Comparison of Continuum and Molecular Approaches for Rarefied Gas Flows

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Abstract

The present work aims at clarifying the domain of validity of two continuum approaches by comparing their results to a reference given by a Direct Simulation Monte Carlo method (DSMC). The first continuum approach is based on the usual Navier-Stokes (NS) equations. The second one is based on the Quasi-Gas-Dynamic (QGD) equations which are derived from Boltzmann equation with an additional diffusion term. The present paper includes a self-consistent presentation of QGD equations. The flow around a flat plate has been considered for a freestream Mach number varying from 1.5 to 20 and a wall temperature taken successively equal to freestream and stagnation temperatures. A criterion is proposed for the validity of the continuum approaches.

1 Introduction

The treatment of rarefied gas flows by means of equations based on the mechanics of continuum media is desirable because solving such equations requires less computational resources than methods based on a molecular description. The present work aims at clarifying the domain of validity of two continuum approaches by comparing their results to a reference given by a Direct Simulation Monte Carlo method (DSMC). The first continuum approach is based on the usual Navier-Stokes (NS) equations, the second one is based on the Quasi-Gas-Dynamic (QGD) equations. The latter ones can be considered as a new model for the description of viscous gas flows. The present report is also an opportunity to give self-consistent presentation of QGD equations.

2 Quasi Gas Dynamic model

QGD equations may be obtained based on Boltzmann equation (BE) with additional diffusion terms, extracted from the collisional integral [4]. Using cartesian coordinates and usual notations, QGD system writes as follows:

$$\rho_t + \nabla_i \rho u^i = \nabla_i \frac{\mu}{p}(\nabla_j \rho u^i u^j + \nabla^i p) \tag{2.1}$$

$$(\rho u^k)_t + \nabla_i \rho u^i u^k + \nabla^k p = \nabla_i \frac{\mu}{p} \nabla_j \rho u^i u^j u^k + \nabla_i \frac{\mu}{p} \nabla^i p u^k + \nabla_i \frac{\mu}{p} \nabla^k p u^i + \nabla^k \frac{\mu}{p} \nabla_i p u^i \tag{2.2}$$

$$E_t + \nabla_i (E+p) u^i = \nabla_i \frac{\mu}{p} \nabla_j (E+2p) u^i u^j + \nabla_i \frac{\mu}{p} \nabla^i \frac{p u^k u_k}{2} + \frac{\gamma}{\gamma - 1} \nabla_i \frac{\mu}{\rho} \nabla^i p + \nabla_i \kappa \nabla^i T \tag{2.3}$$

Note that $\mu/p = \tau$ is the time that characterizes the flow from a molecular point of view and may be interpreted as the local mean collisional time multiplied by a constant of the order of unity, that depends only on the intermolecular potential. Note also that using popular non-dimensional form and introducing Mach number $M = u/a$ and Reynolds number $Re = \rho u L/\mu$ makes the coefficient M/Re appear before all the right-hand terms in Eq. 2.1 - 2.3, as in NS system.

Considering the perfect gas equations

$$E = \rho(\vec{u}^2/2 + \varepsilon), \ \varepsilon = p/\rho(\gamma - 1), \ p = \rho R T$$

and adding finally the initial and boundary conditions, we obtain a closed system of equations which describes the space-time evolution of the macroscopic parameters of the gas: $\vec{u}$ - velocity, ρ - density, p - pressure, E - total energy, T - temperature, ε - internal energy.

The first variant of QGD equations can be found in [6], [7]. A further QGD development is presented in [9], [10] and [11].

Finite-difference schemes for QGD equations are closely related with Kinetical-Consistent Finite Difference (KCFD) schemes constructed by authors [6], [7], [8] earlier and based directly on a model BE or on a finite-difference approximation of BE. The possibility of applying KCFD schemes obtained in the latter way for computing slightly rarefied gases is considered in [12].

