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*Steepest Entropy Ascent Models of the Boltzmann Equation: Comparisons With Hard-Sphere Dynamics and Relaxation-Time Models for Homogeneous Relaxation From Highly Non-Equilibrium States*

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**Citation:** Beretta, Gian Paolo, and Nicolas G. Hadjiconstantinou. "Steepest Entropy Ascent Models of the Boltzmann Equation: Comparisons With Hard-Sphere Dynamics and Relaxation-Time Models for Homogeneous Relaxation From Highly Non-Equilibrium States." 15-21 November, 2013, San Diego, California, USA, ASME, 2013. © 2013 by ASME

**As Published:** <http://dx.doi.org/10.1115/IMECE2013-64905>

**Persistent URL:** <http://hdl.handle.net/1721.1/108757>

**Version:** Final published version: final published article, as it appeared in a journal, conference proceedings, or other formally published context

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**IMECE2013-64905**

**STEEPEST ENTROPY ASCENT MODELS OF THE BOLTZMANN EQUATION.  
COMPARISONS WITH HARD-SPHERE DYNAMICS AND  
RELAXATION-TIME MODELS FOR HOMOGENEOUS RELAXATION  
FROM HIGHLY NON-EQUILIBRIUM STATES**

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**ABSTRACT**

*We present a family of steepest entropy ascent (SEA) models of the Boltzmann equation. The models preserve the usual collision invariants (mass, momentum, energy), as well as the non-negativity of the phase-space distribution, and have a strong built-in thermodynamic consistency, i.e., they entail a general H-theorem valid even very far from equilibrium. This family of models features a molecular-speed-dependent collision frequency; each variant can be shown to approach a corresponding BGK model with the same variable collision frequency in the limit of small deviation from equilibrium. This includes power-law dependence on the molecular speed for which the BGK model is known to have a Prandtl number that can be adjusted via the power-law exponent.*

*We compare numerical solutions of the constant and velocity-dependent collision frequency variants of the SEA model with the standard relaxation-time model and a Monte Carlo simulation of the original Boltzmann collision operator for hard spheres for homogeneous relaxation from near-equilibrium and highly non-equilibrium states. Good agreement is found between all models in the near-equilibrium regime. However, for initial states that are far from equilibrium, large differences are found; this suggests that the maximum entropy production statistical ansatz is not equivalent to Boltzmann collisional dynamics and needs to be modified or augmented via additional constraints or structure.*

**INTRODUCTION**

Recent interest in microscale and nanoscale internal gaseous flows in which kinetic effects are important [1] has renewed the search for collision operator models that are simple yet more accurate than the standard relaxation-time model, typically referred to as the Bhatnagar-Gross-Krook (BGK) model [2–5]. Although very simple, the latter is known [5] to lead to an incorrect value of the Prandtl number, namely 1. As a result, this model is incapable of capturing the interplay between heat and momentum transport in coupled problems. This is particularly important in nanoscale flows where, in contrast to the Navier-Stokes regime where viscosity and temperature effects decouple in the framework of a linearized analysis, a noticeable heat flux can be present even if temperature is uniform [6]. To address this limitation, but also provide a more realistic model of the original Boltzmann hard-sphere (HS) dynamics for near-equilibrium problems, the molecular-velocity-dependent collision frequency variant of the BGK model was developed [7].

In this paper we investigate the strongly non-equilibrium regime of the Boltzmann equation using a simple kinetic problem, namely homogeneous relaxation. Since the BGK model is usually justified [8] as a near-equilibrium approximation of the Boltzmann collision term, we compare its behavior with solutions of the hard-sphere Boltzmann equation in the highly non-equilibrium regime. The latter are obtained using direct simulation Monte Carlo (DSMC), the prevalent method for obtaining solutions of the original Boltzmann equation [9].

Moreover, we investigate a new family of kinetic models that differs significantly from the standard BGK model and its ES (Gaussian) and velocity-dependent collision frequency variants. This new family of kinetic models does not involve a local target Maxwellian, Gaussian, or pseudo-Maxwellian. Rather, the new model selects the direction of the time evolution of the local one-particle phase-space distribution on the basis of the local direction of steepest entropy ascent (SEA) compatible with mass, momentum, and energy conservation. An interesting feature of the SEA principle is its intrinsic thermodynamic consistency. The H-theorem is easily proved to hold for arbitrary deviations from equilibrium. From the theoretical point of view, the SEA model implements in the framework of kinetic theory various possible variants of the so-called maximum entropy production principle (MEPP), that during the last few decades has been advocated as a unifying feature of several classes of irreversible phenomena [10–15].

The geometrical considerations that lead to the construction of the new SEA model equations will be presented elsewhere. The purpose of the present paper is to present the new model, discuss its conservation and H-theorem features, and present some preliminary comparisons with established models in the context of homogeneous relaxation. We specifically compare the constant and variable collision frequency variant of the new model with the corresponding BGK models and with the original Boltzmann equation for hard spheres. We also show that the new model reduces to the corresponding BGK model in the near-equilibrium limit, for both the constant and the velocity-dependent collision frequency variants. The results of these preliminary comparisons suggest that a variable collision frequency improves the agreement between the SEA and the HS model. Further analysis of the SEA principle and further comparisons with standard benchmark problems of kinetic theory, such as shock structure, as well as a Chapman-Enskog-type analysis are necessary before definitive conclusions can be drawn.

