Simulation of gas flows in micro/nano systems using the Burnett equations

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Abstract. The gaseous flow characteristics in micro/nano systems are studied using the Burnett equations. The Burnett equations are the second-order approximation of the Chapman–Enskog solution to the Boltzmann equation. This set of equation is appropriate to describe the rarefied gas flows. Velocity slip and temperature jump boundary conditions are applied on solid surface. Several techniques, including the usage of relaxation method on slip values and Burnett terms, are introduced to increase the stability of the Burnett equations. Hence, convergent results at Knudsen number up to 0.5 are achieved for the first time. The results of the Burnett equations are first verified using the corresponding experimental and the DSMC data. The Navier-Stokes and the Burnett equations give almost the same result when the flow is in slip regime ($Kn<0.01$). But when the flow is in transition regime (0.1<$Kn<0.5$), the results of Navier-Stokes equations deviate from DSMC data while those of Burnett equations still agree very well. The Burnett equations are then used to study the gaseous flows in micro/nano systems. The pressure driven plane Poiseuille and the backward-facing step flows, the flows through micro filters are then studied. Different inlet to outlet pressure ratios, size effects, shape effects and boundary conditions are analyzed. The competitive relations of rarefied and compressible effects in micro gas flows are discussed.

1. Introduction

Micro/nano-scale gaseous flows are always encountered in microfluidic and nanofluidic systems. Flow and heat transfer characteristics in these systems have attracted considerable investigations during the past decade[1-2]. In micro/nano-scale flows, small length scale gives rise to high Knudsen number, $Kn$, which is defined as the ratio of the mean free path to the characteristic length scale. The Knudsen number is usually used to describe the departure from the continuum regime. As the value of $Kn$ increases, rarefaction effect becomes more important. The appropriate flow and heat transfer models are based on the range of $Kn$. A classification of different flow regimes is proposed by Tsien[3]: continuum flow (ordinary density) for $Kn<=0.001$, slip flow regime (slightly rarefied) for $0.001<Kn<=0.1$, transition regime (moderately rarefied) for $0.1<Kn<=10$ and free molecule flow (highly rarefied) for $Kn>10$. The Navier-Stokes equations together with nonslip boundary conditions are appropriate to model the continuum flow. Deviation from the state of continuum is relatively small in slip flow regime and the flow is still governed by the Navier-Stokes equations. The rarefaction effect is modelled through the partial slip at the wall using slip boundary conditions. In free molecule regime, the collisionless Boltzmann equation can be used. While in transition regime, the flow can neither be considered as an absolutely continuous medium nor a free molecule flow.
and is hard to describe.

In micro/nano-scale gaseous flows, the characteristic length scale is comparable to mean free path of gas. The rarefaction effect becomes important and cannot be neglected any more\cite{4,5}. Experiments conducted by Harley et al.\cite{6} and Arkilic et al.\cite{7} on low Reynolds number gas flows in microchannels showed that conventional analyses are unable to predict the observed flow rates with any degree of accuracy. The Navier-Stokes equations, which are based on linear constitutive relationship between shear and stress, cannot describe the gaseous flow in this regime any more\cite{11,4}. The direct simulation Monte Carlo (DSMC) method is widely used nowadays to investigate the flow and heat transfer behaviours in microscale gaseous flows\cite{8,9}. But this method requires a large number of particles for accurate simulation and is very expensive both in computational time and memory requirements, especially for the low-speed flow in MEMS and nanodevices\cite{2}.

As an alternative, higher-order extended or generalized hydrodynamic equations have been proposed which can perform equally well in both the continuum and slip/transition regimes\cite{2,4}. The Burnett equations, which add additional nonlinear second-order terms to the stress and heat flux terms, represent a second order correction to the equilibrium distribution function of gas flow\cite{10}. These equations have been proposed and proved to be suitable to model the flows near equilibrium in slip and early transition regime\cite{11}.