QGD equations differ from NS equations by the structure of the dissipative terms. They were proved to reduce to NS equations in the limiting

case of small Knudsen numbers [9]. The continuity equation 2.1 includes convective and molecular mass transfer and it features additional space derivatives of higher order than the corresponding NS equation. This is the reason why QGD system requires an additional boundary condition (BC) compared with NS. That additional BC was applied to the pressure gradient normal to the wall in the form

$$\partial p/\partial n = 0. \tag{2.4}$$

This relation provides that QGD expressions for mass flow, total energy flux and viscous friction forces on the solid wall are the same as NS ones. So the wall coefficients for heat transfer C_h and skin-friction C_f in both models are defined in the same way. As for NS equations, others BC for velocity vector and temperature can be written, either as $u^i = 0$, $T = T_w$ (no slip) or according (e.g.) to [1] or [3] (velocity slip and temperature jump).

3 Computational work

The comparison of the three above-mentioned models requires an identical physical modelling of the gas for all three calculations. This was obtained by considering a monoatomic hard-sphere gas ($\gamma = 5/3$), whose transport properties were represented in the continuum approaches by a $\mu \propto T^{1/2}$ viscosity law and a constant Prandtl number ($Pr = 2/3$). Temperature T identified with the translational temperature in DSMC.

The configuration retained was a semi-infinite sharp flat plate parallel to the direction of the freestream. Five values of the Mach number were considered ($M = 1.5, 2, 5, 10, 20$). The only length scale of the problem was the mean free path λ. For a given Mach number, the rarefaction level, expressed in terms of any of the usual parameters (Kn, Re_∞, Re_w, $\bar{V}$, χ) could thus be varied by considering different values of the abscissa x, ranging from 0 to approximately $100\,\lambda$. The wall temperature was set equal successively to the freestream temperature ($T_w = T_\infty$) and to the stagnation temperature ($T_w = T_0$). Gas-surface interaction was characterized by diffuse reflection with full accommodation at wall temperature.

NS code uses a finite-volume upwind implicit method with flux vector-splitting of Steger and Warming [5]. QGD code uses second order finite-volume space approximation in explicit form. This numerical method is probably not the most efficient one, but the objective was to examine the validity domain of QGD equations rather than optimizing their numerical solution. Both NS and QGD calculations assumed the gas to be perfect and accounted for velocity slip and temperature jump at the wall [1], [3]. DSMC calculations were carried out using a code developed at the Laboratoire d'Aérothermique du CNRS based on the ideas of Bird [2] and briefly described in [5].

The results are presented in dimensionless form based on freestream values. Lengths are reduced by the freestream mean free path. Due to space limitations, results are presented only for $M = 2$ and $M = 10$. Other results confirm the present conclusions.

The wall pressure distribution for $T_w = T_\infty$ and $T_w = T_0$ has been plotted in Figs.1–2. These figures exhibit two curves obtained from DSMC calculations, namely the thermodynamic pressure of the gas along the wall, as resulted from the equation of state $p = nkT$, and the normal stress F_n due to the exchange of normal momentum between the gas and the wall. In the continuum approaches these two concepts coincide whereas they differ strongly in DSMC results. The distribution of skin-friction coefficient has been plotted in Figs.3–4. Density profiles obtained at reduced abscissas equal to 10, 40 and 80 are presented in Figs.5–6.

4 Discussion and Conclusions

Numerical results show that for small Knudsen numbers (i.e. large abscissas) NS and QGD models give the same results. This is consistent with the fact that NS equations are the asymptotic limit of QGD equations for $Kn \to 0$ [9]. This is also the confirmation of the validity of BC used in the present QGD calculations.

