Proceedings of the ASME 2010 3rd Joint US-European Fluids Engineering Summer Meeting and 8th International Conference on Nanochannels, Microchannels, and Minichannels
FEDSM-ICNMM2010
August 1-5, 2010, Montreal, Canada

FEDSM-ICNMM2010-30178

SIMULATION OF GASEOUS MICROSCALE TRANSPORT PHENOMENA VIA KINETIC THEORY

Sarantis Pantazis and Dimitris Valougeorgis
Department of Mechanical Engineering, University of Thessaly
Pedion Areos, 38334, Volos, Greece, spantazis@mie.uth.gr, diva@mie.uth.gr

ABSTRACT

Kinetic theory of gases, as described by the Boltzmann or model kinetic equations, provides a solid theoretical approach for solving microscale transport phenomena in gases. Due to significant advancement in computational kinetic theory and due to the availability of high speed parallel computers, kinetic equations may be solved numerically with modest computational effort. In this framework, recently developed upgraded discrete velocity algorithms for solving linear and nonlinear kinetic equations are presented. In addition, their applicability in simulating efficiently and accurately multidimensional micro flow and heat transfer problems is demonstrated. Analysis and results are valid in the whole range of the Knudsen number.

INTRODUCTION

Gaseous microflows is a significant chapter in the emerging field of microfluidics [1, 2]. In general, these flows do not have local equilibrium and they are described by different length and time scales associated with different laws of physics. As it is demonstrated in the present work mesoscale approaches based on kinetic theory [3, 4] are capable of handling such problems in a unified manner. The parameter, which quantifies the departure of the gas from local or global equilibrium flow conditions, is the Knudsen number, which is defined as the ratio of the mean free path λ (i.e. the distance that particles travel between collisions) over a characteristic macroscopic length L of the problem ($Kn = \lambda / L$) [1].

When the Knudsen number is much less than one, the mean free path is so small that the gas may be considered as a continuum medium and the well-known Navier-Stokes equations can be applied to model the flow. This flow regime is known as the *hydrodynamic* regime and the solution of the governing equations can be obtained very efficiently implementing advanced numerical approaches.

Although the validity of the Navier-Stokes equations breaks down for $Kn > 10^{-3}$, it is possible to extend their applicability by substituting the no slip with suitable slip boundary conditions [1]. It has been found that in the so-called slip regime, defined by $10^{-3} \le Kn \le 0.1$, the Navier-Stokes equations subject to the velocity slip and temperature jump boundary conditions may provide reliable results. Also, by introducing more advanced high-order slip boundary conditions the validity of the continuum equations may be extended to a wider range of the Knudsen number. However, it is important to note that the implementation of advanced reliable slip boundary conditions depends on the accurate estimation of the slip coefficients, which are obtained only through kinetic theory. Other attempts to facilitate and extend the implementation of macroscopic conservation equations are based on the application of more complicated constitutive laws yielding a set of generalized hydrodynamic equations [1, 5]. It is obvious however, that all this effort is limited by the hydrodynamic assumption and can not be valid in the whole range of the Knudsen number. However, it is fully justified by the fact that there is a lot of knowledge and experience on the numerical solution of nonlinear hydrodynamic equations and whenever applicable the gain in computational effort is significant.

At the other end, when the Knudsen number is much greater than one, and more specifically for $Kn \ge 10$, the mean free path is so large that collisions between molecules and boundaries occur more often than collisions between molecules. This flow regime is known as the *free molecular* regime and in this case it may be considered that each particle travels independently of each other, ignoring the intermolecular collisions. Due to this simplification it is possible following the particle paths and based on the method of characteristics to yield closed form solutions for simple flow configurations. In more complex geometry the Test Particle Monte Carlo (TPMC) method is applied with great success [6].

Finally, when the Knudsen number has intermediate values ($0.1 < Kn < 10$) the gas may not be considered as a continuum medium, neither as a medium consisting of individual particles.

This flow regime is known as the transition regime and it may be modeled by kinetic theory as it is described by the Boltzmann equation or alternatively by simplified kinetic model equations, where the primary unknown is the particle distribution function [3, 4, 7]. Then, the macroscopic quantities of practical interest are easily obtained by taking moments of the distribution function. This is a mesoscale approach since it is characterized by phase space volumes and times, which are small compared to the spatial and time scales on which macroscopic quantities vary but large enough to contain a sufficient number of molecules to allow a statistical description. A kinetic description is self-contained providing that the laws of intermolecular interaction are specified. Traditionally, the computational solution of the kinetic equations is much more demanding and complicated than the solution of the hydrodynamic equations. It is important to note that in the transition and free molecular regimes new transport phenomena, known as cross effects, arise and then they diminish gradually in the slip and hydrodynamic regimes. In gaseous micro devices the Knudsen number may rise due to small length scales or due to low pressures, while all flow regimes may occur in the same micro system.

A typical way to circumvent, when needed, the numerical solution of the kinetic equations, is the implementation of the Direct Simulation Monte Carlo method [6]. The DSMC method is a statistical computational approach where the region of the gas flow is divided into a large number of cells having dimensions such that the change in flow properties across each cell is small. Then, the evolution in space and time of a large number of randomly selected and statistically representative molecules in each cell is considered. The computational molecules, each of which represents a huge number of real molecules move, interact with solid boundaries and collide to each other following basic kinetic principals, so as to statistically mimic the behavior of real molecules. The DSMC method due to its simplicity has attracted considerable attention and although, in general, it requires large computer memory and long CPU time, is by far the most widely used approach when the flow is in the whole range of the Knudsen number. However, in low speed microflows as well as in high frequency unsteady microflows, both of which are quite common in microfluidics, despite the significant improvements and upgrades which have been achieved [8], the DSMC method requires considerably increased computation effort due to statistical noise. Therefore, it is always reasonable to search for reliable alternatives capable of solving any microflow configuration in an accurate and computationally efficient manner.

Such an alternative methodology may be the fully deterministic solution of suitable kinetic model equations [9]. This approach is well developed and advanced in the field of rarefied gas dynamics and can be applied in a straight forward manned in microflows due to the fact that a gas microflow may be considered as a rarefied gas flow. Of course, fully deterministic numerical solutions of kinetic equations, consisting of the discretization of the distribution function in the physical and molecular velocity spaces, are complicated. However nowadays, due to the availability of high speed parallel computers and due to the significant advancement in computational kinetic theory made during the last years, kinetic equations may be solved numerically in an efficient manner. In the case of multi dimensional configurations deterministic numerical schemes include variational, integro-moment and discrete velocity methods [10].

