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Mean-Field Model Beyond Boltzmann-Enskog Picture for Dense Gases

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Abstract. This work proposes an extension to Boltzmann BGK equation for dense gases. The present model has an H-theorem and it allows choice of the Prandtl number as an independent parameter. I show that similar to Enskog equation this equation can reproduce dynamics of dense gases.

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1 Introduction

An overwhelming majority of fluid flow problems of physical and engineering interest cannot be solved using microscopic simulation methods, such as molecular dynamics, due to the enormous number of degrees of freedom constituting the macroscopic systems. In such a scenario, mesoscale descriptions in terms of one particle distribution function, such as Boltzmann equation, provide important tools for understanding transport phenomena beyond phenomenological hydrodynamic descriptions of the Navier-Stokes-Fourier equations. Indeed, the nonlinear Boltzmann kinetic equation can accurately predict a wide range of physical properties and flow profiles for low density gases even in states very far from equilibrium (see for example [1]).

However, technical difficulties encountered in solving (analytically or numerically) the Boltzmann equation, a nonlinear integro-differential equation for the time dependent distribution functions, limits its application in practice. During the last few decades, this technical problem has been solved for the Boltzmann equation in two very important regimes. First, for highly non-equilibrium situations associated with supersonic flows (in general for high Mach number flows), direct simulation Monte Carlo method was applied with remarkable success (see for reviews [2]). Secondly, for very low Mach number

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flows lattice Boltzmann method is remarkably successful in both hydrodynamic regime as well as transitional regime (see for example [3–5]). The lattice Boltzmann method relies on an approximate form of Boltzmann collision term known as Bhatnagar-Gross-Krook (BGK) collision approximation. The model Boltzmann equation with BGK collision term retains almost all qualitative features (such as correct conservation laws, H-theorem) of the Boltzmann equation [1]. Indeed, the BGK model can be classified as the first truly successful phenomenological model at the level of one particle distribution. The mathematical simplicity of this model is often used to obtain exact and semi-exact analytical solutions which can help one understand the hydrodynamics well beyond Navier-Stokes equations [1, 5]. The strength and limitations of this model along with ways to make it quantitatively accurate (without destroying the basic features such as H-theorem) is well understood [1, 6, 7].

In order to describe the fluid transport in the dense regimes, Boltzmann equation was extended by Enskog and further modified by van Beijeren and Ernst (known as the revised Enskog theory (RET)) [8, 9]. Similar to Boltzmann's model of dilute gas, particles motion in these models is decomposed into two parts: propagation at constant velocity followed by collisions in which exchange of momentum between particles happens. However, unlike Boltzmann model, collision are understood to be non-local events due to the presence of finite size particles. This idea of non-local collisions due to finite size of particles behind Enskog or RET extension of Boltzmann equation is borrowed from Van-der Waals' picture of excluded volume in dense gases. However, mainly due to the non-local collisions, Enskog extension of Boltzmann model leads to even more intractable form of nonlinear integro-differential equation. Thus, it is not surprising that it took almost fifty years to prove even the existence of H-theorem [10] and so far only modest engineering and physical applications of dense fluid are modeled via Enskog equation. The non-local nature of collision is difficult to handle both for Monte-Carlo method as well as for kinetic modeling via simplified phenomenological theories of BGK type.

From the engineering perspective, a dense gas model, where non-ideality can be added as extra terms over a rarefied gas model (either of Monte-Carlo type or BGK type or of Fokker-Planck type), is an extremely desirable solution. In case of DSMC model of Boltzmann equation, Alexander et al. proposed a simple modification of propagation step which gave the correct equation of state but failed to reproduce the Enskog transport coefficients [11]. An important progress for such modeling approaches was reported in [12, 13], where BGK like collision terms for Enskog equation were proposed. The main idea behind these works was to compute the effect of Enskog collision term on momentum and energy balance and explicitly add it in momentum and energy balance equation as a correction to the BGK collision term. This approach gave correct viscosity coefficient and equation of state, but neither H-theorem can be proven nor correct thermal conductivity can be derived for these type of models.

The goal of the present work is to fill this gap and construct a phenomenological model of fluid transport at the meso-scale level. Similar to hydrodynamic description given by Navier-Stokes equations, we demand that a good phenomenological theory at

mesoscale should fulfil the following criteria:

- It must obey conservation laws and second law of thermodynamics (H-theorem).
- It must reproduce correct thermodynamic equation of state.
- It must reproduce correct constitutive relations along with Enskog transport coefficients in hydrodynamic regime.

