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An axisymmetric computational model of generalized hydrodynamic theory for rarefied multi-species gas flows

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ABSTRACT

On the basis of the Eu's generalized hydrodynamic (GH) theories for diatomic single species gas and monatomic multi-species gas, an axisymmetric GH computational model for multi-species gas containing monatomic and diatomic molecules is developed for the numerical simulation of hypersonic rarefied gas flows. The multi-species GH computational model includes monatomic and diatomic species of O_2, N_2, NO, O, N. The mass diffusion flux of the gas mixture is included in the GH constitutive relation. In addition, the physical relationship between the mass diffusion and heat fluxes is added to the evolution equation set. The multi-species GH theory includes the rotational nonequilibrium effect of diatomic molecules by introducing excess normal stress associated with the bulk viscosity.

An efficient multi-species GH numerical solver for axisymmetric rarefied flows is then developed by adopting various numerical techniques, such as an adequate nonlinear equation solver for the GH constitutive relation, an accurate flux splitting scheme, multi-grid convergence acceleration and slip-wall boundary conditions. For validation, the proposed computational model is applied to hypersonic rarefied flows over a space shuttle nose, a sphere and a reentry body as well as 1D shock structure. By comparing the results of the multi-species GH model with those of the Navier–Stokes equation and the DSMC, the accuracy and physical consistency of the GH computational model are critically examined.

1. Introduction

In recent past several decades, the study of nonlinear gas flows in rarefied condition has been treated as an important topic. It has been motivated by the needs of tools to efficiently predict aero-thermodynamic loads on vehicles operating in high altitude. From this point of view, the development of computational models to predict gas flows over a large portion of rarefied flow regime is important. The primary physical parameter characterizing the rarefied flow is the Knudsen number [1], which is not small in high altitude condition. Though the Navier–Stokes (N–S) theory is capable of treating flow phenomena in a small deviation from the local equilibrium condition, it is not known to remain valid in the flow regime of a relatively large Knudsen number [2,3].

Much effort has been put into the development of a computational model beyond the N–S equations. Numerical models to predict the rarefied flow can be classified into two categories: the 'full kinetic (or molecular dynamic) model' and the 'fluid dynamic model'. In the former category, the direct simulation Monte Carlo (DSMC) is the most successful and powerful method [4–6]. At least, in terms of accuracy, there seems to be no alternative yet which can provide better results than

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DSMC. However, computational load of DSMC is very costly in comparison with fluid dynamic model, particularly in the regime near continuum limit [7]. Moreover, much experience is required to properly operate many tunable parameters.

On the other hand, fluid dynamic model is more attractive in terms of computational time cost and mathematical modelling. They can be formulated by hyperbolic conservation laws and some additional nonconserved variables. The nonconserved variables, such as the stress, the excess normal stress, the heat flux and the diffusion flux, are determined by the evolution equations which are derived with the help of the Boltzmann equation [2,8]. So far, several fluid dynamic models have been developed, such as the Bahtnagar–Gross–Krook (BGK) method [9,10], Burnett-type equations [11] and the Grad's moment method [2]. BGK method models the molecular collision term of the Boltzmann equation through the evolution process from the initial nonequilibrium to the final equilibrium state over the relaxation time scale. Various computational investigations based on the BGK theories have been carried out [9,10]. Some computations based on the Burnett-type equations, however, have shown several difficulties, such as numerical instability, violation of the second law of thermodynamics and the treatment of boundary condition. While the Maxwell–Grad moment method satisfies the second law of thermodynamics in the near equilibrium condition, it is not assured whether it is also valid in the condition far from the equilibrium [2].

Because physical consistency is as much important as computational efficiency, it is desirable to derive a fluid dynamic model for rarefied gas flows under the constraint of the fundamental physical laws, such as the second law of thermodynamics.

The generalized hydrodynamic (GH) theory developed by Eu [2,8,12–14] is derived under the strict constraint of the second law of thermodynamics. With the help of modern CFD techniques, there have been some effort and progress to establish a GH computational model for a single species gas in two-dimensional setting [7,15]. However, the axisymmetric extension of the diatomic GH model and the development of the multi-species GH model are prerequisite for realistic rarefied flow simulations. In addition, the effects of chemical reaction and the heterogeneous collision between monatomic and diatomic molecules have to be included for an accurate numerical modeling. Thus, the setup of the GH constitutive relations including heterogeneous molecular composition of species is essential.

Keeping these in mind, the GH computational model for multi-species gas including monatomic and diatomic molecules is developed, and it is extended into an axisymmetric formulation in the present work. By combining the monatomic multi-species [2] and diatomic single species GH models [8,7,16], the multi-species GH constitutive relations are formulated. The multi-species GH model takes into account the mass diffusion owing to molecular collision and thermal interaction. The excess normal stress is considered to represent the rotational energy of diatomic molecules.

To assess the reliability of the model and the accuracy of computational approximation, the proposed multi-species GH computational method is applied to the hypersonic rarefied flows over an axisymmetric shuttle nose, a sphere and a reentry body as well as 1D shock structure. The computed results are critically compared with the N–S and DSMC data.

2. Generalized hydrodynamic theory

Fluid dynamic approaches to compute rarefied flows generally start from the Boltzmann equation [2,17]. The formulation of the nonequilibrium distribution function to treat the collision term of the Boltzmann equation provides the foundation of each fluid dynamic theory, such as the BGK method [9], the Burnett equations [11] and the Grad's moment method [2]. In formulating those nonequilibrium distribution functions, there is no explicit constraint on the second law of thermodynamics [2,15], which indicates that some of the methods may not guarantee the positive entropy production.

On the other hand, the GH theory is derived under the strict constraint of the second law of thermodynamics. The nonequilibrium distribution function in the GH theory is defined as the following exponential form [2,12]:

$$f = \exp\left[-\frac{1}{k_B T}\left(\frac{1}{2}mc^2 + H_{rot} + \sum_{\alpha \geqslant 1} X^{(\alpha)} \odot h^{(\alpha)} - \mu_0\right)\right]. \tag{1}$$

A detailed explanation for Eq. (1) will be given later. Following the above definition of the nonequilibrium distribution function, the entropy production can be expressed as

$$\sigma_{ent} = k_B \kappa \sinh \kappa, \tag{2}$$

where k_B is the Boltzmann constant, and κ is the first-order cumulant introduced in deriving the entropy production. The detailed derivation of the entropy production can be found in the Ref. [2].

From Eq. (2), it is clear the entropy production is positive-definite, because κ is proportional to the square root of squared nonconserved variables (κ will be explained in the later part of this paper). This means that the GH theory always satisfies the second law of thermodynamics.

The primary difference between the GH model and the N–S model lies in the level of realizing the nonequilibrium effects in rarefied flow. In rarefied flow, the frequency of molecular collision is substantially reduced, and molecules need a longer time to reach the equilibrium state. The Navier–Stokes equations, on the contrary, assume the 'locally thermal equilibrium', which indicates that the gas model would take a shorter time to reach the equilibrium state. Even for high Knudsen number, the Navier–Stokes equations produce too much stress and heat flux (or too much momentum and energy exchange between