For small Mach numbers both continuum models come rapidly to close agreement with DSMC. However the region near the trailing edge is affected by the differences in formulating the downstream boundary conditions. As M increases, discrepancies appear near the leading edge of the plate. Both these discrepancies and the extent of the region where they appear increase with increasing M. QGD results are generally closer to DSMC than NS ones. This is due to additional dissipation in QGD model. The ratio of additional terms in QGD to the NS one in the right-hand side of Eq.2.2 is proportional to M^2. So the difference between QGD and NS increases with M. Thus QGD equations can be considered as an improvement, compared with the usual NS equations in the domain of large M in slip-flow regimes.

However both continuum models depart from DSMC at abscissas x that correspond to values of $M/\sqrt{Re_x}$ ranging from ≈ 0.5 ($T_w = T_\infty$) to ≈ 1 ($T_w = T_0$). This parameter that can be interpreted as a Knudsen number based on the boundary layer thickness $Kn_\delta = \lambda_\infty/\delta$ appears to be a basis for an approximate validity criterion for continuum approaches. A more complete presentation of the present work (including details on equations and additional numerical results) can be found in [13].

It results from the present work that

- QGD equations can be considered as a model for the description of viscous gas flows. Under some conditions QGD equations bring significant improvement compared with NS ones. Otherwise QGD and NS results tend to collapse.

- For small values of M, continuum models are valid except in the immediate vicinity of the leading edge. More generally a criterion can be proposed for the validity of the continuum approach.

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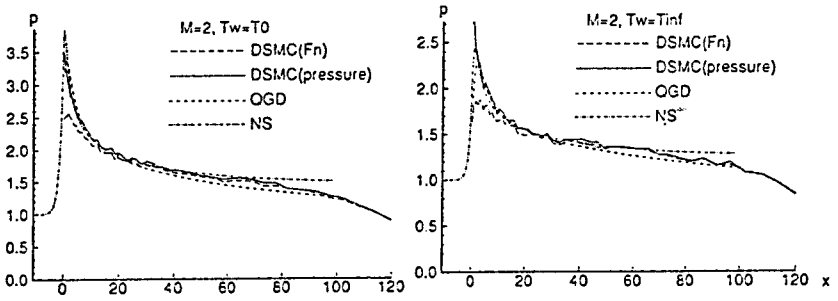