Over the years the discrete velocity method (DVM) [11, 12, 13, 14] and its recently introduced accelerated version [15, 16] have shown to be very efficient numerical algorithms providing accurate results with modest computational effort. They have been applied in a series of linear problems including pressure, temperature and concentration driven fully developed flows of single gases and gaseous mixtures through long channels of various cross sections. Most of this work is based on the BGK [17], Shakhov [10] and McCormack [18, 19] kinetic models, although the numerical solution of the Boltzmann equation in several occasions has been achieved [20, 21, 22]. It may be stated that in the case of low Mach number microflows the implementation of linearized kinetic theory is the most computationally efficient approach. Fully deterministic algorithms based on the discrete velocity method have been also applied in the case of nonlinear configurations including the cylindrical Couette flow [23, 24], flow in a cavity due to discontinuous wall temperature [25] and half space evaporation and condensation [26]. Very recently a methodology has been proposed to upgrade the computational efficiency of the nonlinear DVM solvers [27] in order to be more competitive with respect to the DSMC method even at high speed flows.

Within this framework, in this paper, recently developed upgraded discrete velocity algorithms for solving linear and nonlinear kinetic equations are presented. In addition, their applicability in simulating efficiently and accurately micro transport phenomena is demonstrated by reviewing recent results of rarefied gas flows through channels and heat transfer through rarefied gases confined between cylinders. Analysis and results are valid in the whole range of the Knudsen number. In Section 2 the fundamental kinetic equations with the associated boundary conditions are provided. In Section 3 the basic and the accelerated discrete velocity algorithms are described. Results for the specific problems under consideration with the relative discussion are given in Section 4, followed by brief concluding remarks in Section 5.

GOVERNING EQUATIONS

At the kinetic (or mesoscale) level the state of a monoatomic gas is described by the distribution function $f(t,\boldsymbol{r},\boldsymbol{\xi})$, defined such that $f(t,\boldsymbol{r},\boldsymbol{\xi})d\boldsymbol{r}d\boldsymbol{\xi}$ is the number of molecules which, at time t, have positions lying within the volume $d\boldsymbol{r}$ about $\boldsymbol{r}$ and velocities lying within a velocity-element $d\boldsymbol{\xi}$ about $\boldsymbol{\xi}$. The evolution of the distribution function

obeys the Boltzmann transport equation (BE) [3]

$$\left(\frac{\partial}{\partial t}+\boldsymbol{\xi}\cdot\frac{\partial}{\partial \boldsymbol{r}}+\frac{\boldsymbol{F}}{m}\cdot\frac{\partial}{\partial \boldsymbol{\xi}}\right)f=Q(ff) \tag{1}$$

where the left-hand side represents the streaming motion of the molecules of mass m, along the trajectories associated with the force field $\boldsymbol{F}$ and $Q(ff)$ represents the effect of intermolecular (two-body) collisions taking molecules in and out from the streaming trajectory. Each of the macroscopic quantities is deduced by taking the corresponding moment of the distribution function, while the equation of state is valid for any non-equilibrium state of the gas.

The solution of the BE is a very complicated task and in most occasions simplified collision models are implemented instead. In general, a kinetic collision model must satisfy all three collision invariants, obey the H-theorem and when it is solved by the Chapman-Enskog procedure it should deduce the same expressions for the transport coefficients with the ones obtained by the BE. The most simple and widely used model, providing reliable results in isothermal flows, is the BGK model, where the collision term is written as

$$Q_{BGK}(f)=\nu\left[f^{M}(n,T,\boldsymbol{u})-f(n,T,\boldsymbol{u})\right]. \tag{2}$$

Here, the collision frequency ν is assumed as independent of the molecular velocity,

$$f^{M}(n,T,\boldsymbol{u})=n(t,\boldsymbol{r})\left(\frac{m}{2\pi kT(t,\boldsymbol{r})}\right)^{3/2}\exp\left[-\frac{m\left(\boldsymbol{\xi}-\boldsymbol{u}(t,\boldsymbol{r})\right)^{2}}{2kT(t,\boldsymbol{r})}\right] \tag{3}$$

is the local equilibrium Maxwellian function, while n, $\boldsymbol{u}$ and T denote the local number density, velocity and temperature respectively. A shortcoming of this model is that it does not produce the right expressions for both viscocity and heat conductivity coefficients simultaneously and as a result the right Prandtl number.

The simplest advance on the BGK model is the ellipsoidal statistical (ES) model introduced by Holway [28, 3] where

$$Q_{ES}(f)=\nu\left(f^{ES}-f\right) \tag{4}$$

while

$$f^{ES}=\frac{n}{\pi^{3/2}}\sqrt{|\det A|}\exp\left[-\sum_{i,j=1}^{3}\alpha_{ij}\left(\xi_i-u_i\right)\left(\xi_j-u_j\right)\right] \tag{5}$$

is a local anisotropic 3D Gaussian. The elements α_{ij} of matrix A are obtained by requiring the model to yield the correct Prandtl number and conservation properties. This model provides simultaneously the correct expressions for both viscocity and conductivity, while by setting $\Pr=1$ it yields the BGK model. It has been found recently that the ES model fulfills the H-theorem [29]. Another model, which is recommended for non-isothermal problems, is the Shakhov (S) model, where its collision term is given by [10]

$$Q_S(f)=\frac{P}{\mu}\left\{f^{M}\left[1+\frac{2m}{15n(kT)^{2}}\hat{\boldsymbol{q}}\cdot(\boldsymbol{\xi}-\boldsymbol{u})\left(\frac{m(\boldsymbol{\xi}-\boldsymbol{u})^{2}}{2kT}-\frac{5}{2}\right)\right]-f\right\}. \tag{6}$$

This model yields the correct Prandtl number for monoatomic gases but one cannot prove or disapprove the H-theorem.