The Burnett equations have been a subject of considerable investigation in recent years. They were firstly used to model the shock wave in the transition regime. Fiscko and Chapman\cite{12} showed that the Burnett equations provide much more accurate numerical solutions than the Navier-Stokes equations for one-dimensional hypersonic shock structure in monatomic gases. Agarwal et al.\cite{15} investigated the hypersonic shock structure, hypersonic blunt body flow and axisymmetric hemispherical nose flow using the Burnett equations, and also found that the Burnett equations can present better results than the Navier-Stokes equations in transition regime. Xu\cite{13} showed that the discrepancy between the Navier–Stokes and the DSMC results can be resolved based on the simulation results of higher-order equations, such as Burnett and super-Burnett ones. Ohwada and Xu\cite{14} theoretically showed the consistency between the traditional Chapman–Enskog expansion and the successive approximation for the BGK equation up to the super-Burnett order and they designed a numerical scheme to efficiently solve the Burnett equations.

The necessity of using the Burnett equations for micro/nano flows has been demonstrated by many researcher\cite{15}. The Couette flows between two parallel plates were simulated using the Burnett equations and the results were compared with Navier-Stokes results\cite{16,17}. Agarwal et al.\cite{2} and Fang\cite{18} studied plane Poiseuille flow numerically and found that the velocity profiles agree well with those from μFlow calculations by Beskok and Karniadakis\cite{19}.

However, because of the numerical instability associated with the Burnett equations\cite{20,21}, convergent results in Poiseuille flow can only be obtained at small $Kn$. Agarwal et al.\cite{21} got convergent solutions of the Burnett equations to Poiseuille flow when $Kn=0.2$. But when Knudsen number becomes higher than 0.2, no convergent results could be achieved in the past. However, many gas flows in micro/nano devices fall in the range of $0.2<Kn<0.5$.

In present paper, the Burnett equations were adopted to indicate the gaseous flow characteristics in micro/nano-scale channels. The pressure driven plane Poiseuille flows\cite{22}, the backward-facing step flow and the flows in filters\cite{23} were modelled and analyzed.

### 2. The Burnett equations

The Burnett equations are the second-order approximation of the Chapman-Enskog solution to the Boltzmann equation\cite{10}. The augmented Burnett equations\cite{20} are adopted in present paper. The governing equations of two dimensional unsteady compressible viscous flow can be expressed in Cartesian coordinates as follows,

\[
\frac{\partial Q}{\partial t} + \frac{\partial E}{\partial x} + \frac{\partial F}{\partial y} = 0
\]  

\hspace{2cm} (1)

where
where \( e_t \) is the total energy, \( e_t = \rho C_v T + \frac{1}{2} \rho (u^2 + v^2) \). The viscous stress tensor \( \sigma \) and heat flux vector \( q \) can be derived as approximate solutions of the Boltzmann equation using the Chapman-Enskog expansion. In the Burnett equations,

\[
\sigma = -2\mu \mathbf{e} - \frac{\mu}{p} \left[ \omega_1 \mathbf{v} \cdot \nabla \mathbf{e} + \omega_2 (D \mathbf{e} - 2 \mathbf{v} \cdot \mathbf{e}) + \omega_3 \frac{1}{\rho T} \mathbf{v} \cdot \nabla \mathbf{e} \right] + \frac{\mu^3}{2p} \mathbf{v} \frac{3}{2} \omega_4 \mathbf{v} \nabla (\nabla \cdot \mathbf{v}) \tag{3}
\]

\[
q = -k \nabla T + \frac{R}{p} \left[ \theta_1 \nabla \cdot \mathbf{v} \nabla T + \theta_2 (D \nabla T - \nabla \cdot \mathbf{v} \nabla T) + \theta_3 \frac{T}{p} \mathbf{v} \cdot \nabla \mathbf{e} + \theta_4 \mathbf{v} \cdot \nabla \mathbf{e} + 3 \theta_5 T \mathbf{v} \cdot \nabla \mathbf{e} \right] + \frac{\mu^3}{p \rho} \left[ \theta_6 \mathbf{v} \nabla (\nabla \cdot \mathbf{v}) + \theta_7 \mathbf{v} \nabla (\nabla \cdot T) \right] \tag{4}
\]

where \( \mathbf{e} = \overline{\mathbf{v}^2} \). The double line over a tensor represents a divergence-free symmetric tensor,

\[
f_{ij} = \frac{f_{ij} + f_{ji}}{2} - \frac{\delta_{ij} f_{mn}}{3}.
\]