## THE MAXIMUM ENTROPY LANDSCAPE IN THE KINETIC THEORY OF GASES

The new kinetic model consists of a general rate equation describing a smooth constrained relaxation of the non-equilibrium one-particle phase-space distribution in the direction of maximal local entropy increase compatible with the requirement of mass, momentum, and energy conservation. The latter quantities are related to the well known hydrodynamic fields of entropy  $s(\mathbf{x}, t)$ , mass density  $\rho(\mathbf{x}, t)$ , macroscopic (flow) velocity vector  $\mathbf{v}(\mathbf{x}, t) = (v_x, v_y, v_z)$  and mass-specific internal energy  $u(\mathbf{x}, t)$ . They are calculated as moments of the single-particle distribution function  $f(\mathbf{x}, \mathbf{c}, t)$  in the phase space of position  $\mathbf{x}$  and molecular

velocity  $\mathbf{c}$  via

$$\rho(\mathbf{x}, t) s(\mathbf{x}, t) = -k_B \int_{\Omega_c} d\mathbf{c} f(\mathbf{x}, \mathbf{c}, t) \ln[b f(\mathbf{x}, \mathbf{c}, t)] \quad (1)$$

$$\rho(\mathbf{x}, t) = m \int_{\Omega_c} d\mathbf{c} f(\mathbf{x}, \mathbf{c}, t) \quad (2)$$

$$\rho(\mathbf{x}, t) \mathbf{v}(\mathbf{x}, t) = m \int_{\Omega_c} d\mathbf{c} f(\mathbf{x}, \mathbf{c}, t) \mathbf{c} \quad (3)$$

$$\rho(\mathbf{x}, t) u(\mathbf{x}, t) = m \int_{\Omega_c} d\mathbf{c} f(\mathbf{x}, \mathbf{c}, t) \frac{1}{2} |\mathbf{c} - \mathbf{v}(\mathbf{x}, t)|^2 \quad (4)$$

where  $m$  is the molecular mass,  $k_B$  is the Boltzmann constant, and  $b$  a suitable constant.

In this landscape, i.e., on each intersection surface defined by given values of the local density, barycentric velocity vector, and internal energy, there is one and only one stable equilibrium state, corresponding to the phase-space distribution which maximizes the local entropy density [8]. Of course, the determination of a distribution of maximum entropy subject to a set of linear constraints has a long history of applications in many areas of quantum physics, chemistry, information theory, and probability theory, see e.g. [16–20]. In the framework of kinetic theory and gas dynamics, the maximum entropy distribution represents the local thermodynamic equilibrium state.

By the standard methods of Lagrange multipliers and functional derivatives, it is straightforward to show that the distribution which maximizes the entropy functional (1) subject to the constraints (2), (3), and (4) is

$$f_{MB}(\rho, \mathbf{v}, u) = \frac{\rho}{m} \left[ \frac{1}{2\pi RT} \right]^{3/2} \exp \left[ -\frac{|\mathbf{c} - \mathbf{v}|^2}{2RT} \right] \quad (5)$$

which already satisfies constraints (2) and (3), and substituted in (4) yields the Lagrange multiplier  $T = 2u/3R$ .

The Boltzmann equation describes the time evolution of the single-particle phase-space distribution as a result of the interplay between collisionless advection and collisions. In the absence of body forces, it takes the form

$$\frac{\partial f}{\partial t} + \mathbf{c} \cdot \nabla_{\mathbf{x}} f = Q_{\text{Boltz}}[f] \quad (6)$$

where  $Q_{\text{Boltz}}[f]$  is the well-known Boltzmann collision integral (see, e.g., [5]).

In view of the non-linearity of the Boltzmann collision term  $Q_{\text{Boltz}}[f]$  and the associated numerical challenges in obtaining accurate simulations of its behavior, several model equations have been proposed where the term  $Q_{\text{Boltz}}[f]$  is substituted by a model term  $Q_{\text{model}}[f]$ , which is simpler to handle and treat numerically but featuring as many of the essential properties of  $Q_{\text{Boltz}}[f]$  as possible. The minimal set of such features includes mass, momentum, and energy conservation, the H-theorem and the fact that  $Q_{\text{model}}[f_{MB}] = 0$  for every Maxwellian distribution  $f_{MB}$ .

For example, the standard BGK model [2] is defined by

$$Q_{\text{BGK}}[f] = \frac{\mathcal{M}[f] - f}{\tau} \quad (7)$$

where the target distribution  $\mathcal{M}[f]$  is the Maxwellian (isotropic Gaussian) with the same mass, momentum, and energy densities as the actual non-equilibrium distribution  $f$ . The well-known weakness of this model is that it yields the wrong ratio of thermal conductivity to viscosity  $\kappa/\mu = 5k_B/2m$ .

The Ellipsoidal-Statistical-BGK (ES-BGK) or Gaussian BGK model [4, 21] is defined by

$$Q_{\text{ES-BGK}}[f] = \frac{\mathcal{G}[f] - f}{\tau} \quad (8)$$

where the local target distribution  $\mathcal{G}[f]$  is an anisotropic Gaussian with the same mass and momentum densities as the actual non-equilibrium distribution  $f$  and a stress tensor given by a suitable linear combination of the stress tensor of  $f$  and the isotropic (diagonal) stress tensor corresponding to the temperature of  $f$ . This linear combination introduces a parameter that can be adjusted to achieve a Prandtl number in the range  $2/3 \leq \text{Pr} < \infty$ .

