

## SLIP MODEL PERFORMANCE FOR MICRO-SCALE GAS FLOWS

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### ABSTRACT

The small length scale and bulk gas velocity associated with micro-scale gas flows make it difficult to simulate such flows using accurate and efficient computational methods. To address this problem, slip models have been proposed in the literature as a means to combine numerically efficient continuum flow solvers with corrected boundary conditions. The purpose of this investigation is to evaluate the performance of three popular slip models found in the literature. Analytical solutions using the slip models are compared to DSMC results for one-dimensional Couette and Poiseuille flow. The three slip models tested perform similarly well predicting the velocity profile and mass flux for a Knudsen number  $Kn < 0.1$ . Above this range, the performance deteriorates significantly for all slip models due in part to the error associated with the shear stress closure in the Navier-Stokes equation. Although some slip models yield reasonable results for larger Knudsen numbers, their performance is generally limited to very specific applications. As a result, slip models would not be appropriate for more complex flow geometries for  $Kn > 0.1$ .

### 1. INTRODUCTION

The lack of accurate and efficient simulation methods for micro-scale gas flows is directly due to two factors: the small length scales, and slow bulk gas velocities

associated with micro-scale devices. When the length scale of the flow approaches the mean free path of the operating fluid, there are no longer sufficient collisions between gas molecules to achieve thermodynamic equilibrium. Non-continuum non-equilibrium regions cannot be accurately predicted using the continuum-based Navier-Stokes equations, because thermodynamic equilibrium is assumed for the no-slip boundary condition and the transport closure. Particle simulations, like the Direct Simulation Monte Carlo (DSMC) method of Bird, are correct in non-equilibrium regions but suffer from statistical noise in the bulk velocity because of the random, or thermal speed of the molecules.<sup>1</sup> When the bulk velocity is much slower than the thermal velocity, as is typically the case for gas flows in micro-electro-magnetic systems (MEMS), many independent samples are needed to eliminate the statistical scatter and recover the bulk flow properties. In fact, for nitrogen gas at room temperature, the standard deviation in the thermal speed for one molecule is about 300 m/sec, which would require approximately 9 million independent samples in DSMC to reduce the scatter in the bulk velocity to 0.1 m/sec. For MEMS gas flows that operate in the mm/sec range, the number of required samples can grow to the trillions and simulations on even the world's fastest supercomputers can take weeks. DSMC is impractical in these cases as a tool to evaluate MEMS design iterations rapidly. Overall, the small length scales and slow bulk gas velocity combine to make continuum solutions inaccurate, and particle solutions time-consuming.

Slip models have been proposed to correct the numerically efficient, continuum methods for non-equilibrium regions near solid boundaries. The idea is to relax the traditional no-slip boundary to allow for the presence of slip. Slip models have been around since the beginning of gas kinetic theory, when Maxwell

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derived a relation between the slip velocity at the wall and the local velocity gradient.<sup>2,4</sup> However, in recent times, the desire for physically accurate and numerically efficient simulation of MEMS gas flows has renewed interest in the field and has brought to light a century of work. After Maxwell, many contributed slip models based on extensions of higher-order equations (Deissler 1964, Cercignani 1969, and Kogan 1969), while more recent work by Karniadakis, and Pan has involved empirical models.<sup>4-8</sup> The above research represents only a fraction of the proposed models, yet almost all of them can be considered an extension of Maxwell's original model.

This investigation will focus on the performance of three popular, gradient-based slip model corrections to the Navier-Stokes equations. The slip models chosen for study are our implementation of Maxwell's model and the empirical model proposed by Karniadakis & Beskok, and a first-order empirical model based on DSMC results.<sup>4,10</sup> One-dimensional, low speed, constant temperature Couette and Poiseuille flows are used as test cases because it is straightforward to obtain analytic solutions to the Navier-Stokes equation using the slip models. The velocity profiles of the analytic solutions are compared to DSMC results for Knudsen numbers ranging from 0.01 to 10 to determine the maximum error. In addition, the error in mass flux between the analytic slip model solutions and the DSMC results are found for the Poiseuille flow cases. By understanding the error using the slip models in the non-equilibrium regime, the results from these simple flows can serve as a guide for more complex simulations.

In the subsequent sections of this paper, the three slip models are introduced along with their usage in the analytic solution to the Navier-Stokes equation. The investigation methods, including the DSMC simulation parameters, are explained. Then comparisons are made between the DSMC results and the slip models. From these comparisons, the velocity profile errors are found for Poiseuille and Couette flows, and the mass flux errors for Poiseuille flow. In addition, the model performance is discussed for high Knudsen number flows.