In a number of interesting situations, particularly those involving low-speed flows, the distribution function may still be nearly Maxwellian and linearization of the BE or of the model equations may be appropriate. However, the deviation of the Maxwellian is not of the Chapman-Enskog type. Introducing the perturbed distribution according to

$$f=f_0(1+h),\ \|h\|<1 \tag{7}$$

where

$$f_0=n_0\left(\frac{m}{2\pi kT_0}\right)^{3/2}\exp\left[-\frac{m\left(\boldsymbol{\xi}-\tilde{\boldsymbol{u}}_0\right)^{2}}{2kT_0}\right]. \tag{8}$$

is the absolute Maxwellian the linearized version of the BGK and S models are

$$L_{BGK}(h)=\nu_0\left\{\rho+\frac{m}{kT_0}\boldsymbol{\xi}\cdot\boldsymbol{u}+\tau\left(\frac{m\xi^{2}}{2kT}-\frac{3}{2}\right)-h(t,\boldsymbol{r},\boldsymbol{\xi})\right\} \tag{9}$$

and

$$\begin{aligned}L_S(h)=\frac{P_0}{\mu_0}\Bigg\{&\rho+\frac{m}{kT_0}\boldsymbol{\xi}\cdot\boldsymbol{u}+\tau\left(\frac{m\xi^{2}}{2kT}-\frac{3}{2}\right)\\&+\frac{2}{15}\frac{m}{n_0(kT_0)^{2}}\boldsymbol{q}\cdot(\boldsymbol{\xi}-\boldsymbol{u})\left(\frac{m\xi^{2}}{2kT_0}-\frac{5}{2}\right)-h(t,\boldsymbol{r},\boldsymbol{\xi})\Bigg\}\end{aligned} \tag{10}$$

where ρ, τ and $\boldsymbol{q}$ are the perturbed macroscopic quantities of number density, temperature and heat flow vector.

In the case of gaseous mixtures with N components one has to consider N distribution functions $f_i(t,\boldsymbol{r},\boldsymbol{\xi})$, $1\le i\le N$, satisfying the system of N Boltzmann transport equations [3]

$$\left(\frac{\partial}{\partial t}+\boldsymbol{\xi}\cdot\frac{\partial}{\partial \boldsymbol{r}}+\frac{\boldsymbol{F}}{m_i}\cdot\frac{\partial}{\partial \boldsymbol{\xi}}\right)f_i=\sum_{j=1}^{N}Q_{ij}\left(f_i f_j\right),\ 1\le i\le N, \tag{11}$$

where $Q_{ij}\left(f_i f_j\right)$ is the collision term describing the interaction between particles i and j. Several simplifications may be introduced at the two limits of the Knudsen number. In the hydrodynamic regime the gaseous mixture may be considered as a gas with particles of one species with density $n=\sum_{i=1}^{N}n_i$ and molecular mass $m=\sum_{i=1}^{N}n_i m_i/n$ and tackle the problem using the monoatomic transport theory. In the free molecular regime it may be considered that the various species of the mixture do not interact to each other and apply again the monoatomic transport theory for each component of the mixture and then estimate the overall macroscopic quantities as a summation of the corresponding quantities of each component. However, in the transition regime these simplifications are not valid and the coupled system of the Boltzmann equations must be solved. To simplify things several kinetic models have been proposed [3]. A linearized kinetic model for binary mixtures, which is fulfils all requirements, is the McCormack model [17, 18]. Following a detailed comparison with results obtained by the solution of the

Boltzmann equation, it has been shown that the McCormack model may provide very reliable results with significantly reduced computational effort. In addition, realistic intermolecular potentials can be implemented in the simulation, while the solutions of the BE are based, so far, only on the hard sphere model.

Turning now to the boundary conditions, it is needed to relate the distribution of the incident particles $\left(f^{-}\right)$ with the distribution of the particles $\left(f^{+}\right)$ leaving the boundary surface. A model, which is widely used, is the Mawell specular-diffuse boundary condition given by [3]

$$f^{+} = \alpha f_W^M + \left(1-\alpha\right) f^{-} \tag{13}$$

where f_W^M is the local Maxwellian distribution defined by the macroscopic properties of the wall (i.e. velocity and temperature) and $\alpha \in \left[0,1\right]$ is the well known tangential momentum accommodation coefficient indicating the portion of the particles which are emitted diffusively from the wall. The Maxwellian gas-surface interaction model contains only one free accommodation parameter without clear physical meaning. For example, momentum and energy accommodation are different and this can not be fulfilled with the Maxwell boundary model. In addition, this model contradicts some experimental results on the thermo-molecular pressure difference effect. Another popular boundary models is the one proposed by Cercignani and Lampis (CL), which provides a more physical description of the gas-surface interaction [30]. This model contains two parameters $a_t \in \left[0,2\right]$ and $a_n \in \left[0,1\right]$, which are known as the tangential momentum and energy accommodation coefficients. The combination $a_t = a_n = 0$ corresponds to purely specular reflection, while the combination $a_t = a_n = 1$ corresponds to purely diffuse reflection. Therefore, it is possible to distinguish the momentum and energy accommodation and also to consider back scattering, which may exist at rough surfaces.

Obtaining a kinetic solution of a microflow problem it would require the numerical solution of a kinetic model equation (BGK, S, ES) or of the BE, accordingly adjusted to the flow under consideration, subject to corresponding Maxwell or CL boundary conditions. Such algorithms based on the DVM are presented in the next section.

UPGRADED DISCRETE VELOCITY ALGORITHMS

Typical discrete velocity algorithms are based on a simple iteration scheme between the distribution function defined by the kinetic equation and the macroscopic quantities obtained as moments of the distribution function. However, it is well known to researchers involved in discrete velocity computations that while the convergence of the iteration scheme works well in the free molecular regime, it degrades as into the transition regime and becomes unacceptably slow in the slip and continuum regimes. Due to this computational pitfall in many occasions the applicability of the kinetic methodology has been limited up to certain gas rarefaction. This is a serious drawback since the main advantage of mesoscale kinetic approaches is their ability to deduce results valid in the whole range of the gas rarefaction.

Here two methodologies, one for linear and one for nonlinear kinetic equations, are presented to speed up the slow convergence of the iterative scheme related to discrete velocity algorithms. For clarity purposes these methodologies are demonstrated by their implementation in the solution of two specific well known problems. In particular, linear (fully developed) flow of a gas through a rectangular microchannel and nonlinear heat transfer through a stationary gas confined between two microcylinders are considered.