The velocity-dependent collision frequency BGK model [7, 22, 23],  $v(\mathbf{c})\text{BGK}$ , is defined by

$$Q_{v(\mathbf{c})\text{BGK}}[f] = v(\mathbf{c})(\mathcal{P}[f] - f) \quad (9)$$

where  $v(\mathbf{c})$  is a velocity-dependent collision frequency and the target distribution  $\mathcal{P}[f]$  is a suitable pseudo-Maxwellian that we define below [cf. Eqs. (25-27)]. It has been shown [22] that a power law dependence  $v(\mathbf{c}) \sim |\mathbf{c} - \mathbf{v}|^\alpha$  yields an adjustable ratio of thermal conductivity to viscosity given by

$$\frac{\kappa}{\mu} = \frac{15 k_B}{4 m} \frac{10 - 2\alpha + \alpha^2}{15 - 3\alpha}. \quad (10)$$

For a comparison of these and other models see [24].

## NOTATION

For compactness of notation, let us define the five-vector  $\boldsymbol{\psi}$  of collision invariant phase-space functions  $\psi_i(\mathbf{c})$ , given by

$$\psi_0 = 1, \psi_1 = c_x, \psi_2 = c_y, \psi_3 = c_z, \psi_4 = \frac{1}{2}|\mathbf{c} - \mathbf{v}|^2 = \frac{1}{2}C^2 \quad (11)$$

and the corresponding five-vector  $\langle \boldsymbol{\psi} \rangle$  of local averages

$$\langle \psi_0 \rangle = 1, \langle \psi_1 \rangle = v_x, \langle \psi_2 \rangle = v_y, \langle \psi_3 \rangle = v_z, \langle \psi_4 \rangle = u \quad (12)$$

Here, angled brackets denote average with respect to the distribution  $f(\mathbf{x}, \mathbf{c}, t)$ , namely,

$$\langle F \rangle = \frac{m}{\rho} \int_{\Omega_c} d\mathbf{c} f(\mathbf{x}, \mathbf{c}, t) F(\mathbf{c}) \quad (13)$$

We also define the function

$$S(f) = -k_B \ln(bf + 1_{\{f=0\}}) \quad (14)$$

where  $1_{\{f=0\}} = 1(\mathbf{c})_{\{f(\mathbf{c})=0\}}$  is a Heaviside-like (indicator) function equal to unity over the subset  $\{f=0\}$  of  $\Omega_c$  where  $f$  vanishes, and equal to zero over the rest of  $\Omega_c$ , i.e., over the support of  $f$ . In this way, function  $S(f)$  is defined over the entire phase space even if  $f$  is zero in some regions of it. Then, the local specific entropy is given by

$$s(x) = \langle S(f) \rangle / m \quad (15)$$

The essential features of the collision terms  $Q[f]$  in Eqs. (6-9) are that, for any  $f$ ,

$$m \int_{\Omega_c} d\mathbf{c} Q[f] \psi_j = 0 \quad \text{for } j = 0, 1, \dots, 4 \quad (16)$$

as well as the H-theorem

$$\int_{\Omega_c} d\mathbf{c} Q[f] S(f) \geq 0 \quad (17)$$

where the strict equality holds if and only if  $f$  is a Maxwellian.

## STEEPEST LOCAL ENTROPY ASCENT COLLISION TERM

The kinetic model studied here is defined by

$$Q_{w\text{SEA}}[f] = \frac{1}{k_B \tau} w(\mathbf{c}, f) f M(f) \quad (18)$$

where  $w = w(\mathbf{c}, f)$  is a suitable positive-definite function of  $\mathbf{c}$  and  $f$  (for example  $w = \zeta[f] |\mathbf{c}|^{\alpha[f]}$  or  $w = 1/f$ ),  $M(f)$  is the function of  $f$  defined by

$$M(f) = S(f) - \sum_{j=0}^4 \gamma_j [f] \psi_j \quad (19)$$

and the five-vector  $\boldsymbol{\gamma}[f]$  is defined (for each given  $f$ ) by the solution of the linear system of equations

$$\sum_{j=0}^4 \langle w \psi_i \psi_j \rangle \gamma_j = \langle w S \psi_i \rangle \quad \text{for } i = 0, \dots, 4 \quad (20)$$

We use the letter  $M$  in Eq. (19) because the function  $M(f)$  represents at equilibrium the Massieu characteristic function and off equilibrium its natural generalization.

Using Eqs. (19) and (20), we verify the conservation conditions as follows

$$\begin{aligned} \frac{k_B \tau m}{\rho} \int_{\Omega_c} d\mathbf{c} Q_{w\text{SEA}}[f] \psi_i &= \langle w M \psi_i \rangle \\ &= \langle w S \psi_i \rangle - \sum_{j=0}^4 \gamma_j \langle w \psi_i \psi_j \rangle = 0 \end{aligned} \quad (21)$$

Using the fact that  $\langle w M \psi_i \rangle = 0$  and again Eq. (19), the proof of the H-theorem is as follows

$$\begin{aligned} \frac{k_B \tau m}{\rho} \int_{\Omega_c} d\mathbf{c} Q_{w\text{SEA}}[f] S &= \langle w M S \rangle \\ &= \langle w M S \rangle - \sum_{i=0}^4 \gamma_i \langle w M \psi_i \rangle = \langle w M M \rangle, \end{aligned} \quad (22)$$

which is clearly a non-negative definite functional of  $f$  for any positive  $w$ .

Eq. (22) also shows that the local entropy production rate is zero if and only if  $f w M = 0$ , i.e., for any local equilibrium distribution  $f_{\text{eq}}$  such that  $Q_{w\text{SEA}}[f_{\text{eq}}] = 0$ .