## 2. SLIP MODELS

Continuum flow has sufficient molecular collisions throughout the fluid to be considered in local thermodynamic equilibrium (LTE). The degree that a gas flow deviates from LTE is typically measured by the Knudsen number (Kn), which is defined as  $Kn = \lambda/L$ , where  $\lambda$  is the mean free path of the gas molecules

between collisions, and  $L$  is the characteristic length scale of the problem. As the Knudsen number increases, there are fewer collisions occurring within the length scale of interest, and the gas deviates further from LTE. A flow with a higher Knudsen number is said to be more rarefied because the number of molecules within the volume of interest is lower.

The Navier-Stokes equation describes the conservation of momentum for continuum flow (eq. 1), with a Newtonian shear stress closure (eq. 2).<sup>9</sup>

$$\frac{\partial \rho \vec{v}}{\partial t} + \nabla(\rho \vec{v} \otimes \vec{v}) = -\nabla p + \rho \vec{f} + \nabla \bar{\bar{\tau}} \quad (1)$$

$$\bar{\bar{\tau}} = \tau_{ij} = \mu \left( \frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} \right) \quad (2)$$

In the above equations,  $\rho$  is the fluid density,  $v$  is the fluid velocity vector,  $p$  is the fluid pressure,  $f$  is the external body force acting on the fluid, and  $\tau$  is the stress tensor. The Newtonian shear stress closure assumes that the shear stress is equal to the local velocity gradient tensor times the fluid viscosity. Flow interacting with a solid surface is said to have a no-slip boundary condition, meaning that the relative gas velocity at the surface is zero. Both the stress closure and the no-slip boundary assumptions breakdown as the flow deviates from LTE.

In Fig. 1, the Couette flow results for  $Kn = 0.1$  illustrate the breakdown of the no-slip condition at the wall. The DSMC results show a slip velocity equal to about 10% of the difference between wall velocities. This slip velocity cannot be predicted using the Navier-Stokes equation. If the boundary conditions were altered, then it would be possible to obtain good agreement with the DSMC data. In Fig. 1, a least squares fit of the Navier-Stokes solution to the DSMC data is found in order to show the best possible results of a slip model. However for the same conditions, the error in the shear stress for the no-slip solution is 30% higher than DSMC, while even the best-fitting solution over-predicts the shear stress by 7%, as shown in Fig. 2. This break down of the shear stress closure cannot be predicted by any slip model, or the Navier-Stokes equations.

For small enough Knudsen numbers the effects of non-equilibrium are limited to a region within a couple of mean free paths of the boundary surfaces. This thin region is called the Knudsen layer. If this region is small compared to the rest of the flow domain, then it is reasonable to use the Navier-Stokes equation with altered boundary conditions to correct for the non-equilibrium effects. This correction, based on a thin

Knudsen layer assumption, is often referred to as a slip model because it allows for a non-zero relative gas velocity at the boundary surface.

The three slip models tested for this investigation are first-order, velocity gradient-based corrections to the no slip boundary conditions. These include our implementation of Maxwell's model and the empirical model proposed by Karniadakis & Beskok, and an empirical correction to Maxwell's model based on DSMC results.<sup>4,10</sup> All three models can be represented as boundary conditions of the same form:

$$u_{wall} = C(Kn) \cdot L \cdot \frac{2 - \sigma_v}{\sigma_v} \frac{\partial u}{\partial n} \Big|_{wall} \quad (3)$$

where  $u_{wall}$  is the tangential velocity component at the boundary surface,  $C(Kn)$  is a function of Knudsen number and is defined by the slip model,  $L$  is the characteristic length scale of the flow,  $\sigma_v$  is the tangential momentum accommodation coefficient (TMAC), and  $\partial u / \partial n$  is the tangential velocity gradient in the direction normal to the boundary. The TMAC represents the fraction of incident gas molecules on the wall that are assumed to undergo a diffuse reflection instead of a specular reflection. A diffuse reflection is an idealization of a collision process with a rough surface. The reflected molecule is assumed to have been in contact with the wall long enough to equilibrate to the wall temperature and lose all memory of its incident trajectory. A specular reflection on the other hand is perfectly reflected with no loss of energy, or tangential velocity.

Maxwell's model is derived from kinetic theory and predicts that the slip velocity at the boundary is equal to the product of the mean free path and the velocity gradient for full accommodation ( $\sigma_v = 1$ ):

$$u_{wall} = \frac{2 - \sigma_v}{\sigma_v} \lambda \cdot \frac{\partial u}{\partial n} \Big|_{wall} \quad (4)$$

and in the form of (eq. 3):

$$C_{Maxw}(Kn) = Kn \quad (5)$$

Karniadakis and Beskok's (K&B) model (eq. 6) is an empirical model that is designed to give accurate velocity profiles normalized by the average velocity over a wide range of Knudsen numbers for Poiseuille flow:

$$C_{K\&B}(Kn) = \frac{Kn}{Kn + 1} \quad (6)$$

However, the normalization eliminates the dependence on viscosity and any associated error in the shear stress closure. As a result, for high Knudsen numbers it cannot predict the correct mass flux, or any dimensional result without a separate correction made for the shear stress closure. The empirical model derived in this work and given by equation 7 is designed to best match the slip model results to the DSMC results for a range of conditions by adding a correction factor to Maxwell's model.