The work is organized as follows: in Section 2, basic framework for the kinetic description is given. In Section 3, briefly I remind about conceptual problem associated with the existing approaches. In Section 4, the present model will be outlined. In Section 5, the physical modification behind the current model will be presented. In Section 6, conservation laws will be derived from the present description. In Section 7, I will show that H-theorem exist for the present model. Finally, in Section 8, hydrodynamic limit for the proposed kinetic equation will be derived.

2 Basic set-up for the kinetic equation

The basic starting point for such modeling is exact dynamics of one particle distribution function f (defined as probability of finding a particle at location $\mathbf{x}$ with velocity $\mathbf{v}$ at time t) as a function of phase variable $\mathbf{z}\equiv(\mathbf{x},\mathbf{v})$, given by BBGKY hierarchy as

$$\partial_t f(\mathbf{z}_1,t)+\partial_\alpha\left[f(\mathbf{z}_1,t)\mathbf{v}_1\right]=-\hat{A}_1 f_2(\mathbf{z}_1,\mathbf{z}_2,t), \tag{2.1}$$

where f_2 denotes the two particle distribution function and $\hat{A}_1$ is an operator whose exact form is not important for the present discussion (for details of this equation see for example [14]) and $\partial_\alpha\equiv\partial/(\partial x_\alpha)$. The hydrodynamic fields $\{\rho,\mathbf{j},T\}$ are defined in terms of one particle distribution function f as

$$\int d\mathbf{v} f\left\{1,\mathbf{v},\frac{v^2}{2}\right\}=\{\rho,\mathbf{j},E\}, \tag{2.2}$$

with energy of hard-sphere as

$$E=\frac{j^2}{2\rho}+\frac{\rho D K_{\mathrm{B}} T}{2m}, \tag{2.3}$$

where D is the dimension and K_{B} is Boltzmann constant. The velocity $\mathbf{u}$ is defined as $\mathbf{u}=\mathbf{j}/\rho$. A closed form kinetic equation is obtained if we set $\hat{A}_1 f_2=\mathcal{J}(f)$, where $\mathcal{J}$, typically collision integral, maps functions onto functions [14]. Thus for example, $f_2=f_2(\mathbf{z}_1,\mathbf{z}_2,f)$ with explicit time dependence of f_2 entirely contained in f was proposed by Bogoliubov to derive the Boltzmann equation. The traditional mechanistic view-point starting from BBGKY hierarchy is that non-ideality coming from the repulsive part of molecular forces needs to be modeled via three-particle and other higher order collision and free-flight of molecules remains unaffected by it. However, so far the only widely used model is

mean-field approximation of Enskog, where all higher order effects are lumped in non-local collisions. In the present work, I am advocating an alternate mean-field picture of non-ideality in dense system. According to this picture, in the dense system, dominant change is alteration of free flight of a hard sphere particle. Before formulating a BGK type model for dense gases, I will review the problem associated with current modeling approaches.

3 In-admissibility of force driven Boltzmann equation

A typical temptation which might arise in writing simplified kinetic theories is to think of dense gas contribution as a self consistent force added on the Boltzmann equation (or BGK equation). Here, I remind the reader that a Vlasov type force term of the form can always be added to the Boltzmann kinetic equation. Thus, an engineering approach, popularized by Lattice Boltzmann type modeling, is to tune such a force in such a way that the correct hydrodynamics equation is obtained (see for example [4]).

It is obvious that such an approach is not going to be self-consistent [15]. Any attempt to add dense gas contribution via Vlasov type force term is physically wrong as the hard-core part of the interaction cannot be represented in the conservative force form. This happens because dense gas contributions need to increase entropy production in the system.

In the next section, I will formulate a thermodynamically correct extension of Boltzmann BGK equation.