The distributions that satisfy this local equilibrium condition are the partial-Maxwellians

$$f_{\text{eq}}[\omega_c] = \frac{1_{\omega_c} \exp[-\sum_{k=1}^4 \lambda_k \psi_k]}{\int_{\Omega_c} d\mathbf{c} 1_{\omega_c} \exp[-\sum_{j=1}^4 \lambda_j \psi_j]} \quad (23)$$

where  $1_{\omega_c}$  is the Heaviside-like (indicator) function defined after Eq. (14) and  $\omega_c$  is any subset of  $\Omega_c$  (notice that  $1_{\omega_c} = 1_{\omega_c}^2$ ).

It can be easily shown that distributions (23) are unstable (in the sense of Lyapunov [25]) except when  $\omega_c = \Omega_c$ , i.e.,  $1_{\omega_c} = 1$ , in which case the distribution is a Maxwellian. As a result, the Maxwellians emerge as the only stable equilibrium distributions and we can assert that the  $Q_{w\text{SEA}}[f]$  collision term implements the Hatsopoulos-Keenan statement of the second law [26, 27] at the level of description of the Boltzmann equation.

The model just introduced was obtained by adapting the geometrical reasoning and formulation developed in [15, 28] to the present objective. The derivation and the geometrical background of the model will be discussed elsewhere. To conclude this section we give a few general comments without proofs.

The new term  $Q_{w\text{SEA}}[f]$  models the effect of collisions by attracting the phase-space distribution towards the path of steepest local entropy ascent compatible with the constraints of mass, momentum, and energy conservation. In other words, within the subset of the trajectories in state space that satisfy the conservation constraints, it selects the trajectory which for a given “traveled length”  $d\ell$  in the given time lapse  $dt$  yields the maximal local entropy production density. To measure the traveled length in state space we must equip the state space with the definition (choice) of a suitable metric. This choice is not unique and it is related to the weight function  $w$  in the model. For example, the most unbiased metric, i.e., the Fisher-Rao metric considered in [28], corresponds in the present context to the choice of a uniform weight function  $w = 1$ . This is one of the two SEA cases we study numerically in this paper, which reduces to the standard BGK model in the near-equilibrium limit and hence yields the wrong ratio of thermal conductivity to viscosity  $\kappa/\mu = 5k_B/2m$ . The other case we will consider corresponds to  $w = \xi C^\alpha$ , where in our notation  $C = \sqrt{2\psi_4}$ , with  $\alpha = (\sqrt{21} - 1)/2$ . The reason for this choice is that in the near-equilibrium limit the model reduces to a  $v(\mathbf{c})$ BGK model exhibiting the correct ratio  $\kappa/\mu = 15k_B/4m$  (correct Prandtl number for a monoatomic gas). The relation between the metric in state space and the weight function will be discussed elsewhere.

Whereas to our knowledge the SEA principle has never been applied in the context of kinetic theory, these ideas were originally conceived within the quantum context by one of the authors [28–33] and have been considered to some extent also in

other contexts. Therefore, the present study is to be considered a very preliminary exploration in order to extract some information useful for further development and comparisons.

The empirical validity of the maximum entropy production principle at the phenomenological level has been affirmed (explicitly or implicitly) as well as criticized by various authors in the past few decades in different fields and frameworks, with a variety of interpretations (see, e.g., [10–15]).

## NEAR EQUILIBRIUM LIMIT

In order to investigate the near equilibrium limit of the SEA model, we define the function  $\phi$  representing the relative deviation from the local pseudo-Maxwellian, such that

$$\phi = \frac{f - f_P}{f_P} \quad \text{i.e.,} \quad f = (1 + \phi) f_P \quad (24)$$

Here  $f_P = \mathcal{P}[f]$  is defined by the condition

$$S_P = -k_B \ln(b f_P) = \sum_{j=0}^4 \gamma_j^P \psi_j \quad (25)$$

where the set of  $\gamma_j^P$ 's is determined by  $f$  from the conditions

$$\langle w \psi_j \rangle_P = \langle w \psi_j \rangle \quad \text{for } j = 0, \dots, 4 \quad (26)$$

where

$$\langle F \rangle_P = \frac{m}{\rho(\mathbf{x}, t)} \int_{\Omega_c} d\mathbf{c} f_P(\mathbf{x}, \mathbf{c}, t) F(\mathbf{c}) \quad (27)$$

Notice that by its definition (25),  $f_P$  is nonzero everywhere in  $\Omega_c$ , i.e., we can write  $1_{\{f_P=0\}} = 0$ .

Multiplying Eq. (25) by  $w \psi_i$  and averaging with respect to  $f$  we obtain the system

$$\sum_{j=0}^4 \langle w \psi_i \psi_j \rangle \gamma_j^P = \langle w S_P \psi_i \rangle \quad \text{for } i = 0, \dots, 4 \quad (28)$$

We note that all averages can be expressed as averages with respect to the pseudo-Maxwellian  $f_P$  by using the identity

$$\langle F \rangle = \langle (1 + \phi) F \rangle_P \quad (29)$$

We may also write

$$S(f) = S_\phi + S_P \quad (30)$$

where

$$S_\phi = -k_B \ln(1 + \phi + \frac{1}{f_P} 1_{\{\phi=-1\}}) \quad (31)$$

and we used the fact that  $1_{\{f=0\}} = 1_{\{\phi=-1\}}$ . Subtracting Eqs. (28) from (20) and making use of Eqs. (29) and (30) we obtain

$$\sum_{j=0}^4 \langle w(1 + \phi) \psi_i \psi_j \rangle_P (\gamma_j - \gamma_j^P) = \langle w(1 + \phi) S_\phi \psi_i \rangle_P \quad \text{for } i = 0, \dots, 4 \quad (32)$$

In the limit  $\phi \rightarrow 0$ ,  $1_{\{\phi=-1\}} = 0$  and, to first order in  $\phi$ ,  $S_\phi = -k_B \phi$  so that the rhs of system (32) can be written as

$$-k_B \langle w \phi \psi_i \rangle_P = -k_B (\langle w \psi_i \rangle - \langle w \psi_i \rangle_P) = 0 \quad (33)$$

In Eq. (33) the first equality follows from Eq. (29), while the second equality follows from Eqs. (26). Since the matrix  $\langle w(1 + \phi) \psi_i \psi_j \rangle_P$  is in general non-singular, we conclude that, to first order in  $\phi$ ,  $\gamma_j = \gamma_j^P$ .

