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# The influence of Knudsen number on the hydrodynamic development length within parallel plate micro-channels

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## Abstract

One of the major difficulties in predicting the flow of gases through micron-sized channels can be attributed to the breakdown of the continuum flow assumption in the Navier-Stokes equations. If the dimensions of a channel are comparable to the mean free path of the gas molecules, the fluid can no longer be regarded as being in thermodynamic equilibrium and a variety of non-continuum or rarefaction effects will occur. Velocity profiles, mass flow rates and boundary wall shear stresses are all influenced by the non-continuum regime. In addition, the length of the hydrodynamic development region at the entrance to a channel may also be affected.

The present study examines the role of the Reynolds and Knudsen numbers on the hydrodynamic development length at the entrance to parallel plate micro-channels. Numerical simulations are carried out over a range of Knudsen numbers covering the continuum and slip-flow regimes ($0 \leq Kn \leq 0.1$). The results demonstrate that at the upper limit of the slip-flow regime ($Kn \approx 0.1$), the entrance development region is almost 25% longer than that predicted using continuum flow theory.

## 1 Introduction

The development of precision fabrication techniques for constructing Micro-Electro-Mechanical–Systems (MEMS) has emerged as one of the most exciting and revolutionary new areas of technology. For example, the use of *microfluidic* systems to manipulate small volumes of fluid will generate significant benefits in the chemical engineering and bio-chemical industries by enabling faster mixing

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and reaction times, increased chemical yields and faster throughput rates for chemical assays. In addition, the small length scales of microfluidic systems offer the prospect of developing miniaturised pressure sensors and chemical detectors with extremely high frequency responses.

Advanced microfluidic components currently under development include miniaturised heat-exchangers to cool integrated circuits, micro-reactors to generate small quantities of dangerous or expensive chemicals, 'lab-on-a-chip' bio-chemical sensors which perform complex biological assays on sub-nanolitre samples and hand-held gas chromatography systems for the detection of trace concentrations of air-borne pollutants. A common link between these examples is the requirement to move fluid through the device in a controlled manner. However, one of the emerging research issues is the realisation that the fluid mechanics at such small scales is not the same as that experienced in the macroscopic world.

Early investigations of non-continuum gas flows in channels were conducted by researchers in the rarefied gas community who were primarily interested in low-density applications such as high-altitude aircraft or vacuum technology. However, advances in micromachining technology have enabled flow channels to be constructed with sub-micron depths leading to a new area of research where rarefied gas behaviour is relevant. For example, recent experiments conducted by Pfahler *et al.* [1], Harley *et al.* [2] and Arkilic *et al.* [3,4,5] on the transport of gases in silicon micro-machined channels confirm that conventional (continuum) analyses are unable to predict flow rates in micron-sized devices with any degree of accuracy.

## 2 Non-continuum analysis

For an ideal gas modelled as rigid spheres, the mean free path of the molecules, $\mathcal{L}$, can be related to the temperature, $T$, and pressure, $p$, via

$$\mathcal{L} = \frac{kT}{\sqrt{2}\,\pi\, p\, \sigma_c^2} \tag{1}$$

where,

$k$ = Boltzmann's constant = $1.380662\times10^{-23}$ J K$^{-1}$,
$T$ = temperature (K),
$p$ = pressure (Nm$^{-2}$) and
$\sigma_c$ = collision diameter of the molecules (m).

The continuum assumption in the Navier-Stokes equations is valid provided the mean free path of the molecules is smaller than the characteristic dimension of the flow domain. If this condition is violated, the fluid will no longer be under local thermodynamic equilibrium and the linear relationship between the shear stress and rate of shear strain (Newton's law of viscosity) cannot be applied. Velocity profiles, boundary wall shear stresses, mass flow rates and pressure differences will then be influenced by non-continuum effects. In addition, the

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conventional no-slip boundary condition imposed at the solid-gas interface will begin to break down even before the linear stress-strain relationship becomes invalid (Gad-el-Hak [6]).