4 Present model

The key new ingredient, I propose is that $\hat{A}_1 f_2$ will also modify the free propagation step of the Boltzmann type equations. In particular, we propose to write generalized kinetic equation for $f(\mathbf{z},t)$ as

$$\partial_t f(\mathbf{z},t) + \partial_\alpha \left[f(\mathbf{z},t)\hat{\mathbf{v}} \right] = \mathcal{J}, \tag{4.1}$$

where $\hat{\mathbf{v}}$ is some unknown propagation velocity. The physical picture behind such a modification of free propagation can be understood using Bogoliubov hypothesis for the equilibration of a non-equilibrium gas, which assumes separations of time scale by considering mean free time τ of a molecule to be much larger than mean time spent in the interaction domain of the another molecule [14]. In dilute region, where reduced density is small, he derived Boltzmann equation using this hypothesis. Now for hard-sphere in dense region the dynamics in mean free time τ has to be more complex due to collective effects. In this time scale, for dense system we also need to consider the effect of collective motion (hydrodynamics) on individual particles. Such corrections from local collision can also be incorporated by analyzing the short time motion of tagged particle due to entropic force generated by particle-particle correlations and hydrodynamics force

generated by other particles. In other words, apart from usual hydrodynamic forces the tagged particle might also experience effective forces, which have purely entropic origin. Unlike ring kinetic theory approach, I am not trying to derive such an equation from the first principle but am trying to model it based on physical intuitions and limiting behaviors of the system. First, we know the two limiting behavior of such a system in rarefied and extremely dense regime quantified by compressibility factor χ defined as

$$\chi = \frac{p}{\rho RT} - 1 \equiv \frac{1}{\rho R}\left(s^{\rm nid} - \rho \frac{\partial s^{\rm nid}}{\partial \rho}\right), \tag{4.2}$$

where the excess entropy $s^{\rm nid}(\rho)$ and pressure $p(\rho,T)$ as a function of density ρ and temperature T is known from equilibrium statistical mechanics (for example Van-der-Waals or Carnhann-Starling approximation). In a rarefied system $(\chi \to 0)$, present model should recover Boltzmann description of free propagation step ($\hat{\mathbf{v}} = \mathbf{v}$), while for extremely dense system $(\chi \to \infty)$, all hard-spheres should pack together and move with the collective velocity of the system, which means $\hat{\mathbf{v}} = \mathbf{v} = \mathbf{u}$.

In the present work, I ask the question what is the most general form of the propagation velocity $\hat{\mathbf{v}}$ (which can be a function of the moments of f) in the kinetic equation (4.1). In order to do so, the propagation velocity is written as a formal Hermite expansion in terms of dimensionless peculiar velocity $\xi_\alpha = (v_\alpha - u_\alpha)/\sqrt{2RT}$ as

$$\hat{\mathbf{v}} = \mathbf{v} + \sum_{n=0}^{\infty} \mathbf{a}^{(n)} \mathbf{H}^{(n)}(\boldsymbol{\xi}). \tag{4.3}$$

Furthermore, we need to recognize that the condition of having correct continuity equation (obtained by integrating Eq. (4.1) over $\mathbf{v}$) itself severely restricts the choice of $\hat{\mathbf{v}}$. For example, $\mathbf{a}^{(0)} = 0$ and $\mathbf{a}^{(n)} = 0$ for all $n > 2$. For $n = 2$ only the trace part survives and the most general form of $\hat{\mathbf{v}}$, consistent with the conservation laws, is

$$\hat{v}_\alpha - v_\alpha = \underbrace{\chi(v_\alpha - u_\alpha)}_{A} + \underbrace{(v_\beta - u_\beta)\frac{P^{(\rm I)}_{\alpha\beta}}{\rho RT}}_{B} + \underbrace{u^{(\rm I)}_\alpha \left(\xi^2 - \frac{D}{2}\right)}_{C}, \tag{4.4}$$

where precise form of second order tensor $P^{(\rm I)}_{\alpha\beta}$ and fictitious velocity $u^{(\rm I)}_\alpha$ need to be determined with the requirements of correct H-Theorem.

In subsequent section, I will show that these conditions are fulfilled if

$$u^{(\rm I)}_\alpha = -\lambda^{(\rm q)} \tau T \partial_\alpha \log T, \qquad P^{(\rm I)}_{\alpha\beta} = -k_1 \tau \Lambda_{\alpha\beta} - k_2 \tau \partial_\gamma u_\gamma \delta_{\alpha\beta}, \tag{4.5}$$

where k_1, k_2 and $\lambda^{(\rm q)}$ are positive definite scalars related to transport coefficients of the fluid and the traceless part of the strain tensor is

$$\Lambda_{\alpha\beta} = \left(\partial_\beta u_\alpha + \partial_\alpha u_\beta - \frac{2}{D}\partial_\gamma u_\gamma \delta_{\alpha\beta}\right). \tag{4.6}$$

Here, it needs to be noted that the physical picture behind the present model envisions that both $P^{(\mathrm{I})}_{\alpha\beta}$ and $u^{(\mathrm{I})}_{\alpha}$ are corrections of the order of mean free time τ. We can relate these new transport coefficients with that of real fluid by performing the Chapman-Enskog expansion. The kinetic equation Eq. (4.1) along with expression of $\hat{\mathbf{v}}$ given by Eq. (4.4) and Eq. (4.5), are the main result of this work.