In equations (3) and (4), \( D \) is the material derivative. The coefficients in equations (3) and (4) for a hard sphere gas are: \( w_1 = 10/3 \), \( w_2 = 2 \), \( w_3 = 3 \), \( w_4 = 0 \), \( w_5 = 8 \), \( w_6 = 2/9 \), \( \theta_1 = 75/8 \), \( \theta_2 = -45/8 \), \( \theta_3 = -3 \), \( \theta_4 = 3 \), \( \theta_5 = 117/4 \), \( \theta_6 = -5/8 \), \( \theta_7 = 11/16 \).

The pressure in above equations obeys the ideal gas law,

\[
p = \rho RT \tag{5}
\]

Equations (1) to (5) form a closed set of equations, and \( \rho, u, v \) and \( T \) can be solved with appropriate boundary conditions.
3. Slip boundary conditions
Non-slip boundary conditions are generally unrealistic in slip and transition regime flows as there are not enough collisions near the wall to equilibrate the flow field. So, slip boundary conditions are specified at the wall. The classical slip boundary conditions are the Maxwell-Smoluchowski first-order slip conditions:

\[
\begin{align*}
    u_s - u_w &= \frac{2 - \sigma_v}{\sigma_v} \frac{\partial u}{\partial n_w} + \frac{3}{4} \frac{\mu}{\rho T} \frac{\partial T}{\partial n_w} \\
    T_s - T_w &= \frac{2 - \sigma_T}{\sigma_T} \frac{2\gamma}{Pr(\gamma + 1)} \frac{\partial T}{\partial n_w}
\end{align*}
\]  

(6) (7)

where the subscripts s and w denote the slip and wall values. \(\sigma_v\) and \(\sigma_T\) are, respectively, the tangential momentum and thermal accommodation coefficients. The second term on the right of equation (6) is thermal creep contribution to slip velocity.

Analytical models derived using the first-order slip boundary condition have been shown to be relatively accurate up to Knudsen numbers of approximately 0.1. For \(Kn>0.1\), however, experimental studies have shown that models based on the first-order slip condition show considerable discrepancies against observed data. In the present study, the following general slip boundary condition proposed by Beskok is adopted,

\[
\begin{align*}
    u_s &= \frac{1}{2} \left[ \left( 2 - \sigma_v \right) u_\lambda + \sigma_v u_w \right] \\
    T_s &= \frac{2 - \sigma_T}{Pr} \frac{2\gamma}{\gamma + 1} T_\lambda + \sigma_T T_w \\
         &= \frac{\sigma_T + \frac{2 - \sigma_T}{Pr} \frac{2\gamma}{\gamma + 1}}{\sigma_T}
\end{align*}
\]  

(8) (9)

where, the subscript \(\lambda\) represents the value calculated one mean free path away from the wall. This kind of slip boundary condition corresponds to a high-order slip boundary condition by simply expanding \(u_\lambda\) in terms of \(u_s\), using Taylor series expansion. The tangential momentum and thermal accommodation coefficient are both set to 1.0 in present study.

4. Numerical Algorithm
The present computation is based on the SIMPLE algorithm. The Burnett terms are treated as source terms. Slip boundary conditions are adopted to describe the velocity slip and temperature jump phenomena at wall. Generally, the Reynolds number and Mach number in microscale gas flows are small. But because of the large pressure drop along the channel, the density varies greatly and the effect of compressibility must be taken into consideration. The convergent Navier-Stokes results are used as initial values to increase the convergence.

As mentioned by many researchers, the computation of Burnett equations is unstable at fine grids. Convergent solutions can only be achieved on very coarse grids in their simulations. In rarefied gas flows, the largest departure from thermal dynamics equilibrium takes place near the boundary. As to the proposal of Lockerby and Reese, a relaxation method for the boundary values is first adopted in the present computation. The relaxation factor, \(R_f\), is introduced to modify the boundary value of the new iteration as follows:

\[
B_{\text{new}} = B_{\text{old}} + R_f \left( B - B_{\text{old}} \right)
\]  

(10)

where \(B_{\text{old}}\) represents for the values of previous iteration. \(B\) represents for the value calculated from present values.