The function  $M$  defined by Eq. (19) can be rewritten in general as follows

$$M(f) = S_\phi - \sum_{j=0}^4 (\gamma_j - \gamma_j^P) \psi_j \quad (34)$$

Therefore, to first order in  $\phi$ ,  $M(f) \rightarrow -k_B \phi$  and

$$Q_{w\text{SEA}}[f] \rightarrow -\frac{1}{\tau} f_P w \phi = \frac{1}{\tau} w (f_P - f) \quad (35)$$

which we may call  $w$ BGK approximation in that it coincides with the standard BGK model for  $w = 1$  and with the  $v(\mathbf{c})$ BGK model for  $w = \tau v(\mathbf{c})$ . This also proves, in turn, that the  $w$ BGK approximation near equilibrium is  $w$ SEA, for any  $w$ .

## NUMERICAL EXPERIMENT SETUP AND RESULTS

Our preliminary comparisons are based on homogeneous relaxation from a highly non-equilibrium initial distribution  $f(\mathbf{x}, \mathbf{c}, t = 0) = f_0$  with zero macroscopic velocity. This initial condition is constructed by mixing two Maxwellian distributions with density  $n_0$ , temperature  $T_0$ , and non-zero but opposite mean flow velocities in the  $x$ -direction, namely

$$f_0 = \frac{1}{2} [f_{MB}(n_0, (v_{\text{shift}}, 0, 0), T_0) + f_{MB}(n_0, (-v_{\text{shift}}, 0, 0), T_0)] \quad (36)$$

where  $v_{\text{shift}} = \text{Ma} \sqrt{5k_B T_0 / 3m}$ . From energy conservation, it can be deduced that the final stable equilibrium state reached at the end of the relaxation process is the Maxwellian with density  $n_0$ , zero macroscopic velocity and temperature  $T_\infty = (1 + 5\text{Ma}^2/9) T_0$ . For the results reported here, we set  $k_B = 1.38 \times 10^{-23}$  J/K,  $m = 6.63 \times 10^{-26}$  kg,  $T_0 = 273$  K.

In [22] it is shown that if  $v(\mathbf{c}) = \zeta C^\alpha$  in the  $v(\mathbf{c})$ BGK model, Chapman-Enskog analysis yields the following expressions for the viscosity and the thermal conductivity

$$\mu = \frac{1}{2} \frac{\rho}{\zeta} \left( \frac{2k_B T}{m} \right)^{\frac{2-\alpha}{2}} \frac{\Gamma(\frac{7-\alpha}{2})}{\Gamma(\frac{7}{2})} \quad (37)$$

$$\kappa = \frac{k_B \rho}{m \zeta} \left( \frac{2k_B T}{m} \right)^{\frac{2-\alpha}{2}} \frac{10 - 2\alpha + \alpha^2}{8} \frac{\Gamma(\frac{5-\alpha}{2})}{\Gamma(\frac{5}{2})} \quad (38)$$

where the constants  $\alpha$  and  $\zeta$  can be adjusted to match both viscosity and thermal conductivity, and hence the Prandtl number.

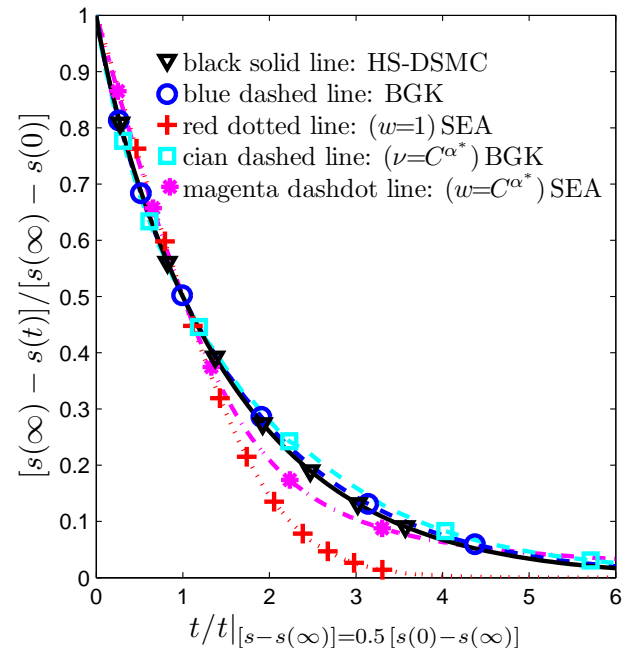
For  $\alpha = 0$  and  $\zeta = 1/\tau$  we recover the Chapman-Enskog expressions for the standard BGK model