5 Physical motivation

Before analyzing the model further, let us try to understand the physical meaning of Eq. (4.4). The physical picture behind first term on the right hand side of Eq. (4.4) (underlined term A) can be understood in the framework of social force model created by Helbing and Molnár in the context of traffic dynamics [16]. The goal of this term is to keep tagged particle separated from other particles, and such crossing of particles can be avoided (only in an average sense) by introducing a force which tries to remove them from dense regions. What we want is that at the time τ after any collision, the probability of having a particle in denser region is smaller. A system mimicking such a motion is the trajectory of an individual moving on a street trying to avoid being very close to crowded region after time t. Suppose he is moving very fast in a region of high density, then he can avoid being in the region of high density at the end of time t by moving even more faster. In other words, he experiences a social force which accelerates him in the region of high density if he is moving too fast. In the opposite limit, where the individual is moving too slow compared to the crowd in dense regions. He can avoid being in the region of high density at the end of time t, if he gets decelerated in the regions of high density. For hard-spheres such an effect can be modeled by underlined term A in Eq. (4.4). The third term C is a hydrodynamic effect and can be understood as microscopic analog of thermophoretic forces [17]. The difference from macroscopic expression is that in stead of transport coefficient a direct dependence on heat velocity appears. This may be due to the fact that the current description (Eq. (4.4)) is for short-time motion, whereas transport coefficients appear only in long time limit. Similarly, the term B in Eq. (4.4) is a hydrodynamic force which reflects the tendency to resist locally generated flow field (shear stresses and compression).

6 Conservation law

It is easy to check that the present formulation gives correct conservation laws for dense gas. Before, showing that, let us recall that the kinetic part of the stress tensor and heat flux are conveniently defined in terms of second and third order traceless Hermite tensor

$$\mathcal{H}^{(3)}_{\alpha}(\boldsymbol{\xi}) = \xi_{\alpha}\left(\xi^2 - \frac{D+2}{2}\right), \qquad \mathcal{H}^{(2)}_{\alpha\beta}(\boldsymbol{\xi}) = \left(\xi_{\beta}\xi_{\alpha} - \frac{1}{D}\xi^2\delta_{\alpha\beta}\right). \tag{6.1}$$

In terms of these tensors kinetic part of the stress tensor $\sigma^{(\mathrm{K})}_{\alpha\beta}$ and the heat flux $q^{(\mathrm{K})}_{\alpha}$ are

$$\sigma^{(\mathrm{K})}_{\alpha\beta} = 2RT\int d\mathbf{v} f \mathcal{H}^{(2)}_{\alpha\beta}, \qquad q^{(\mathrm{K})}_{\alpha} = (2RT)^{\frac{3}{2}}\int d\mathbf{v}\frac{f}{2}\mathcal{H}^{(3)}_{\alpha}. \tag{6.2}$$

By taking moments of the kinetic equation Eq. (4.1), we have time evolution equation for the locally conserved fields as

$$\partial_t \rho + \partial_\alpha j_\alpha = 0, \tag{6.3a}$$
$$\partial_t j_\gamma + \partial_\alpha \left[\rho u_\alpha u_\gamma + p\delta_{\alpha\gamma} + \sigma_{\alpha\gamma}\right] = 0, \tag{6.3b}$$
$$\partial_t E + \partial_\alpha \left[(E+p)u_\alpha + \sigma_{\alpha\gamma}u_\gamma + q_\alpha\right] = 0, \tag{6.3c}$$

where

$$\sigma_{\alpha\gamma} = (1+\chi)\sigma^{(\mathrm{K})}_{\alpha\gamma} + P^{(\mathrm{I})}_{\alpha\gamma} + P^{(\mathrm{I})}_{\alpha\beta}\frac{\sigma^{(\mathrm{K})}_{\beta\gamma}}{\rho RT} + u^{(\mathrm{I})}_{\alpha}\left(\frac{q^{(\mathrm{K})}_{\gamma}}{RT}\right), \tag{6.4a}$$

$$q_\alpha = \left\{(1+\chi)\delta_{\alpha\beta} + \frac{P^{(I)}_{\alpha\beta}}{\rho RT}\right\}q^{(\mathrm{K})}_{\beta} + eu^{(\mathrm{I})}_{\alpha} + q^{II}_{\alpha}, \tag{6.4b}$$

$$q^{II}_{\alpha} = RTu^{(\mathrm{I})}_{\alpha}\int d\mathbf{v} f\left[\xi^2\left(\xi^2 - \frac{D+2}{2}\right)\right]. \tag{6.4c}$$