The ratio between the mean free path, $\mathcal{L}$, and the characteristic dimension of the flow geometry, $L$, is commonly referred to as the Knudsen number, $Kn$:

$$Kn = \frac{\mathcal{L}}{L} \ . \tag{2}$$

The value of the Knudsen number determines the degree of rarefaction of the gas and the validity of the continuum flow assumption. For $Kn \leq 0.001$, the continuum hypothesis is appropriate and the flow can be analysed using the Navier-Stokes equations with conventional no-slip boundary conditions. However, for $0.001 \leq Kn \leq 0.1$ (commonly referred to as the *slip-flow* regime) rarefaction effects start to influence the flow and the Navier-Stokes equations can only be employed provided tangential *slip-velocity* boundary conditions are implemented along the walls of the flow domain [6,7]. Beyond $Kn = 0.1$, the continuum assumption of the Navier-Stokes equations begins to break down and alternative simulation techniques such as particle based DSMC (Direct Simulation Monte Carlo) approaches must be adopted. Finally, for $Kn \geq 10$, the continuum approach breaks down completely and the regime can then be described as being a free molecular flow.

The analysis of developing flows at the entrance to rectangular ducts has received considerable attention over the years. Whilst most researchers have concentrated their efforts on the no-slip (continuum) flow regime, several studies have considered the hydrodynamic entrance problem under rarefied conditions where the momentum transport starts to be affected by the discrete molecular composition of the gas. For example, Ebert & Sparrow [8] formulated an analytical slip-flow solution for a rectangular channel whilst Quarmby [9] and Gampert [10] used finite-difference simulations to investigate developing slip-flow in circular pipes and parallel plates. In the present investigation, the role of the Reynolds and Knudsen numbers on the hydrodynamic development length at the entrance to a parallel plate micro-channel is investigated.

The parallel-plate micro-channel is an important geometry as it forms the limiting flow condition for large aspect-ratio rectangular ducts commonly encountered in silicon micro-machined components. Knowledge of the expected hydrodynamic development length is particularly important when designing the layout of microfluidic inlet structures or when choosing a suitable location for the upstream boundary of a numerical model.

## 3 Governing hydrodynamic equations

The governing hydrodynamic equations for a continuous (infinitely divisible) fluid can be written in tensor notation as follows:

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*continuity:*

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u_k)}{\partial x_k} = 0 \tag{3}$$

*momentum:*

$$\frac{\partial(\rho u_i)}{\partial t} + \frac{\partial(\rho u_k u_i)}{\partial x_k} = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ik}}{\partial x_k} \tag{4}$$

where $u$ is the velocity, $p$ is the pressure, $\rho$ is the fluid density and $\tau_{ik}$ is the second-order stress tensor. For a Newtonian, isotropic fluid, the stress tensor is given by

$$\tau_{ik} = \mu\left(\frac{\partial u_i}{\partial x_k} + \frac{\partial u_k}{\partial x_i}\right) + \lambda\left(\frac{\partial u_j}{\partial x_j}\right)\delta_{ik} \tag{5}$$

where $\mu$ and $\lambda$ are the first and second coefficients of viscosity and $\delta_{ik}$ is the unit second-order tensor (Kronecker delta). Implementing Stokes' continuum hypothesis allows the first and second coefficients of viscosity to be related via

$$\lambda + \frac{2}{3}\mu = 0 \tag{6}$$

although the validity of the above equation has occasionally been questioned for fluids other than dilute monatomic gases (Gad-el-Hak [11]).

### 3.1 Slip-velocity boundary conditions

To account for non-continuum effects in the slip-flow regime ($Kn \leq 0.1$), the Navier-Stokes equations are solved in conjunction with the tangential slip-velocity boundary condition first proposed by Basset [12]:

$$\tau_t = \beta u_t \tag{7}$$

where $u_t$ is the tangential slip-velocity at the wall, $\tau_t$ is the shear stress at the wall and $\beta$ is the slip coefficient. Schaaf & Chambre [13] have shown that the slip coefficient can be related to the mean free path of the molecules as follows:

$$\beta = \frac{\mu}{\left(\frac{2-\sigma}{\sigma}\right)\mathcal{L}} \tag{8}$$

where $\sigma$ is the tangential momentum accommodation coefficient (TMAC) and $\mathcal{L}$ is the mean free path. The tangential momentum accommodation coefficient is introduced to account for the reduction in the momentum of gas molecules colliding with the wall as described by Schaaf & Chambre [13]. For an idealised surface (perfectly smooth at the molecular level), the angles of incidence and reflection are identical and therefore the molecules conserve their tangential momentum. This is referred to as *specular reflection* and results in perfect slip at the boundary ($\sigma \to 0$). Conversely, in the case of an extremely rough surface, the molecules are reflected at totally random angles and lose, on average, their

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entire tangential momentum: a situation commonly referred to as *diffusive reflection* ($\sigma = 1$). The crystalline surfaces found in silicon micro-machined components often exhibit sub-unity tangential momentum accommodation, with $\sigma$ typically ranging from 0.8 to 1.0 (Arkilic et al. [5]).