Linear accelerated discrete velocity algorithm

The pressure driven fully developed flow of a gas through a rectangular microchannel may be described by the dimensionless linearized BGK model equation [11]

$$\zeta\left[\cos\theta\frac{\partial\Phi^{(t+1/2)}}{\partial x}+\sin\theta\frac{\partial\Phi^{(t+1/2)}}{\partial y}\right]+\delta\Phi^{(t+1/2)} = \delta F_{00}{}^{(t)} - \frac{1}{2}, \tag{14}$$

where $\Phi = \Phi\left(x,y,\zeta,\theta\right)$ is the unknown reduced distribution function, with x,y denoting the spatial variables and ζ,θ the magnitude and the polar angle of the molecular velocity vector, $\delta \in \left[0,\infty\right)$ is the rarefaction parameter (proportional to the inverse of the Knudsen number) and $F_{00}\left(x,y\right)$ is the macroscopic velocity defined by the zeroth moment of Φ according to

$$F_{00}{}^{(t+1)} = \frac{1}{\pi}\int_0^{2\pi}\int_0^{\infty}\Phi^{(t+1/2)}\exp\left[-\zeta^2\right]\zeta\, d\zeta\, d\theta\,. \tag{15}$$

The integro-differential system defined by Eqs. (14) and (15), is solved in an iterative manner as indicated by the iteration index t. In particular, at the beginning of each iteration, one introduces an old estimate $F_{00}{}^{(t)}$ in the right hand side of Eq. (14). Using this estimate Eq. (14) is solved to obtain an estimate for $\Phi^{(t+1/2)}$, which is introduced into Eq. (15) to obtain the new estimate $F_{00}{}^{(t+1)}$. This iteration process, which is named "*kinetic iteration*" is repeated until the difference between successive estimates of $F_{00}{}^{(t)}$ is less than a pre-assigned convergence criterion. It has been shown that the above described iteration process converges fast for small values of δ and unacceptably slow for large values of δ [15, 16, 31]. This situation is remedied by the fast iteration scheme introduced in the following acceleration scheme.

The rapidly convergent iteration scheme involves, in each iteration, an additional step. In particular, following the calculated value of $\Phi^{(t+1/2)}$ from Eq. (14), the updated velocity $F_{00}{}^{(t+1)}$ instead of applying Eq. (15), is obtained by solving the diffusion equation

$$\frac{\partial^2 F_{00}^{(t+1)}}{\partial x^2}+\frac{\partial^2 F_{00}^{(t+1)}}{\partial y^2}=-\frac{1}{2}\frac{\partial^2 F_{20}^{(t+1/2)}}{\partial x^2}-\frac{\partial^2 F_{11}^{(t+1/2)}}{\partial x\partial y}-\frac{1}{2}\frac{\partial^2 F_{02}^{(t+1/2)}}{\partial y^2} \quad (16)$$

where at the right hand side of Eq. (16) the higher-order moments F_{20}, F_{11} and F_{02} are defined by

$$F_{mn}^{(t+1/2)}(x,y)=\frac{1}{\pi}\int_0^{2\pi}\int_0^{\infty}H_m(\zeta\cos\theta)H_n(\zeta\sin\theta) \times\Phi^{(t+1/2)}(x,y,\zeta,\theta)exp(-\zeta^2)\zeta d\zeta d\theta \quad (17)$$

Equation (16) has been derived by taking the zeroth- and first-order moments of Eq. (1) and manipulating accordingly the resulting moment equations. In Eq. (17), H_m and H_n are Hermite polynomials of m-th and n-th order respectively [15].

The iteration process, which now consists of two stages, is defined as follows. In the first stage of the iteration, since $F_{00}^{(t)}$ is known from the previous iteration, Eq. (14) is solved to yield $\Phi^{(t+1/2)}$ and then the higher-order moments are calculated from Eq. (17). In the second stage of an iteration, Eq. (16) is solved for the updated velocity $F_{00}^{(t+1)}$. The iteration process, which is named "*synthetic iteration*", is terminated when the pre-assigned convergence criterion is fulfilled. It is obvious that a synthetic compared to a kinetic iteration is more costly. However, it has been shown, that the number of required iterations in the synthetic scheme is significantly reduced and therefore, the overall efficiency of the scheme is increased.

The spectral radius of the typical and accelerated iteration schemes has been estimated theoretically by applying a Fourier mode stability analysis and they have been equal to one and 0.32 respectively [15]. These theoretical findings have been also confirmed by numerical investigation where by applying the upgraded scheme the number of iterations is significantly reduced. Detailed results are presented in the Section 4.

Nonlinear accelerated discrete velocity algorithm

The problem of heat transfer through a rarefied gas, confined between coaxial cylindrical surfaces at different temperatures may be described by the dimensionless coupled nonlinear Shakhov kinetic equations

$$\zeta\cos\theta\frac{\partial\phi^{(t+1/2)}}{\partial r}-\frac{\zeta\sin\theta}{r}\frac{\partial\phi^{(t+1/2)}}{\partial\theta}+\delta\rho\sqrt{\tau}\phi^{(t+1/2)}=\delta\rho\sqrt{\tau}\phi_S^{(t)} \quad (18)$$

$$\zeta\cos\theta\frac{\partial\psi^{(t+1/2)}}{\partial r}-\frac{\zeta\sin\theta}{r}\frac{\partial\psi^{(t+1/2)}}{\partial\theta}+\delta\rho\sqrt{\tau}\psi^{(t+1/2)}=\delta\rho\sqrt{\tau}\psi_S^{(t)} \quad (19)$$

where $\phi=\phi(r,\zeta,\theta)$ and $\psi=\psi(r,\zeta,\theta)$ are the unknown reduced distribution functions, r is the spatial variable, ζ,θ and δ the same quantities as previously defined, while

$$\rho^{(t+1)}=\int_0^{2\pi}\int_0^{\infty}\phi^{(t+1/2)}\zeta d\zeta d\theta \quad (20)$$

and

$$\tau^{(t+1)}=\frac{2}{3\rho(r)}\int_0^{2\pi}\int_0^{\infty}\left(\zeta^2\phi^{(t+1/2)}+\psi^{(t+1/2)}\right)\zeta d\zeta d\theta \quad (21)$$

are the macroscopic distributions of number density and temperature respectively. Also, the functions

$$\phi_S=\phi^M\left[1+\frac{4}{15}\frac{1}{\rho\tau^2}q\zeta\cos\theta\left(\frac{\zeta^2}{\tau}-2\right)\right] \quad (22)$$

and

$$\psi_S=\psi^M\left[1+\frac{4}{15}\frac{1}{\rho\tau^2}q\zeta\cos\theta\left(\frac{\zeta^2}{\tau}-1\right)\right], \quad (23)$$

while

$$\phi^M=\frac{\rho}{\pi\tau}\exp\left(-\zeta^2/\tau\right) \text{ and } \psi^M=\frac{\rho}{2\pi}\exp\left(-\zeta^2/\tau\right) \quad (24)$$

are the local Maxwellians. Equations (18-24), along with the associated boundary conditions, constitute the basic set of equations to be solved in an iterative manner.

