Commun. Comput. Phys.
doi: 10.4208/cicp.301009.240910s

Vol. **9**, No. 5, pp. 1106-1116
May 2011

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

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Received 30 October 2009; Accepted (in revised version) 24 September 2010

Available online 24 December 2010

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.

AMS subject classifications: 52B10, 65D18, 68U05, 68U07

Key words: Microflows, lattice Boltzmann method.

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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