FOR RELAXATION PROBLEMS**

BGK-type models replace the Boltzmann collision term with a simple relaxation expression. This relaxation expression then determines the validity of the model. Analyzing the relaxation process of the distribution function is probably a good approach to evaluate the models.

The relaxation process in BGK-type models is governed by

\begin{equation}
\text{(23)}
\end{equation}
where the convection and acceleration terms are neglected. Relaxation problems are designed to investigate the performance of the collision term.

**Anisotropic Maxwellian Distribution**

The first case is an anisotropic Maxwellian distribution specifically, the distribution in each velocity component is Maxwellian, but has different temperature value:

\[
f(u) = \frac{\beta_u}{\sqrt{\pi}} \exp\left(-\beta^2 u^2\right) \frac{\beta_{u'}}{\sqrt{\pi}} \exp\left(-\beta_{u'}^2 u'^2\right),
\]

where \( \beta = \sqrt{m/2kT} \) and \( T_1 = 2730K, T_2 = 273K \) is set.

Figure 1 shows the comparison of the x-component velocity distribution function of BGK-type models with DSMC at \( t = 0.2\tau_g \) and \( t = \tau_g \). Parameters of the G-model are chosen as \( \alpha = 1, C_{ES} = 1/3 \) with (18) and (19) satisfied to recover the N-S-F equations. It is clear that the model can not recover the Burnett equations. The distribution profiles of the S-model and BGK model coincide with each other and are close to DSMC with the maximum distribution a bit bigger; however, the ES-model does not do well for this problem with a steeper distribution profile and a larger maximum distribution than DSMC. It seems that the anisotropy introduced into the temperature tensor of the ES-model does not help it behave well in capture of relaxation process of a highly non-equilibrium distribution despite hydrodynamic equations can be recovered by making the parameter \( C_{ES} = -1/2 \). A contrast is the BGK model with an isotropic temperature scalar, which is even incorrect in the N-S-F limit. But numerical experiments shows that by adjusting the parameter \( C_{ES} \) with a value of 1/3 in the G-model, the relaxation process of the anisotropic distribution can be captured. The distribution profile agrees well with DSMC.

![Comparison of x-component distribution function of BGK-type models with DSMC when \( t = 0.2\tau_g \) and \( t = \tau_g \).](image)

**FIGURE 1.** Comparison of x-component distribution function of BGK-type models with DSMC when \( t = 0.2\tau_g \) and \( t = \tau_g \).
Tailored Half-normal Distribution

The comparison is next done on a tailored half-normal distribution case. This case is similar to the first one except that the Maxwellian in one direction is replaced by a double-half-Maxwellian of which the discontinuity is removed by adjusting the amplitude of half distributions:

$$f(0) = \frac{2}{\sqrt{\pi}} \frac{\beta_2}{\beta_1} \left( \exp\left(-\beta_1^2 u^2\right) + \exp\left(-\beta_2^2 u^2\right) \right) \frac{\beta_1^2}{\sqrt{\pi}} \exp\left(-\beta_1^2 u^2\right) \frac{\beta_2^2}{\sqrt{\pi}} \exp\left(-\beta_2^2 u^2\right)$$

(25)

where $T_e = 2730K$, $T_i = 273K$ is set.

Figure 2 shows the comparison of the x-component velocity distribution function of BGK-type models with DSMC at $t = \tau_B$. Parameters of the G-model are set $\alpha = 1$, $C_{ES} = 1/3$ too. From the distribution curves, it is not easy to give a certain answer to the question which model is better. To answer this question, the moments and fluxes can be compared. It is for sure that the first and second order moments of all models are the same with the Boltzmann equation due to conservation of momentum and energy and to achieve this, the relaxation time is adjusted according (19). On the third order moment which is illustrated in Figure 3, only the G-model agrees well with DSMC and the BGK model, ES-model and S-model show some distinction, despite it is believed that the latter two models can do very well in the continuum limit. The reason for this is that the introduction of new parameters in the G-model gives the model more space to ensure its properties simultaneously for both continuum and non-equilibrium flow. The mass, momentum and energy fluxes also agree well with DSMC as they can be easily expressed in terms of the first three order moments of the distribution function. In Figure 4, comparison of the energy flux is demonstrated.
CONCLUSION

In this paper, a generalized BGK-type model is addressed by linearly combining the BGK model, S-model and ES-model. Through Chapman-Enskog expansion, the Navier-Stokes-Fourier and Burnett equations can be recovered by properly choosing the parameters in the G-model. Also, the collision term of the different models is evaluated for designed relaxation problems. Results show that comparing to other models, the G-model either improves the distribution function profile or better the capture of the third order moment. This is evidence to that by introducing new parameters into BGK-type models, good performance could be achieved simultaneously on the hydrodynamic limit and non-equilibrium situation. Although our proposal of the G-model proves to be successful, it should be mentioned that it is also an approximation of the Boltzmann equation by its nature and can not replace the Boltzmann equation in most non-equilibrium flows. Thus the model needs to be further analyzed and tested using other means.

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REFERENCES