It is important to note that the synthetic algorithm implemented in Section 3.1 for linearized equations is not applicable in the case of nonlinear kinetic equations. Nonlinear accelerated algorithms are needed. Therefore, the typical iteration algorithm, which is identical as in the linear problem has been upgraded by implementing the Romberg integration rule and the Wynn-epsilon (Wε) acceleration algorithm [32, 33]. In particular, the Romberg rule provides very accurate estimates of integration in the macroscopic quantities, even when coarse angle and spatial grids are used, while the Wε algorithm speeds up the slow convergence of the typical iteration scheme. Both methodologies result to a significant reduction of CPU time.

The Romberg integration rule is carried out by the expression

$$T_k(m)=\left[4^k T_{k-1}(2m)-T_{k-1}(m)\right]/\left(4^k-1\right),\ k=1,2,3\ldots, \quad (25)$$

where $T_k(m)$ denotes the estimation of an integral with m intervals after k integration steps, while $T_0(m)$ is the original trapezoidal rule with m intervals. This treatment can be implemented in both the spatial and angular domains and the resulting accuracy is of $O\left(\Delta r^{2k+2},\Delta\theta^{2k+2}\right)$. The Romberg rule is applied at the macroscopic quantities (20-21), where the computation is performed initially on a coarse spatial and angular grid and, after convergence has been reached, it is repeated in a refined mesh, where the grid parameters have been doubled. This refinement is repeated $k-1$ times and the results are combined according to Eq. (25) at each spatial point until the final number of total discrete angles and space nodes is reached. It is also noted that in each grid refinement the results of the previous grid have been used as an initial condition to speed up convergence. This procedure has lead to an accurate solution with a moderately dense grid.

The Wε acceleration is a strongly nonlinear sequence accelerator that can exhibit spectacular acceleration for some sequences and has been described as the most elegant of all convergence acceleration methods [34]. The convergence of a

series S_j, $j=1,...,J$, can be accelerated by forming a tableau whose even columns are estimations of the sequence limit

$$\varepsilon_{l+1}^{(j)} = \varepsilon_{l-1}^{(j+1)} + \left[\varepsilon_l^{(j+1)} - \varepsilon_l^{(j)} \right]^{-1}, \tag{26}$$

with $\varepsilon_{-1}^{(j)} = 0$ and $\varepsilon_0^{(j)} = S_j$. This algorithm is imposed inside the typical iteration loop on the macroscopic quantities. Thus, a value of each sequence is stored in regular intervals between the iterations and a transitional stage is allowed before each application of the algorithm.

Comparing the computational efficiency of the typical and the upgraded algorithms it has been found that while keeping the same accuracy in the results, the CPU time of the latter ones is reduced by at least one order of magnitude. Furthermore, both Romberg and Wε schemes are easily applied in both linearized and non-linear kinetic problems. Finally, it is noted that for more demanding problems the upgraded algorithm can be further improved by extending and optimizing the implementation of the Romberg rule.

RESULTS AND DISCUSSION

Using linearized kinetic theory, fully developed flows through long channels of various cross sections have been investigated. Following the early results of flows through circular tubes [10], solutions have been obtained for flows through rectangular [11], triangular [14] ellipsoidal [35], annular [36] and trapezoidal [37] cross sections. Very good agreement with corresponding experimental results has been demonstrated [37, 38]. Some indicative results for the dimensionless flow rate in terms of the rarefaction parameter covering all flow regimes are shown in Fig. 1. In all cases the hydraulic diameter has been used as the characteristic length.

All these flow configurations have been solved using discrete velocity algorithms involving the typical *kinetic* iteration, while the cases of rectangular and triangular cross sections have been also solved using the upgraded *synthetic* iteration [15, 16]. To demonstrate the efficiency of the synthetic algorithm a comparison on the computational performance of two algorithms is provided for the case of flow through rectangular cross section. The problem has been solved based on the formulation described in Section 3.1. In Fig. 2 the required number of iterations to satisfy the convergence criterion in the computed results is plotted as a function of the convergence criterion for $\delta = 10$ (slip regime) and $\delta = 100$ (hydrodynamic regime). It is seen that in both cases the required number of iterations in the kinetic scheme is significantly larger than the corresponding one in the synthetic scheme. More specifically for a relative convergence criterion of about 10^{-4} the required iterations for the synthetic with regard to the kinetic scheme are reduced roughly by a factor of 10 for the case of $\delta = 10$ and by a factor of 10^3 for the case of $\delta = 100$. It is also noted that the required number of synthetic iterations for $\delta = 10$ (slip regime) and $\delta = 100$ remains actually constant even when very strict convergence criteria are applied, while the corresponding ones in the kinetic scheme are increased by at least one order of magnitude. In Fig. 3 the required CPU time to satisfy the convergence criterion in the computed results is plotted in terms of the convergence criterion for the most computationally demanding case of $\delta = 100$. It is seen that the reduction in the overall computational time is of the same order of magnitude with the reduction in the required number of iterations. This is easily explained by the fact that the additional computational effort per iteration is insignificant compared to the computational gain due to the small number of iterations required. In the same figure the corresponding results in the case of the S model are shown and they are very similar with those of the BGK model. This is an interesting fact indicating that the effectiveness of the acceleration algorithm is computationally independent of the complexity of the kinetic model. Overall, it is clearly seen that, by implementing the synthetic discrete velocity algorithm, this type of problems described by linearized kinetic equations may be numerically solved in a few minutes of CPU time.