High-order derivatives will bring large variations. The third-order and fourth-order derivatives in the
Burnett equations result in large change of Burnett terms and lead to the divergence of computation. So the relaxation method is also applied to the Burnett terms in present study. By applying the relaxation method to boundary values and Burnett terms, the convergent results of the Burnett equations can be achieved up to \( Kn = 0.5 \). The general slip boundary condition in equation (8) and (9) are not appropriate any more when \( Kn \) is larger than 0.5 since the slip value are calculated from the location one mean free path away from the wall. This kind of boundary condition is not suitable if the channel width is less than one mean free path.

5. Results and Discussions

5.1. Poiseuille flow

The plane Poiseuille flow is driven by the pressure difference between the inlet pressure and outlet pressure. The ratio of these two pressures is defined as \( \Pi \). Pong et al.\[27\] studied the pressure distributions along planar microchannels using an array of surface micromachined piezoresistive pressure sensors. In the experiments they found that pressure distributions are nonlinear in the microchannels due to compressibility. The present computed pressure distributions along the stream-wise direction for nitrogen flow are compared with experimental results of Pong et al. in figure 1. Five inlet pressures are compared ( \( p_i = 135, 170, 205, 240 \) and \( 275 \)kPa). Our present numerical results agree very well with experimental data. When the pressure ratio is small, the effect of compressibility is small and the pressure gradient is almost constant. The trend towards a nonlinear distribution is clear when the pressure ratio becomes large.

The detailed flow properties in microchannels in transition flow regime are beyond the present experiment technology. As a result, the molecule-based DSMC method is usually considered as an accurate method. Velocity profiles at \( \Pi = 2.28 \), non-dimensionalized with the inlet velocity, \( u_i \), at three different locations, are shown in figure 2, compared with DSMC results of Beskok\[19\]. The results of the Navier-Stokes with the same boundary conditions are also presented in the figure. The Knudsen number based on the outlet pressure is 0.20. It is found that the centerline velocities of the Navier-Stokes equations are slightly under predicted compared to DSMC results, while the Burnett results agree very well with DSMC, at all these three locations.

![Figure 1. Pressure distribution along the channel at five inlet pressures.](image1)

![Figure 2. Velocity profiles at three locations, \( x/L = 0.2, 0.5 \) and 0.8.](image2)

The velocity profiles at \( x/L = 0.5 \) at five Knudsen numbers (\( Kn = 0.01, 0.1, 0.2, 0.3, 0.4 \)) are shown in figure 3 to give a detailed description of slip velocity. These velocities are non-dimensionalized with corresponding average velocities, \( u_{ave} \) at \( x/L = 0.5 \). When Knudsen number is small, the maximum velocity is about 1.5 time the averaged value. But when \( Kn = 0.4 \), this value falls to only 1.1. The velocity profile is flatter at higher Knudsen number. Also, we can found from the figure that the results of these two methods
agree with each other at small $Kn$, e.g. $Kn=0.01$. But when $Kn$ is larger, e.g. $Kn=0.4$, the results are different.

The axial variation of local Poiseuille number at different $Kn$ is showed in figure 4. The Reynolds numbers in these cases are 2.2. Because of the difference in dimension, the inlet pressure is chosen to keep $Re$ constant. The local Poiseuille number decreases when proceeding along the channel. At small $Kn$ (e.g. $Kn=0.01$), $Po$ decrease rapidly first near the inlet and then tends to a constant. But at large $Kn$ (e.g. $Kn=0.3$), $Po$ decreases along the channel, not only in the entrance region, but in the whole channel. The fluid accelerates along the channel because of the density reduction brought about by the pressure drop. The normal velocity gradient at the wall also increases along the channel. The numerical results in figure 4 reveal that the increase in $\alpha$ outweighs the increase in normal velocity gradient when $Kn$ is large.