Equations (7) and (8) can be combined and rearranged to give

$$u_t = \frac{2-\sigma}{\sigma}\frac{\mathcal{L}}{\mu}\tau_t \ . \tag{9}$$

At this stage it is convenient to recast the mean free path in the above equation in terms of a non-dimensionalised Knudsen number, *Kn*. The choice of the characteristic length scale depends upon the flow geometry under consideration. In the case of non-circular ducts, a convenient length scale can be found by invoking the concept of the *hydraulic diameter* of the cross-section, $D_h$:

$$D_h = \frac{4 \times \text{area}}{\text{wetted perimeter}} = \frac{4A}{P} \ . \tag{10}$$

For the specific case of flow between parallel plates separated by a distance, $H$, it can readily be shown that the hydraulic diameter equals twice the plate separation. The Knudsen number, *Kn*, can therefore be defined as the ratio of the mean free path of the gas molecules to the hydraulic diameter of the duct:

$$Kn = \frac{\mathcal{L}}{D_h} = \frac{\mathcal{L}}{2H} \ . \tag{11}$$

Substituting equation (11) into (9) allows the tangential slip-velocity at the solid perimeter wall to be written as

$$u_t = \frac{2-\sigma}{\sigma}\frac{Kn\,2H}{\mu}\tau_t \ . \tag{12}$$

The governing hydrodynamic equations were solved using THOR-2D – a two-dimensional finite-volume Navier-Stokes solver developed by the Computational Engineering Group at CLRC Daresbury Laboratory. Since most microfluidic devices operate at extremely low Mach numbers, compressibility effects were ignored in the present study. In addition, isothermal conditions were assumed throughout the flow domain.

### 3.2 Inflow/outflow boundary conditions

At the entrance to the duct, a uniform non-dimensionalised velocity distribution was prescribed parallel to the longitudinal axis of the channel:

$$u = 1 \quad \text{and} \quad v = 0 \qquad \text{at} \qquad x = 0 \ , \ 0 \le y \le H \tag{13}$$

whilst at the outlet, the axial gradients of the flow variables were set to zero:

$$\frac{\partial u}{\partial x} = 0 \quad \text{and} \quad \frac{\partial v}{\partial x} = 0 \qquad \text{at} \qquad x = l \ , \ 0 \le y \le H \tag{14}$$

where $l$ is the total length of duct.

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### 3.3 Hydrodynamic development length

When a viscous fluid enters a duct, the uniform velocity distribution at the entrance is gradually redistributed towards the centreline due to the retarding influence of the shear stresses along the side walls. Ultimately the fluid will reach a location where the velocity profile no longer changes in the axial-direction, and under such conditions the flow is said to be *fully-developed*. Theoretically, the required distance to reach the fully-developed solution is infinitely large. However, for practical engineering calculations, the *hydrodynamic development length, L,* is arbitrarily defined as the axial distance required for the centre line velocity to reach 99% of the fully-developed value.

The fully-developed slip-velocity profile in a parallel plate micro-channel can readily be obtained from the axial direction Navier-Stokes equation. It can be shown that the theoretical velocity profile across a micro-channel of height, $H$, is given by

$$u(y) = 6\bar{u}\left(\frac{y}{H} - \frac{y^2}{H^2} + 2\frac{2-\sigma}{\sigma}Kn\right)\Bigg/\left(1 + 12\frac{2-\sigma}{\sigma}Kn\right) \qquad (15)$$

where $\bar{u}$ is the mean velocity in the duct. In addition, the maximum velocity along the centreline of the duct ($y$=$H$/2) can be derived as

$$u_{\max} = \frac{3}{2}\bar{u}\left(1 + 8\frac{2-\sigma}{\sigma}Kn\right)\Bigg/\left(1 + 12\frac{2-\sigma}{\sigma}Kn\right). \qquad (16)$$

As an aside, in the limit of $Kn \to 0$ (i.e. under continuum flow conditions), equation (16) reverts to the familiar no-slip (NS) solution given by Poiseuille theory:

$$u_{\max(\mathrm{NS})} = \frac{3}{2}\bar{u}\ . \qquad (17)$$

Using equation (16) in conjunction with a 99% velocity cut-off point allows the hydrodynamic development length to be defined as the location where the longitudinal velocity at the centre of the duct reaches a value of

$$u = 1.485\,\bar{u}\left(1 + 8\frac{2-\sigma}{\sigma}Kn\right)\Bigg/\left(1 + 12\frac{2-\sigma}{\sigma}Kn\right). \qquad (18)$$