$$\mu = \tau \rho \frac{k_B T}{m} \quad (39)$$

$$\kappa = \frac{5}{2} \frac{k_B}{m} \tau \rho \frac{k_B T}{m} \quad (40)$$

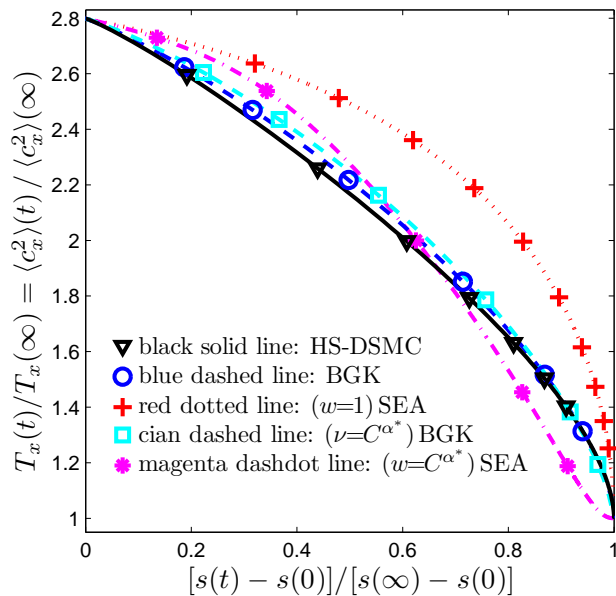
where  $\tau$  is the time between collisions assumed in the BGK model.

In our implementation of the variable collision-frequency SAE model, we set  $\alpha = \alpha^* = (\sqrt{21} - 1)/2$  to facilitate direct comparison with the equivalent BGK model with  $\text{Pr} = 2/3$ .

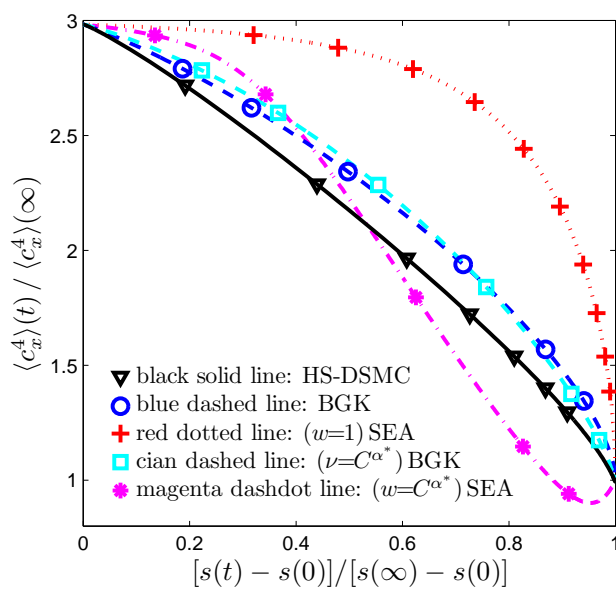


**FIGURE 1.** Normalized entropy as a function of time for different collision operators for relaxation from the highly non-equilibrium initial distribution given by (36) with  $\text{Ma} = 4$ .  $s(\infty)$  denotes the entropy of the final ( $t \rightarrow \infty$ ) equilibrium state. Time is scaled by  $t|_{[s-s(\infty)]=0.5[s(0)-s(\infty)]}$ , the time for which the entropy change is half of the total change due to the relaxation.

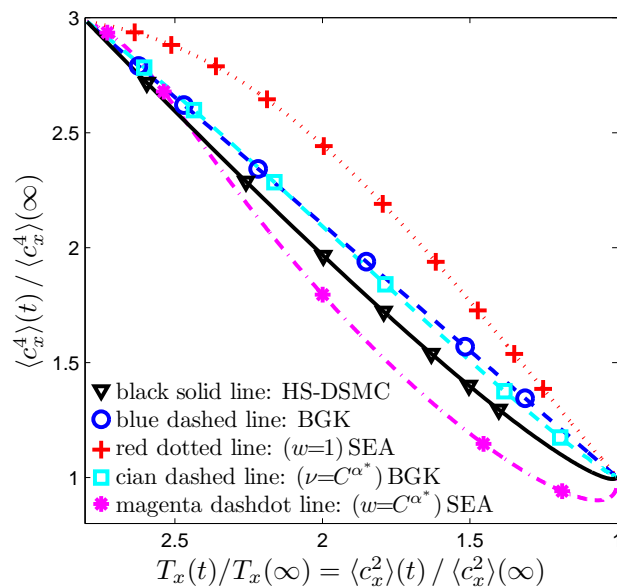
Figure 1 shows plots of entropy versus time for relaxation from initial condition (36) for  $\text{Ma} = 4$ . For the sake of a more direct comparison, we plot time nondimensionalized by the time  $t|_{[s-s(\infty)]=0.5[s(0)-s(\infty)]}$  at which, according to each model, the entropy change reaches half of the total entropy change  $s(t = 0) - s(t \rightarrow \infty)$  due to the relaxation. The entropy is normalized by the magnitude of the total entropy change during the relaxation process. The HS results shown in this and the following figures were obtained using DSMC. The SEA and BGK models were