We can show that the stress tensor and heat flux has same expression as RET if k_1, k_2 and $\lambda^{(\mathrm{q})}$ are chosen properly. As for example, in case of BGK collision model, it will be shown later that

$$k_1 = \frac{\eta}{\tau} - (1+\chi)p, \tag{6.5}$$

where η is the shear viscosity and τ is the relaxation time. Similarly for the BGK model k_2 in terms of the bulk viscosity η_b is given as

$$k_1 = \frac{\eta_b}{\tau}. \tag{6.6}$$

Before deriving the transport coefficient, in the next section, we shall prove the H-theorem for the present model.

7 H-theorem

Résibois [10] showed that in order to prove H-theorem for the Enskog equation, it is important to decompose the H-function for the dense gas into a kinetic part (same as Boltzmann's H-function)

$$H^{\mathrm{id}}(\mathbf{x},t) = \int d\mathbf{v} f(\mathbf{x},\mathbf{v},t)\left[\log f(\mathbf{x},\mathbf{v},t) - 1\right] \tag{7.1}$$

and a correlation part which depends on the one particle distribution function only via density of the fluid. The correlation part is essentially equilibrium excess entropy of the dense gas. This idea was explored further by Grmela et al. in [18], where it was shown that with this choice of H-function the Enskog equation is consistent with traditional non-equilibrium thermodynamics.

Thus, in order to show the existence of H-theorem for the present model, I define the H-function for dense system as

$$H(\mathbf{x},t) = H^{\rm id} - \frac{s^{\rm nid}(\rho(\mathbf{x},t))}{R}. \tag{7.2}$$

By noting that non-ideal part of entropy is a function of density only, using continuity equation, we obtain

$$\partial_t\Big(\frac{s^{\rm nid}}{R}\Big) + \frac{d\big(s^{\rm nid}/R\big)}{d\rho}\partial_\alpha j_\alpha = 0. \tag{7.3}$$

In order to write the evolution equation for the kinetic part of the H function, I multiply Eq. (4.1) with $\log f$ and integrate over $\mathbf{v}$, which gives

$$\partial_t H^{\rm id} + \partial_\alpha \int d\mathbf{v}\big[f\log f\hat{v}_\alpha\big] - \int d\mathbf{v}\hat{v}_\alpha f\partial_\alpha \log f = \int \mathcal{J}\log f d\mathbf{v}. \tag{7.4}$$

Furthermore, using Eq. (4.4), we have:

$$\begin{aligned}\int d\mathbf{v}\hat{v}_\alpha\partial_\alpha f = \int d\mathbf{v}v_\alpha\partial_\alpha f - \partial_\alpha\Big(\frac{s^{\rm nid}}{R}u_\alpha\Big) + \frac{d\big(s^{\rm nid}/R\big)}{d\rho}\partial_\alpha j_\alpha \\ - \Big(\frac{P^{(\rm I)}_{\alpha\beta}}{RT}\Big)\partial_\alpha u_\beta - u^{(\rm I)}_\alpha\int d\mathbf{v}\Big(\xi^2 - \frac{D}{2}\Big)\partial_\alpha f.\end{aligned} \tag{7.5}$$

Finally, by subtracting Eq. (7.3) from Eq. (7.4) and simplifying resulting expression using Eq. (7.5), we have evolution equation for the total H function as

$$\partial_t H + \partial_\alpha J^{\rm H}_\alpha = \int \mathcal{J}\log f d\mathbf{v} + \frac{D}{2}\rho u^{(\rm I)}_\alpha\partial_\alpha\log T + \Big(\frac{P^{(\rm I)}_{\alpha\beta}}{RT}\Big)\partial_\alpha u_\beta, \tag{7.6}$$

with the flux of H-function (analog of entropy flux) is

$$J^{\rm H}_\alpha = -\Big(\frac{s^{\rm nid}}{R}u_\alpha\Big) + \int d\mathbf{v}\big[f(\log f - 1)\hat{v}_\alpha\big]. \tag{7.7}$$