Figure 4 also demonstrates that the $Po$ decreases with the increase of $Kn$. The velocity profile at larger $Kn$ is flatter than that at smaller $Kn$. The normal velocity gradient at the wall decreases with the increase of $Kn$ number. So the friction factor or the shear stress decreases with the increase of $Kn$.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{velocity_profiles.png}
\caption{Velocity profiles of the Burnett and Navier-Stokes equations at different $Kn$.}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{poiseuille_number.png}
\caption{Variation of $Po$ along the channel at different $Kn$.}
\end{figure}

5.2. Micro-filter flow

The flows in and around microfilter are then studied. Usually, the width of filter hole is much larger than the height, $h$. So, only two-dimensional flow is considered here. Considering that the filter holes repeat periodically, the single micro/nano-filter shown in figure 5 is studied in present paper. The opening factor of filter is defined as $\beta = h/H$. The flow is driven by the pressure difference between inlet and outlet. The outlet pressure is $10^5$Pa throughout this section.

The present work first compares the velocity and pressure profiles obtained from the Burnett simulations with those of DSMC method\textsuperscript{28}. The filter geometry and boundary conditions are all set the same in these two methods. The $Kn$ of the flow in the simulation is 0.057. The distributions of centerline velocity and pressure are shown in figure 6. As can be seen from the figure, the velocity and pressure calculated from the Burnett equations agree well with DSMC results, which indicates that the Burnett equations are able to describe the gas flow characteristics in micro/nano-filters.
The variation of non-dimensional pressure drop, $K$, with Reynolds number, $Re$, is then analyzed, where $K$ is defined as $K = \Delta P / \frac{1}{2} \rho U^2_0$. The opening factor, $\beta$, and the ratio of the filter thickness to height, $t/h$, are kept the same in the calculation. Three kinds of micro/nano-filter are investigated. The variation of $K$ with $Re$ are shown in figure 7, at different $Kn$ numbers. As can be find from the simulation results, $K$ is proportional to $1/Re$. The relation between them can be fitted according to the simulation as follows:

$$K = C_1 \left( \frac{1}{Re} + 1 \right)^{1.78}$$

where $C_1$ is a function of factor $\beta$ and the ratio $t/h$. It can also be found that the non-dimensional pressure drop is independent of $Kn$. This conclusion is different from that of Mott\textsuperscript{[29]}, in which $K$ varies at different $Kn$.

The variation of $K$ with opening factor, $\beta$, are then analyzed, with $Re$ and $t/h$ kept the same. Non-dimensional pressure drops at different $\beta$ are calculated and the variations of pressure drop with factor $\beta$ are shown in figure 8. As can be found from the figure, the pressure drop $K$ decreases with the increase of factor $\beta$. According to the numerical results, the following relation between $K$ and $\beta$ can be achieved at different $Re$ and $t/h$

$$C_1 = k \left( \frac{11}{Re} + 1 \right) = C_2 \beta^{1.78}$$

Figure 5. Schematic view of the micro/nano-filter

Figure 6(a). Centerline velocity distribution.  
Figure 6(b). Centerline pressure distribution.
The effect of the ratio of filter thickness to height on pressure drop are analyzed at last. Different ratios \( t/h \) are calculated and we can find from the results that the non-dimensional pressure drop increases proportionally with \( t/h \). According to the numerical results, the following relation between \( K \) and \( t/h \) can be achieved at different \( Re \) and \( \beta \).

\[
C_z = K \beta^{1.78} \left( \frac{11}{Re} + 1 \right) = 1.91 \frac{t}{h} + 1.25
\]  

(13)

The variations of \( K \) with ratio \( t/h \) are shown in figure 9, with above fitting curve also included.

In conclusion, according to the numerical results, the variations of non-dimensional pressure drop \( K \) with \( Re \), opening factor \( \beta \) and the ratio \( t/h \) can be characterized as follows,

\[
K = \beta^{1.78} \left( 1.91 \frac{t}{h} + 1.25 \right) \left( \frac{11}{Re} + 1 \right).
\]  

(14)
5.3. **Backward-facing step flow**

The flow characteristics of backward-facing step flow are then studied. As shown in figure 10, the channel height is 0.5\( \mu \)m and the step ratio\((s/h)\) is 0.5. The outlet pressure is 100KPa and the pressure ratio is 2. The Kn at inlet and outlet are both 0.136. The Re number based on the mass flow rate per unit width is 0.74.