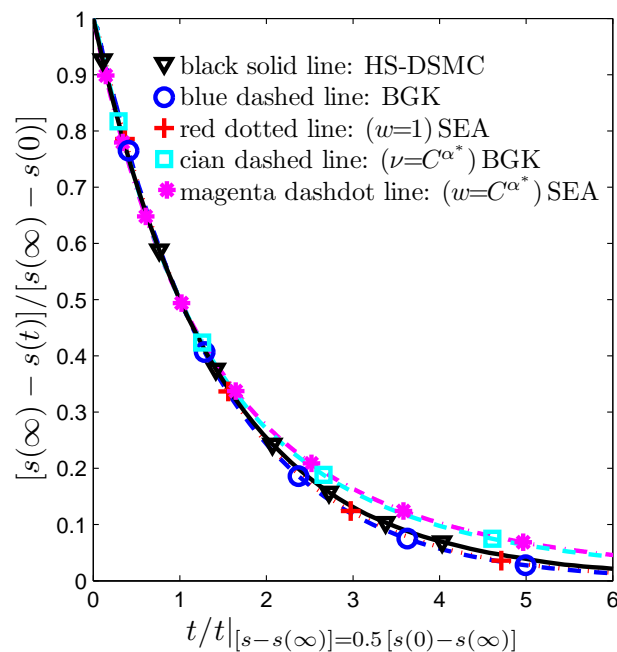
**FIGURE 2.** Normalized parallel kinetic temperature as a function of normalized entropy for different collision operators for relaxation from the highly non-equilibrium initial distribution given by (36) with  $Ma = 4$ .



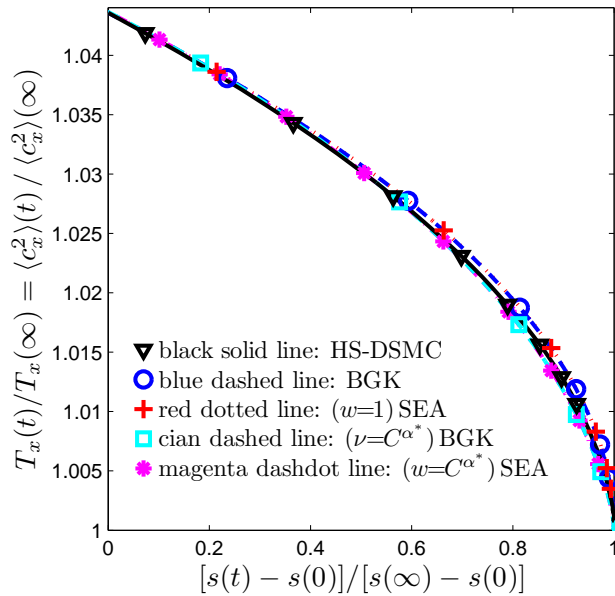
**FIGURE 3.** Normalized moment  $\langle c_x^4 \rangle(t) / \langle c_x^4 \rangle(\infty)$  as a function of normalized entropy for different collision operators for relaxation from the highly non-equilibrium initial distribution given by (36) with  $Ma = 4$ .



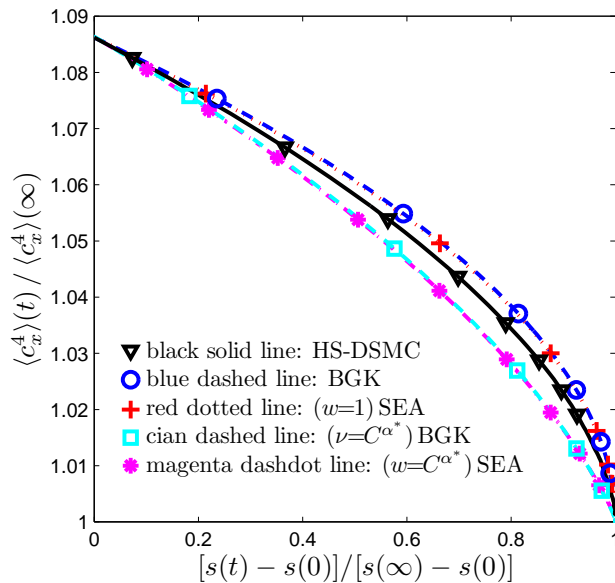
**FIGURE 4.** Normalized moment  $\langle c_x^4 \rangle(t) / \langle c_x^4 \rangle(\infty)$  as a function of normalized parallel kinetic temperature for relaxation from the highly non-equilibrium initial distribution given by (36) with  $Ma = 4$ .



**FIGURE 5.** Normalized entropy as a function of time for different collision operators for relaxation from the near-equilibrium initial distribution given by (36) with  $Ma = 0.2$ .  $s(\infty)$  denotes the entropy of the final ( $t \rightarrow \infty$ ) equilibrium state.

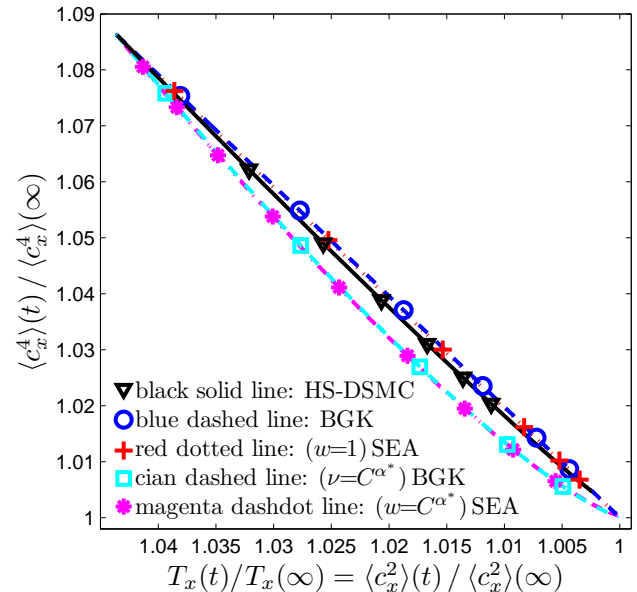


**FIGURE 6.** Normalized parallel kinetic temperature as a function of normalized entropy for different collision operators for relaxation from the near-equilibrium initial distribution given by (36) with  $Ma = 0.2$ .