It is interesting to see here that similar to H-function the flux of it also has a contribution totally dependent on macroscopic variable ρ and $\mathbf{j}$. For H-theorem to be valid, we need to show that entropy production is positive, which means right hand side of Eq. (7.6) must be negative. For Boltzmann collision term or BGK collision term, the first term on the right term is negative. However, this is possible for the last two terms if Eq. (4.5) is valid. Thus, we have proved the H-theorem. Here, it is interesting to note that the as compared to Boltzmann kinetic theory, the new ingredient required to prove H-theorem is just the same as that used in linear irreversible thermodynamics (see for a modern perspective [19]).

8 Hydrodynamics

The goal of any kinetic theory is not complete without understanding the properties of the underlying fluid. In this section, I would like to show that the present kinetic theory results in correct hydrodynamics. The first step in C-E expansion is to write

$$\frac{\partial f}{\partial t}+\partial_\alpha(\hat{v}_\alpha f)=\frac{1}{\mathrm{Kn}}\mathcal{L}f, \tag{8.1}$$

where $\mathcal{L}$ is the linearized collision integral. We expand the distribution function in power of smallness parameter

$$f=f^0+\mathrm{Kn}f^{(1)}+\cdots, \tag{8.2}$$

with condition:

$$\int d\mathbf{v}f\begin{pmatrix}1\\ \mathbf{v}\\ v^2\end{pmatrix}=\int d\mathbf{v}f^0\begin{pmatrix}1\\ \mathbf{v}\\ v^2\end{pmatrix}=\begin{pmatrix}\rho\\ \mathbf{u}\\ \rho u^2+\rho DRT\end{pmatrix}, \tag{8.3}$$

and for any $i>0$,

$$\int d\mathbf{v}f^{(i)}\begin{pmatrix}1\\ \mathbf{v}\\ v^2\end{pmatrix}=\begin{pmatrix}0\\ 0\\ 0\end{pmatrix}. \tag{8.4}$$

Similarly the time derivative acting on any variable ϕ is expanded as

$$\partial_t\phi=\partial_t^{(0)}\phi+\mathrm{Kn}\partial_t^{(1)}\phi+\cdots. \tag{8.5}$$

The solvability condition is

$$\int d\mathbf{v}\begin{pmatrix}1\\ \mathbf{v}\\ v^2\end{pmatrix}\left[\partial_t^{(0)}f^{(0)}+\partial_\alpha(\hat{v}_\alpha f^{(0)})\right]=\begin{pmatrix}0\\ 0\\ 0\end{pmatrix}, \tag{8.6}$$

which using Eq. (6.3a) can be written as

$$\partial_t^{(0)}\rho=-\partial_\alpha j_\alpha, \tag{8.7a}$$

$$\partial_t^{(0)}u_\alpha=-u_\beta\partial_\beta u_\alpha-\frac{1}{\rho}\partial_\alpha p, \tag{8.7b}$$

$$\partial_t^{(0)}T=-u_\alpha\partial_\alpha T-\frac{2p}{\rho RD}\partial_\alpha u_\alpha. \tag{8.7c}$$

At this stage, we need to provide the exact form of collision operators. Although not restrictive to BGK-model, for further analysis I chose to work with BGK collision model, which allows us to write the next approximation for f as

$$f^{(1)}=-\frac{\tau(1+\chi)}{\mathrm{Kn}}f^{eq}\left(2\mathcal{H}^{(2)}_{\alpha\beta}\partial_\alpha u_\beta+\sqrt{2RT}\mathcal{H}^{(3)}_\alpha\partial_\alpha\log T\right), \tag{8.8}$$

so, up to first order in Knudsen number:

$$\sigma_{\alpha\beta} = -\eta\left(\partial_\beta u_\alpha + \partial_\alpha u_\beta - \frac{2}{D}\partial_\gamma u_\gamma \delta_{\alpha\beta}\right) - k_2\tau\partial_\gamma u_\gamma \delta_{\alpha\beta}, \tag{8.9a}$$

$$q_\alpha = -\tau\left\{\frac{D}{2}\rho T\lambda^{(q)} + p(1+\chi)C_p\right\}\partial_\alpha T, \tag{8.9b}$$

where shear viscosity

$$\eta = (k_1 + (1+\chi)p)\tau, \tag{8.10}$$

and, Prandtl number is

$$\mathrm{Pr} = \frac{k_1 + (1+\chi)p}{(D/2C_p)\rho T\lambda^{(q)} + p(1+\chi)}. \tag{8.11}$$

This means in present model, we are allowed to set shear and bulk viscosity and Prandtl number independent of each other. So unlike Dufty et al. [12], in the present model we are allowed to set heat conductivity and viscosity coefficients independently. It is interesting to note here that the present model provide a natural generalization to the BGK model in the case of dilute gas too.