Using the nonlinear formulation of Section 4.2, the heat transfer problem through a gas between two concentric cylinders with radii R_A and R_B ($R_A < R_B$) maintained at different temperatures T_A and T_B ($T_A > T_B$) may be solved. The three parameters governing this heat transfer problem are the temperature difference between the cylindrical walls $\beta = (T_A - T_B)/T_B$, the ratio of the two cylindrical radii $\gamma = R_A / R_B$ and the rarefaction parameter δ_0. Typical results for the behaviour of the radial heat flow $q(r=\gamma)$, in terms of δ_0 is shown in Fig. 4 for $\gamma = 0.1$, 0.2, 0.5 and $\beta = 0.1$, 10. The nonlinear kinetic solution covers the whole range of rarefaction, several ratios of cylindrical radii with practical interest and more important large temperature differences which are not covered by the corresponding linearized solution.

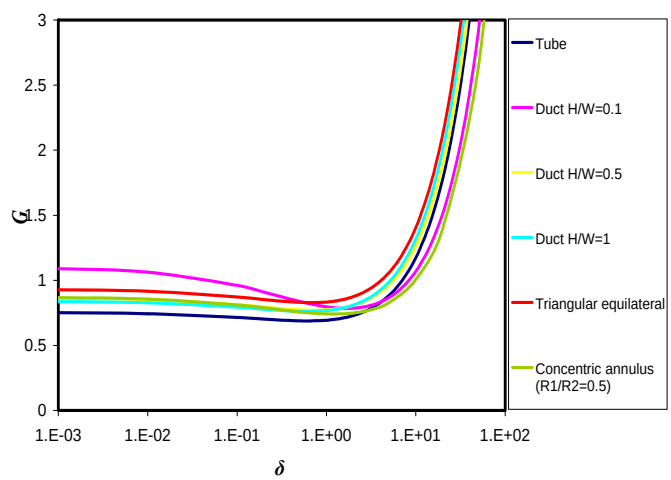

Figure 1: Dimensionless flow rates in long channels of various cross sections, based on the hydraulic diameter as the characteristic length.

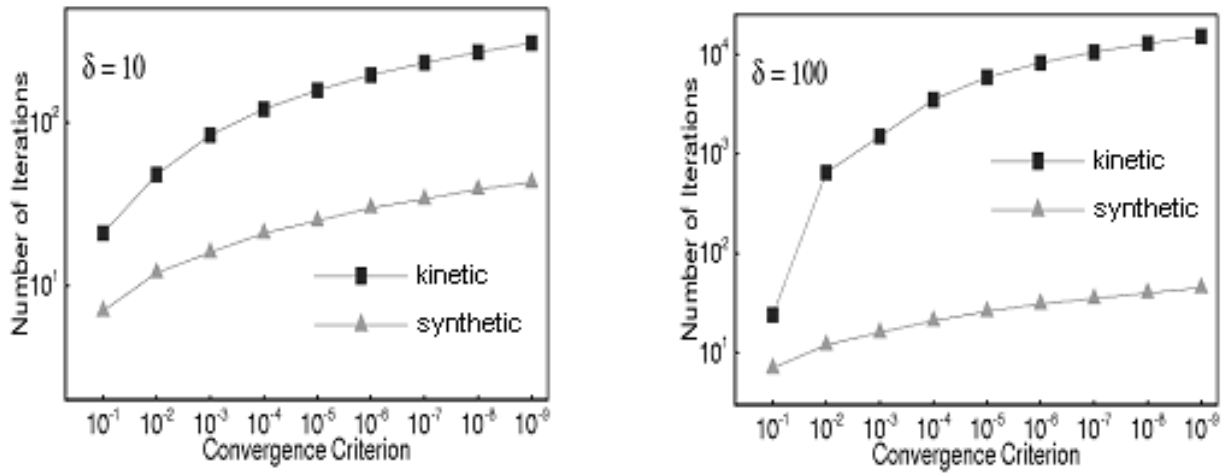

Figure 2: Comparison between the *kinetic* and *synthetic* schemes in terms of required number of iterations for solving the 2D flow through a rectangular channel.

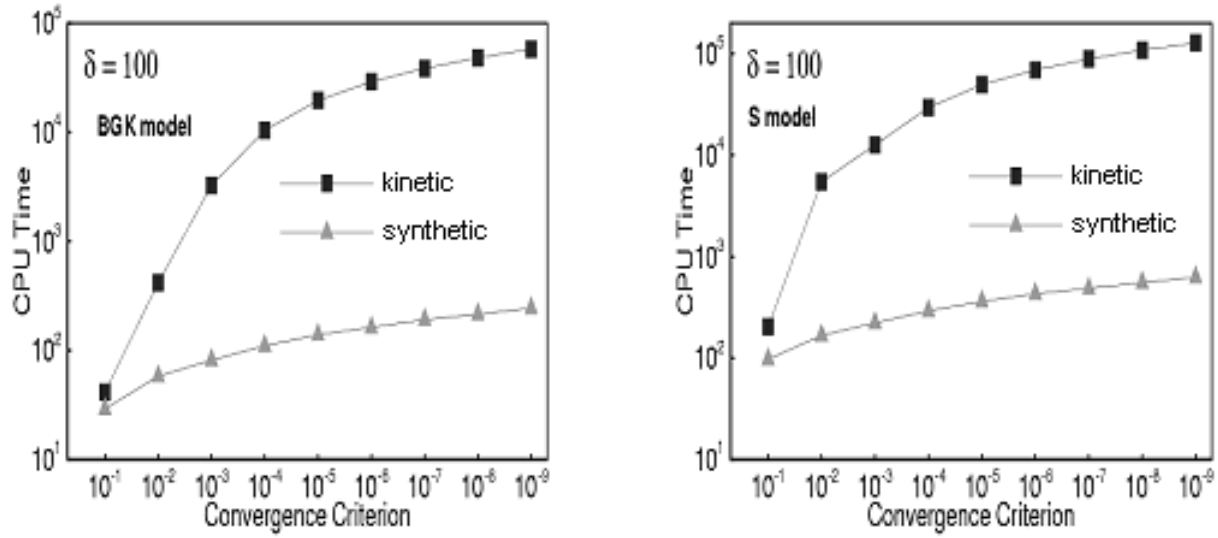

Figure 3: Comparison between the *kinetic* and *synthetic* schemes in terms of required CPU time for solving the 2D flow through a rectangular channel.