**FIGURE 7.** Normalized moment  $\langle c_x^4 \rangle(t) / \langle c_x^4 \rangle(\infty)$  as a function of normalized entropy for different collision operators for relaxation from the near-equilibrium initial distribution given by (36) with  $Ma = 0.2$ .

numerically integrated using the Matlab package ode45; noting the symmetry of the relaxation problem, the distribution function was discretized in the variables  $c_x$  and  $c_r = \sqrt{c_y^2 + c_z^2}$ . Following a number of numerical experiments, the following discretiza-



**FIGURE 8.** Normalized moment  $\langle c_x^4 \rangle(t) / \langle c_x^4 \rangle(\infty)$  as a function of normalized parallel kinetic temperature for different collision operators for relaxation from the highly non-equilibrium initial distribution given by (36) with  $Ma = 0.2$ .

tion was determined as sufficient:  $c_x$  was discretized in the range  $\pm 10\sqrt{2k_B T_0/m}$  using 30 cells, while  $c_r$  was discretized in the range  $0 \leq c_r \leq 10\sqrt{2k_B T_0/m}$  using at least 180 cells. Doubling the number of cells in both directions has a negligible effect on the solution. Integration of the resulting discrete system in time, as well as all numerical integration in velocity space was based on cell mid-point values.

Figure 2 shows relaxation of the “parallel kinetic temperature” (the temperature based on the molecular velocity in the  $x$  direction—the direction of the distribution shift) for the same initial condition ( $Ma = 4$ ). Figure 3 shows comparison of the 5 models for a higher parallel moment. In both figures, moments are plotted against the normalized entropy change during the relaxation process. In Figure 4 the two moments are plotted against each other.

The results of the standard BGK model are surprisingly close to those of the HS model, even for relaxation from highly non-equilibrium ( $Ma = 4$ ) conditions, in spite of the fact that this model does not provide the correct Prandtl number. The constant-collision-frequency SEA model ( $w = 1$ ) is not close to the HS model, even though for late times (close to equilibrium) it becomes equivalent to the BGK model. At the initial time it appears to take a clearly different “direction” than the HS model.

This is perhaps to be expected, given the different origin of the SEA model. For example, a basic difference between the HS and BGK models compared to the constant-collision-



frequency SEA model, is that, in the latter, if the distribution is zero in a region of  $\Omega_c$  it remains zero for all times; in fact, more generally, in the SEA model, in regions of phase space where the distribution approaches zero the rate of repopulation by the collision term also approaches zero. Due to this feature (which persists in all weighted variants except for choices of  $w(f)$  such that  $\lim_{f \rightarrow 0} w(f) f \neq 0$ ) the plain SEA model preserves the non-negativity of the phase-space distribution even when solved backwards in time. Mathematically this means that a given initial distribution belongs to a unique trajectory in state space defined for all times  $-\infty < t < \infty$ . The BGK model does not have this feature. Indeed, when solved backwards in time, the solution becomes meaningless (negative) and must be stopped as soon as the distribution becomes zero somewhere in  $\Omega_c$ . In future work, we will investigate whether choices of  $w(f)$  such that  $\lim_{f \rightarrow 0} w(f) f \neq 0$  as well as using the actual HS collision frequency,  $\tau^{-1}w(\mathbf{c}, f) = \sqrt{2\pi k_B T / m^3} \rho d^2 [\exp(-C^2) + 0.5\sqrt{\pi}(2C + 1/C)\text{erf}(C)]$ , where  $d$  is the hard-sphere diameter, provide better agreement with the HS model.

Figures 5-8 repeat the comparisons of Figures 1-4 for the case  $Ma = 0.2$ . At this low Mach number the differences between the models are significantly smaller. We also observe validation that the SEA model reduces to the BGK model with the same collision frequency in the small deviation from equilibrium (Mach number) limit.

## CONCLUSIONS

We introduced a new family of models of the collision integral in the Boltzmann equation that implement the principle of steepest entropy ascent (SEA). The models preserve the usual collision invariants (mass, momentum, energy), as well as the non-negativity of the phase-space distribution, and satisfy the H-theorem in general. We proved that in the near-equilibrium limit each member of the new family of models reduces to the corresponding variable-collision-frequency BGK model. To compare the SEA and BGK models in the far non-equilibrium regime, we considered a simple case of homogeneous relaxation from a highly non-equilibrium state. We compared numerical solutions of the constant and velocity-dependent collision frequency variants of the SEA model with the standard BGK model, the variable collision frequency variant of the BGK model, and a Monte Carlo simulation of the original Boltzmann equation for hard spheres. Good agreement is confirmed between all models in the near-equilibrium regime. The BGK model provides surprisingly good agreement with the HS model even away from equilibrium. Instead, far from equilibrium the constant collision frequency variant of the SEA model exhibits large departures from the HS model. The variable collision frequency variant which leads to the correct Prandtl number yields results closer to the HS model but still qualitatively different, especially at early times. This suggests that the SEA is not equivalent to Boltzmann

collisional dynamics and needs to be modified or augmented via additional constraints or structure.

## ACKNOWLEDGMENT

The authors gratefully acknowledge the Cariplo–UniBS–MIT–MechE faculty exchange program co-sponsored by UniBS and the CARIPLO Foundation, Italy under grant 2008-2290. GPB did this work also as part of the Italian MIUR PRIN-2009-3JPM5Z-002.

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