Figure 1. Pressure distributions, $M = 2$

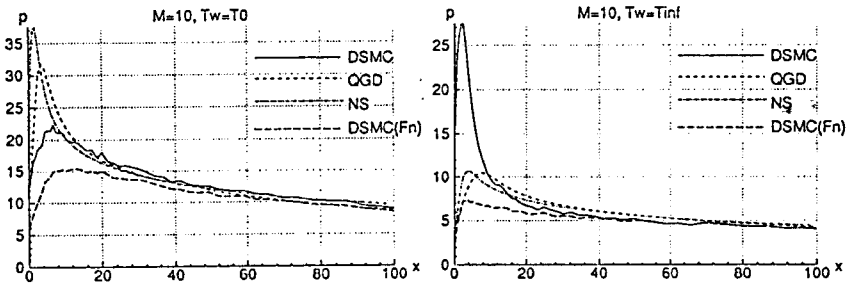

Figure 2. Pressure distributions, $M = 10$

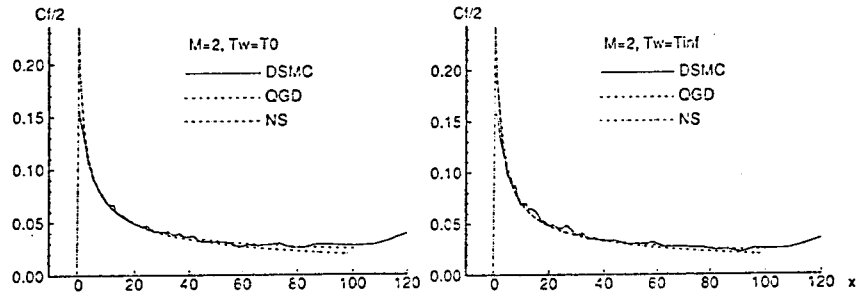

Figure 3. Distribution of skin-friction coefficient, $M = 2$

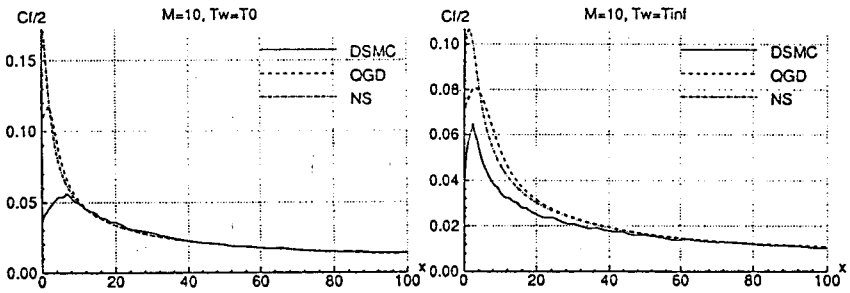

Figure 4. Distribution of skin-friction coefficient, $M = 10$

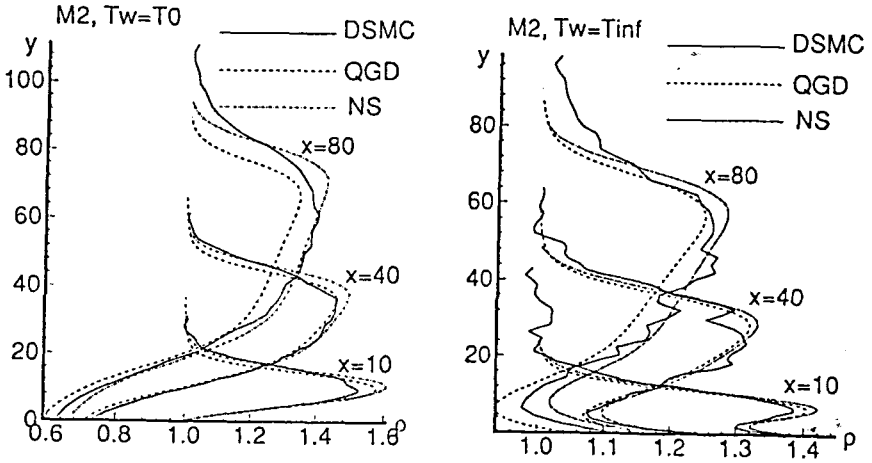

Figure 5. Density profiles, $M = 2$

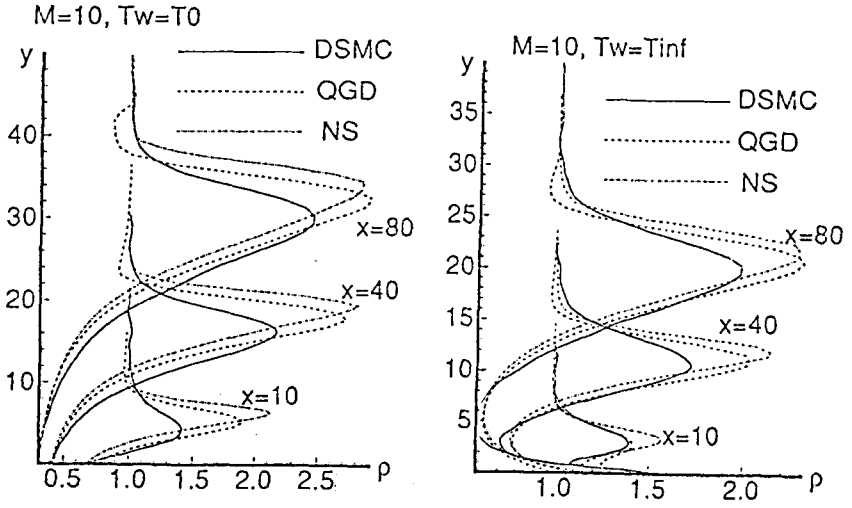

Figure 6. Density profiles, $M = 10$

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