The streamwise velocities at five transverse locations are shown in figure 11(a). It can be found from the figure that the streamwise velocity is always positive, which indicates that no reverse flow exits after the step. The adverse pressure gradient after the step is very small, too small to stagnate the flow. This is different from macro backward-facing step flow.

The slip velocities at top and bottom wall are coincidental in most regions, as illustrated in the figure. The effect of step can be neglected when \(x/h\) is large enough. The transverse velocities at different \(y/h\) locations are shown in figure 11b. The transverse velocity is negative and asymmetric toward the bottom wall, which results from the momentum transfer downward owing to the appearance of downward expansion. The max nondimensional transverse velocity is about 0.9. The transverse velocity becomes zero at about \(x/h=4.5\). The streamwise velocities at different streamwise locations are shown in figure 11c. The velocity profile across the channel are symmetrical when \(x/h=5\).

![Velocity profiles](image)

**Figure 11.** Velocity profiles in backward-facing step flow: (a) streamwise velocities at different transverse locations, (b) transverse velocities at different transverse locations, (c) streamwise velocities at different streamwise locations, (d) transverse velocities at different streamwise locations. The transverse velocities at different streamwise locations are shown in figure 11d. When \(x/h=5\), the
transverse velocities is zero. The effect of step can be neglected when \( x/h = 4.5 \) in present case. This location changes with pressure ratio, \( Kn \) number and step ratio \( s/h \). In present simulation, \( x/h = 8 \) is used to ensure that the characteristics of backward-facing step flow can be fully described.

The backward-facing step flows at different pressure ratios are then analyzed. The channel height is 0.5\( \mu \)m and the step ratio \( (s/h) \) is 0.5. Different pressure ratios are studied, from 1.12 to 5. The \( Kn \) at outlet is 0.136 and the \( Kn \) at inlet is a function of inlet pressure. \( Kn \) decreases with the increase of pressure. The variation of mass flow rate with pressure ratio is shown in figure 12. The mass flow rate increases with the increase of pressure ratio. The relation is not linear as in traditional flow. The gradient increases with the pressure ratio.

The backward-facing step flows at different step ratios are then studied. The channel height is 0.5\( \mu \)m and the pressure ratio is 2. The \( Kn \) at outlet is 0.136. The variations of slip velocity at top wall are first illustrated in figure 15, nondimensionalized with average outlet velocity. The average velocities at seven step ratios, \( s/h = 0.2, 0.3, 0.4, 0.5, 0.6, 0.7 \) and 0.8 are 49.80m/s, 40.63m/s, 30.01m/s,

![Figure 12. Variation of mass flow rate with pressure ratio.](image)

![Figure 13. Centerline velocities along the channel at different pressure ratios.](image)
21.68m/s, 13.38m/s, 6.83m/s and 2.42m/s, respectively. The velocity profiles are parabolic and the Knudsen number (Kn) is the same at outlet. The nondimensional slip velocity at outlet are the same, us/uo = 0.42, as can be seen in the figure. The slip velocity before the step increases with the increase of step ratio.

The velocity gradient is larger in the front part of the backward-facing step flow. That’s because the pressure are mainly drop in the front part of the step flow at large step ratio. The pressure gradient is much larger in the front part of the backward-facing step flow.

6. Conclusions

The gaseous flow characteristics in two dimensional micro/nano systems are investigated using the Burnett equations. Velocity slip and temperature jump boundary conditions are applied on solid surface. The relaxation method on slip values and Burnett terms are introduced to increase the stability of the Burnett equations. Convergent results at Knudsen number up to 0.5 are achieved for the first time in the present study.

The pressure driven plane Poiseuille flow, the backward-facing step flows and the flows in and around micro filters are studied. Different inlet to outlet pressure ratios, size effects, shape effects and boundary conditions are analyzed. The competitive relations of rarefied and compressible effect in micro gas flows are discussed. The Burnett equations are high efficiency method to model the gaseous flow in slip and early transition flow regimes in micro/nano-scale devices.

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