To conclude, in the present manuscript, I have presented an alternate mean-field model of hydrodynamics at the mesoscale level. It can be safely claimed that this model is first complete phenomenological model consistent with non-equilibrium thermodynamics for describing hard-sphere hydrodynamics at the mesoscale level.

Finally, In the manuscript, for moderately dense gases, it was shown that correct hydrodynamic limit (as predicted by Enskog description) is obtained for near equilibrium situations. However, it needs to be reminded that similar to any BGK type model, what would happen far away from equilibrium is not obvious. In those cases, a detailed case by case study is needed.

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References

[1] C. Cercignani, The Boltzmann Equation and Its Applications, Springer, Berlin, 1988.
[2] E. S. Oran, C. K. Oh, and B. Z. Cybyk, Direct simulation monte carlo: recent advances and applications, An. Rev. Fluid. Mech., 30 (1998), 403–441.
[3] H. Chen, S. Kandasamy, S. Orszag, R. Shock, S. Succi, and V. Yakhot, Extended Boltzmann kinetic equation for turbulent flows, Science., 301 (2003), 633–636.
[4] S. Succi, The Lattice Boltzmann Equation for Fluid Dynamics and Beyond, Oxford University, 2001.

[5] S. Ansumali, I. V. Karlin, S. Arcidiacono, A. Abbas, and N. I. Prasianakis, Hydrodynamics beyond Navier-Stokes: exact solution to the lattice Boltzmann hierarchy, Phys. Rev. Lett., 98 (2007), 124502.
[6] A. N. Gorban, and I. V. Karlin, General approach to constructing models of the Boltzmann equation, Phys. A., 206 (1994), 401–420.
[7] S. Ansumali, S. Arcidiacono, S. S. Chikatamarla, N. I. Prasianakis, A. N. Gorban, and I. V. Karlin, Quasi-equilibrium lattice Boltzmann method, EuroPhys. J. B., 56 (2007), 135–139.
[8] S. Chapman, and T. G. Cowling, The Mathematical Theory of Non-uniform Gases, Cambridge University Press, New York, 1991.
[9] H. van Beijeren, and M. H. Ernst, The modified Enskog equation, Phys., 68 (1973), 437–456.
[10] P. Résibois, *H*-theorem for the (modified) nonlinear Enskog equation, Phys. Rev. Lett., 40 (1978), 1409–1411.
[11] F. J. Alexander, A. L. Garcia, and B. J. Alder, A consistent Boltzmann algorithm, Phys. Rev. Lett., 74 (1995), 5212–5215.
[12] J. W. Dufty, A. Santos, and J. J. Brey, Practical kinetic model for hard sphere dynamics, Phys. Rev. Lett., 77 (1996), 1270–1273.
[13] J. F. Lutsko, Approximate solution of the Enskog equation far from equilibrium, Phys. Rev. Lett., 78 (1997), 243–246.
[14] R. L. Liboff, Kinetic Theory: Classical, Quantum, and Relativistic Descriptions, Springer, Berlin, 2003.
[15] L. S. Luo, Unified theory of the lattice Boltzmann models for nonideal gases, Phys. Rev. Lett., 81 (1998), 1618–1621.
[16] D. Helbing, and P. Molnár, Social force model for pedestrian dynamics, Phys. Rev. E., 51 (1995), 4282–4286.
[17] I. Goldhirsch, and D. Ronis, Theory of thermophoresis. I. general considerations and mode-coupling analysis, Phys. Rev. A., 27 (1983), 1616–1634.
[18] M. Grmela, and L. S. Garcia-Colin, Compatibility of the Enskog kinetic theory with thermodynamics. I, Phys. Rev. A., 22 (1980), 1295–1304.
[19] H. C. Ottinger, Beyond Equilibrium Thermodynamics, Wiley-Interscience, Hoboken, NJ 2005.