This nonlinear problem has been solved using discrete velocity algorithms based on the typical iteration scheme as well as on the upgraded one involving the Romberg integration rule and the Wynn-epsilon (Wε) acceleration algorithm. As seen in Fig. 5, the required CPU time is significantly reduced in comparison to the typical scheme for any convergence criterion and rarefaction parameter. It has been found that the implementation of the upgraded scheme is particularly beneficial for high values of the rarefaction parameter, reducing the computational time by at least an order of magnitude (values up to $\delta_0 = 650$ have been considered).

CONCLUDING REMARKS

A brief review on basic kinetic modeling and associated discrete velocity algorithms has been provided. By simulating a linear flow and a nonlinear heat transfer problem it has been demonstrated that kinetic modeling is a powerful approach in gas microflows and it is capable of providing reliable results in the whole range of the Knudsen number with modest computational effort. Overall, the development of advanced highly parallelized kinetic algorithms capable of handling non-equilibrium phenomena in complex geometry and boundaries is an interesting and demanding research field with a lot of potential.

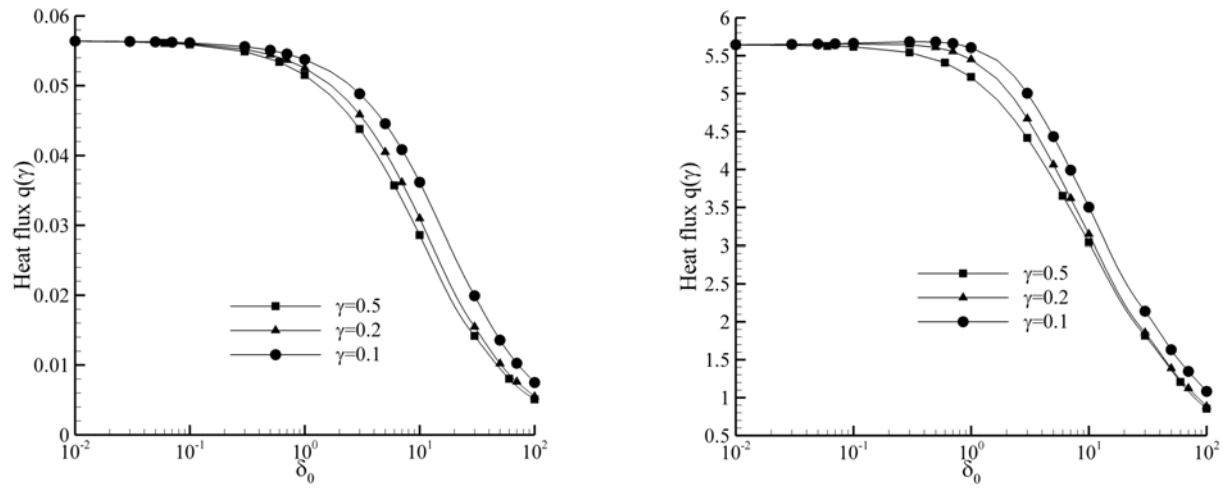

Figure 4: Dimensionless radial heat flow q at $r=\gamma$ in terms of δ for various γ, with $\beta=0.1$ (left) and $\beta=10$ (right).

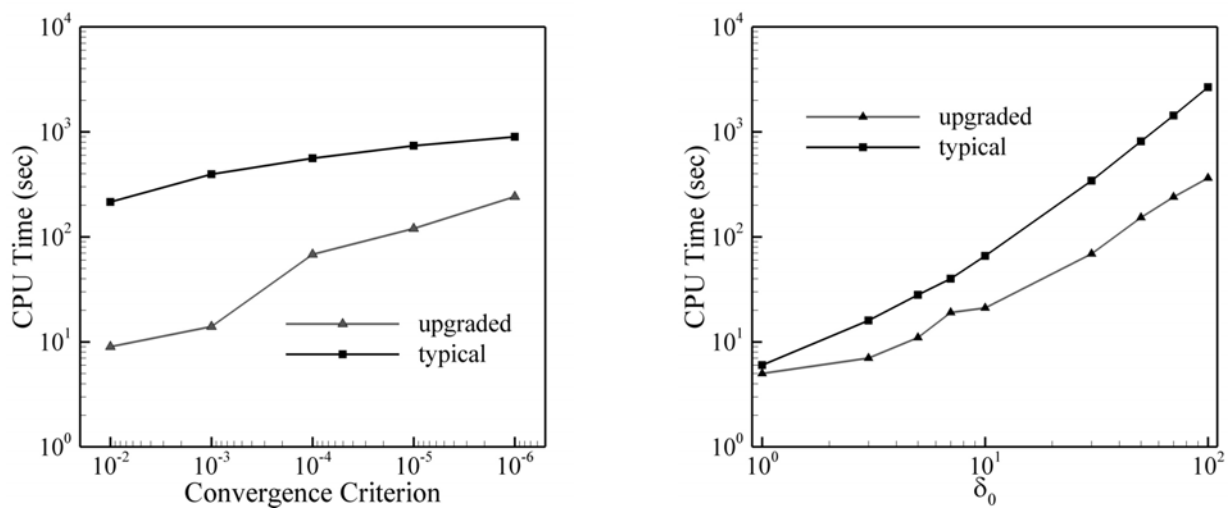

Figure 5: Comparison between the *typical* and *upgraded* schemes in terms of required CPU time for solving the cylindrical heat transfer problem, with $\gamma=0.5$.

REFERENCES

[1] S. G. Kandlikar, S. Garimella, D. Li, S. Colin and M. R. King, Heat transfer and fluid flow in minichannels and microchannels, Elsevier, Oxford (2006).

[2] J. M. Reese, M. A. Gallis and D. A. Lockerby, New direction in fluid mechanics: non-equilibrium aerodynamic and microsystem flows, Phil. Trans. R. Soc. Lond. A, 361, 2967-2988 (2003).

[3] J. H. Ferziger and H. G. Kaper, Mathematical theory of transport processes in gases, North-Holland Publishing Company (1972).

[4] C. Cercignani, The Boltzmann equation and its applications, Springer-Verlag (1988).

[5] H. Struchtrup, Macroscopic transport equations for rarefied gas flows, Springer (2005).