$$C_{Emp}(Kn) = 1.253 \cdot Kn \quad (7)$$

The slip coefficient factor of 1.253 is found to best fit the DSMC data for Poiseuille and Couette flows with Knudsen numbers ranging from 0.01 to 0.1 and speeds less than Mach 0.3 as reference cases. This coefficient is about 10% higher than that found by Pan using just Couette flow results for several monatomic gases.<sup>8</sup> It is important to note that none of the slip models presented here can correct for the error in the shear stress closure.

### 3. INVESTIGATION METHOD

The purpose of the investigation is to assess the performance of the three slip models. In order to achieve a suitable means of comparison, one-dimensional Couette and Poiseuille flows, Figs. 3-4, are used as test cases. Analytic solutions to the Navier-Stokes equation are readily available for these geometries when the flow is assumed incompressible and isothermal. The analytic solutions using the slip models are then compared to DSMC results for the same flow conditions. All cases presented in this investigation are low speed (below 30 m/s), which is within the incompressible limit. For the one-dimensional geometry and the incompressible, isothermal approximation (eqs. 1-3) can be combined to solve for the velocity profiles for Couette (eq. 8) and Poiseuille (eq. 9) flow.

$$u_{Couette} = U_1 + \frac{U_2 - U_1}{1 + 2C(Kn)} \left[ \frac{y}{h} + C(Kn) \right] \quad (8)$$

$$u_{Poiseuille} = -\frac{\rho f h^2}{2\mu} \left[ \left( \frac{y}{h} \right)^2 - \frac{y}{h} - C(Kn) \right] \quad (9)$$

In the above equations,  $h$  is the channel height and the characteristic length of the flow,  $U_1$  is the velocity of the wall at  $y=0$ , and  $U_2$  is the velocity of the wall at  $y=h$ . The body force  $f$  is used to drive the Poiseuille flow instead of the pressure gradient so as to be consistent with the DSMC simulation.

The DSMC results are obtained from a modified version of the one-dimensional code provided by Bird.<sup>1</sup> The working fluid is monatomic argon gas with the collision dynamics modeled with the variable soft sphere (VSS) model. All DSMC simulations use 150 cells and 4500 numerical particles. The time step is chosen so that a particle will cross a cell on average in three time steps. The results are sampled until the statistical scatter in the velocity profile is less than 1% (typically over 15 million samples). The simulation is one-dimensional and it is assumed that the velocity distribution function is the same everywhere along planes parallel to the boundary walls. As a result, a pressure gradient cannot be applied to drive the Poiseuille flow; instead, the accelerative body force  $f$  is used. This driving force varies with Knudsen number, and was found through trial and error until the DSMC results appeared to have a maximum velocity of 25 m/s. Each collision with the wall boundaries is calculated as either specular or diffusive with the fraction of each to be determined by the TMAC. The geometry of all the cases is fixed and varying the number density of the flow controls the Knudsen number.

All cases presented in this investigation are in the incompressible limit with velocities ranging from 20 m/sec to 30 m/sec. At higher speeds, the error associated with the velocity magnitude is dominated by the error due to deviation from LTE.<sup>10</sup> In order to determine the sensitivity of the slip models to the wall surface interaction the tangential momentum accommodation coefficient (TMAC) is varied. The velocity profile and total mass flux (Poiseuille only) are calculated using DSMC and an analytic solution of the Navier-Stokes equation for the following conditions:

- Argon gas with the VSS collision model
- Knudsen numbers ranging from 0.01 to 10
- TMAC of 0.5, 0.8, and 1.0
- Fixed wall temperature of 273°K
- Fixed Poiseuille channel height of 2 mm
- Fixed Couette channel height of 1 mm

## **4. RESULTS AND DISCUSSION**

Many slip models share a common foundation with the original model first proposed by Maxwell. Other

features are added to the models to offer higher-order accuracy, or better agreement with certain data. These differences cause the models to diverge as the Knudsen number increases. However in the continuum limit (Kn tending toward zero), all models are consistent with the continuum solution and the difference between the models is insignificant. It is then expected that below a sufficiently small Knudsen number that the choice of model is irrelevant. For  $Kn \leq 0.03$ , all models predict a velocity within 8% of the DSMC data for all cases.