## 4 Results and discussion

The simulations assessed the entrance development length over a range of Reynolds and Knudsen numbers in the laminar slip-flow regime. In the present study, the Reynolds number was varied from $Re$ = 1 to $Re$ = 400 whilst the Knudsen number was varied from $Kn$ = 0 (continuum flow) to $Kn$ = 0.1 (a frequently adopted upper bound for the slip-flow regime). The upper limit of $Re$ = 400 was chosen since previous experimental work by Wu & Little [14] has

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suggested that the transition to turbulence in micro-geometries may occur at Reynolds number as low as 400. In the absence of additional information, the tangential momentum accommodation coefficient, $\sigma$, was assumed to have a value of unity. The Reynolds and Knudsen numbers were defined using the hydraulic diameter of the cross-section as the characteristic length scale, i.e.

$$Re = \frac{\rho \bar{u}\, 2H}{\mu} \quad \text{and} \quad Kn = \frac{\mathcal{L}}{2H} \; . \tag{19}$$

Preliminary validation of the hydrodynamic code was accomplished by comparing the analytical velocity profile across the duct (equation 15) against predictions from the downstream boundary of the numerical model. The tests involved a number of different grid resolutions, including meshes composed of $51 \times 21$, $101 \times 41$ and $201 \times 81$ nodes. In addition, numerical experimentation was used to decide upon a suitable length of duct, $l$. The computational domains were curtailed a finite distance downstream of the entrance, with the location chosen so as not to affect the computed entrance length. For Reynolds numbers up to 400, it was found that duct lengths of $l = 20D_h$ were sufficient to achieve a reliable estimate of hydrodynamic development length. In addition, an exponential stretching of the meshes in the axial-direction was implemented to achieve a finer grid resolution in the critical boundary-layer formation zone at the entrance.

Hydrodynamic development lengths were computed for three separate Knudsen numbers ( $Kn = 0$ , 0.05 and 0.10 ) and a range of Reynolds numbers between 1 and 400. Figure 1 illustrates the non-dimensionalised entrance development length as a function of Reynolds number for the $201 \times 81$ mesh. Superimposed on the results are the continuum ($Kn = 0$) development length equations presented by Atkinson *et al.* [15] and Chen [16]. Atkinson et al. found that the non-dimensionalised development length for a parallel-plate duct could be related to the Reynolds number via the following linear relationship:

$$\frac{L}{D_h} = 0.3125 + 0.011\, Re \tag{20}$$

whereas Chen [16] proposed a more elaborate function of the form:

$$\frac{L}{D_h} = \frac{0.315}{0.0175\, Re + 1} + 0.011\, Re \; . \tag{21}$$

Figure 1 indicates that the present continuum results ($Kn = 0$) are in good agreement with the hydrodynamic entrance lengths predicted by Chen. It can also be seen that Atkinson *et al.'s* solution tends to over-predict the development length at all but the lowest Reynolds numbers. More importantly, the present results show that the Knudsen number has a significant effect on the length of the development region. Inspection of Figure 1 reveals that at a Reynolds number of 400, the entrance length for a Knudsen number of 0.1 is approximately 25% longer than the corresponding no-slip solution. Even at relatively low Reynolds numbers, the increase in the length of the development region may still be important. It can therefore be concluded that the formulae proposed by Atkinson

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*et al.* [15] and Chen [16] for the parallel-plate geometry are no longer valid in the slip-flow regime and consequently a new development length equation accounting for both the Reynolds number and Knudsen number must be evaluated.