[6] G. A. Bird, Molecular gas dynamics and the direct simulation of gas flows, Oxford University Press (1994).

[7] C. Shen, Rarefied gas dynamics – Fundamentals, simulations and microflows, Springer (2005).

[8] T. M. M. Homolle and N. G. Hadjiconstantinou, A low variance deviational simulation Monte Carlo for the Boltzmann equation, J. Comput. Phys., 226, 2341-2358 (2007).

[9] V. V. Aristov, Direct methods for solving the Boltzmann equation and study of nonequilibrium flows, Springer (2001).

[10] F. Sharipov and V. Seleznev, Data on internal rarefied flows, J. Phys. Chem. Ref. Data, 27, 657-706 (1998).

[11] F. Sharipov, Rarefied gas flow through a long rectangular channel, J. Vac. Sci. Technol. A, 17, 3062-3066 (1999).

[12] S. Naris and D. Valougeorgis, Boundary driven non-equilibrium gas flow in a grooved channel via kinetic theory, Phys. Fluids, 19, 067103.1-067103.15 (2007).
[13] S. Lorenzani, L. Gibelli, A. Frezzotti and C. Cercignani, Kinetic approach to gas flows in microchannels, Nanoscale and Microscale Thermophysical Engineering, 11, 211-226 (2007).
[14] S. Naris and D. Valougeorgis, Rarefied gas flow in a triangular duct based on a boundary fitted lattice, Eur. J. Mech. B/Fluids, 27, 810-822 (2008).
[15] D. Valougeorgis and S. Naris, S, Acceleration schemes of the discrete velocity method: Gaseous flows in rectangular microchannels, SIAM J. Scient. Comp., 25, 534-552 (2003).
[16] L. Szalmas and D. Valougeorgis, A fast iterative model for discrete velocity calculations on triangular grids, J. Comp. Phys., 229, 4315-4326, (2010).
[17] P. L. Bhatnagar, E. P. Gross and M. A. Krook, A model for collision processes in gases, Phys. Rev., 94, 511-525 (1954).
[18] F. J. McCormack, Construction of linearized kinetic models for gaseous mixture and molecular gases, Phys. Fluids, 16, 2095-2105 (1973).
[19] S. Naris, D. Valougeorgis, D. Kalempa and F. Sharipov, Flow of gaseous mixtures through rectangular microchannels driven by pressure, temperature and concentration gradients, Phys. Fluids, 17, 100607.1-100607.12 (2005).
[20] I. N. Ivchencko, S. K. Loyalka and R. V. Tompson, Boundary slip phenomena in a binary gas mixture, Phys. Fluids, 16, 2095-2105 (2002).
[21] S. Takata, S. Yasuda, S. Kosuge and K. Aoki, Numerical analysis of thermal-slip and diffusion-slip flows of a binary mixture of hard-sphere molecular gases, Phys. Fluids A, 15, 3745-3766 (2003).
[22] F. Sharipov and G. Bertoldo, Numerical solution of the linearized Boltzmann equation for an arbitrary intermolecular potential, J. Comp. Phys., 28, 3345-3357 (2009).
[23] F. Sharipov and G. M. Kremer, Nonlinear Couette flow between two rotating cylinders, Transport Theory and Statistical Physics, 25, 217-229 (1996).
[24] K. Aoki, H. Yoshida and T. Nakanishi, Inverted velocity profile in the cylindrical Couette flow of a rarefied gas, Physical Review E, 68, 016302 (2003).
[25] K. Aoki, S. Takata and H. Aikawa, A rarefied gas flow caused by a discontinuous wall temperature, Phys. Fluids, 13, 2645-2661 (2001).
[26] S. Taguchi, K. Aoki and S. Takata, Vapor flows condensing at incidence onto a plane condensed phase in the pressure of a noncondensable gas. I. Subsonic condensation, Phys. Fluids, 15, 689-705 (2003).
[27] S. Pantazis and D. Valougeorgis, Non-linear heat transfer through rarefied gases between coaxial cylindrical surfaces at different temperatures, Eur. J. Mech. B-Fluids, (to appear).
[28] L. H. Holway, Approximation procedure for kinetic theory, Ph.D. thesis, Harvard University (1963).
[29] P. Andries, P. L. Tallec, J. P. Perlat and B. Perthame, The Gaussian-BGK model of Boltzmann equation with small Prandtl number, Eur. J. Mech. B-Fluids, 19, 813-830 (2000).
[30] C. Cercignani and M. Lampis, Kinetic models for gas-surface interactions, Transport Theory and Statistical Physics, 1, 101-114 (1971).
[31] J. Lihnaropoulos, S. Naris and D. Valougeorgis, Formulation and stability analysis of rapidly convergent iteration schemes for the 2D linearized BGK equation, Transport Theory and Statistical Physics, 36 513-528 (2007).
[32] E. Süli and D. F. Mayers, An Introduction to Numerical Analysis, Cambridge University Press (2003).
[33] B. D. Ganapol, Analytical Benchmarks for Nuclear Engineering Applications - Case Studies in Neutron Transport Theory (OECD, NEA No. 6292, Nuclear Energy Agency Organization for Economic Co-operation and Development, ISBN 978-92-64-99056-2, 2008).
[34] F. Borneman, A. Laurie and J. Wagen, The SIAM 100-digit Challenge, SIAM, Philadelphia, USA (2004).
[35] Graur and F. Sharipov, Gas flow through an elliptical tube over the whole range of the gas rarefaction, Eur. J. Mech. B/Fluids, 27, 335-345 (2008).
[36] G. Breyiannis, S. Varoutis and D. Valougeorgis, Rarefied gas flow in concentric annular tube: Estimation of the Poiseuille number and the exact hydraulic diameter, Eur. J. Mech. B/Fluids, 27, 609-622 (2008).
[37] S. Varoutis, S. Naris, V. Hauer, C. Day and D. Valougeorgis, Experimental and computational investigation of gas flows through long channels of various cross sections in the whole range of the Knudsen number, J. Vac. Sci. Technol. A, 27, 89-100 (2009).
[38] J. Pitakarnnop, S. Varoutis, D. Valougeorgis, S. Geoffroy, L. Baldas, S. Colin, A novel experimental setup for gas microflows, Microfluid. Nanofluid., 8, 57-72 (2010).