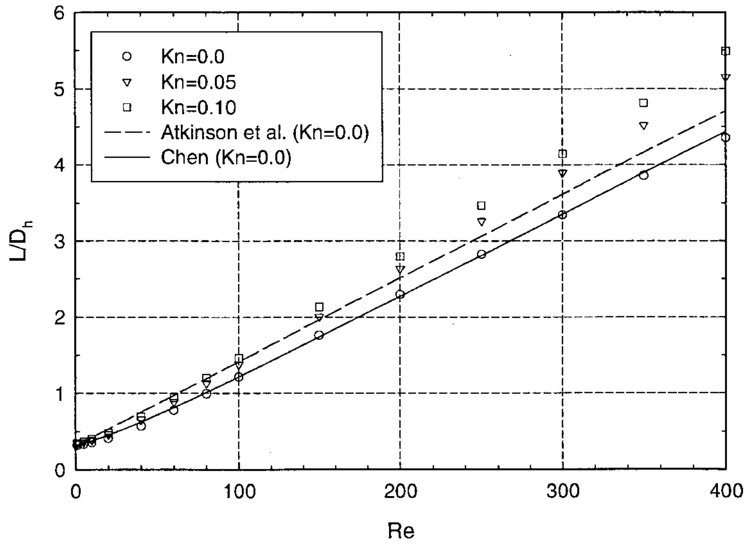


Figure 1: Non-dimensionalised development length for rarefied slip-flow in a parallel plate micro-channel.

A non-linear least-squares curve-fitting procedure employing the Levenberg-Marquardt method was used to determine the relationship between $L/D_h$, $Re$ and $Kn$. The effect of the Knudsen number was taken into account by multiplying the coefficient in the second term of Chen's development length equation (21) by a correction factor of the form:

$$\left(\frac{1 + A\ Kn'}{1 + B\ Kn'}\right) \tag{22}$$

where $A$ and $B$ are constants and $Kn'$ is defined as

$$Kn' = \frac{2-\sigma}{\sigma} Kn \ . \tag{23}$$

The Knudsen number correction shown in equation (22) was chosen because the analytical expression for the fully-developed centreline velocity has a similar Knudsen number modification factor. Applying the Levenberg-Marquardt least-squares technique yields the following expression for the hydrodynamic development length:

$$\frac{L}{D_h} = \frac{0.332}{0.0271\, Re + 1} + 0.011\, Re \left(\frac{1 + 14.78\, Kn'}{1 + 9.78\, Kn'}\right) . \tag{24}$$

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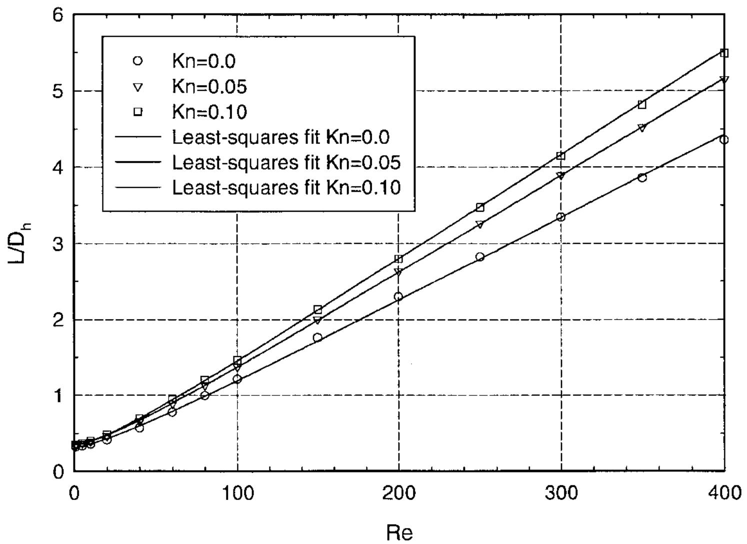


Figure 2: Least-squares fit of non-dimensionalised development length for rarefied slip-flow in a parallel plate micro-channel.

Figure 2 illustrates the results of the Levenberg-Marquardt least squares fit. It can be seen that the proposed equation provides a good representation of the numerical development length data. Moreover, the linearity of the Reynolds number dependency in the second term of equation (24) implies that the expression will provide a reliable estimate of hydrodynamic development length up to the transition to turbulence. The proposed entrance length equation should therefore be appropriate for the entire laminar slip-flow regime.

## 5 Conclusions

An investigation of low Reynolds number rarefied gas behaviour at the entrance of a parallel-plate micro-channel has been conducted using a specially adapted two-dimensional Navier-Stokes solver. The hydrodynamic model is applicable to the slip-flow regime which is valid for Knudsen numbers between $0 < Kn \leq 0.1$. Within this range, rarefaction effects are important but the flow can still be modelled using the Navier-Stokes equations provided tangential slip-velocity boundary conditions are implemented along the walls of the flow domain.

The numerical model has indicated that the Knudsen number has a significant effect on the hydrodynamic development length at the entrance to parallel plates. At the upper limit of the slip-flow regime $(Kn \approx 0.1)$, entrance lengths have been shown to be approximately 25% longer than those experienced in the continuum (no-slip) regime.

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