### **4.1 Poiseuille flow**

As the flow becomes more rarefied, the Knudsen layer grows, and cannot be effectively captured by the boundary correction alone. Since slip models only serve to correct the boundary conditions, it is expected that their performance deteriorates when the Knudsen layer becomes sufficiently large. For  $Kn = 0.01$ , as shown in Fig. 5, all models are in agreement with the DSMC velocity profiles with a maximum error less than 4%. If the Knudsen number increases to 0.1, as shown in Fig. 6, the Knudsen layer represents 20% of the total flow area. At this condition, Maxwell's model and the K&B model under-predict the maximum velocity by 17%. The least squares empirical model performs slightly better than the others with a maximum error of 10% for a TMAC of unity.

### **4.2 Couette flow**

The slip models perform better on the Couette flow than the Poiseuille flow for the same Knudsen number. Couette flow is independent of the fluid viscosity, which means the solution is unaffected by any error in the shear stress closure. For  $Kn = 0.1$ , all the models are in excellent agreement with the DSMC velocity profiles with a maximum error less than 2%, Fig. 7. Even at  $Kn = 1$ , when the Knudsen layer encompasses the entire domain, which is well out of the range of a thin layer assumption, all models are within 10% of the DSMC data, Fig. 8.

### **4.3 Mass flux error**

The error in mass flux for Poiseuille flow is related to the error in the velocity profiles. As the Knudsen number increases the mass flux error grows. In Figs. 9-11, the Knudsen number dependence of the error is plotted for TMAC equal to 0.5, 0.8, and 1.0. The TMAC has little effect on the performance of the models. The mass flux error is less than 20% for all models when  $Kn \leq 0.1$ . For large Knudsen numbers the models diverge, with the least squares empirical model out performing the others over the entire Knudsen number range tested.

#### 4.4 High Knudsen number usage

For  $Kn > 0.1$ , the continuum and near continuum assumptions of a thin Knudsen layer begin to break down. Above  $Kn = 1$ , there is no physical basis to justify the use of the Navier-Stokes solution with the slip models. However, in certain circumstances the slip models do yield acceptable solutions. If the viscosity dependence of the solution can be eliminated, then the slip models can be tuned to correctly predict the slip velocity over a wide range of Knudsen numbers. The slip models yield reasonable solutions for Couette flow ( $Kn = 10$ ) and the normalized Poiseuille flow ( $Kn = 1$ ), both of which are independent of viscosity, Figs. 12 and 13. The Maxwell and least squares empirical model are within 10% of the DSMC solution for Couette flow while the K&B model is within 10% for the normalized Poiseuille flow. The normalized solution of the Poiseuille flow cannot be used alone to obtain the mass flux or other dimensional quantities at large Knudsen numbers because the error in the shear stress closure dominates. In Fig. 14, the dimensional velocity profiles illustrate the error at  $Kn = 1$ . The K&B model which does so well for the normalized profiles is now off by a factor of 5. It is sometimes possible to obtain reasonable results using slip models outside the thin Knudsen layer approximation, but these instances only occur when the Navier-Stokes solution is independent of viscosity. The error due to the shear stress closure is eliminated when there is no viscosity dependence. This limitation makes the slip model performance specific to the flow type and will not be reliable for predicting more complicated flow geometries.

#### 5. CONCLUSION

The goal of this investigation was to determine the range of applicability of various slip models for Navier-Stokes prediction of MEMS flows. Three popular models were tested: Maxwell's model, Karniadakis & Beskok's model, and an empirical model derived to match the DSMC results over a range of Knudsen numbers. It was found that no one model significantly outperformed the rest. At  $Kn = 0.1$  all the models under-predict the maximum DSMC velocity by 10% to 17% for Poiseuille flow. The models performed significantly better on Couette flow than Poiseuille flow. The effect of any errors found in the shear stress closure are not present in Couette flow, or in the normalized Poiseuille flow because they do not depend on the fluid viscosity. The thermal momentum accommodation coefficient (TMAC) has little impact

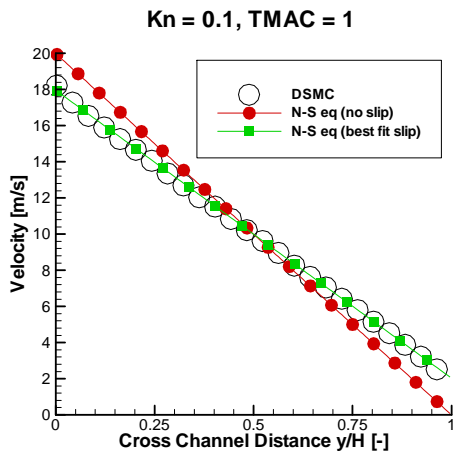
on the effectiveness of the slip models. Furthermore, the investigation showed that care must be taken when applying the slip models outside the limit of the thin Knudsen layer approximation. If dimensional quantities are to be found for  $Kn > 0.1$  the shear stress closure must be modified as well.

#### ACKNOWLEDGEMENTS

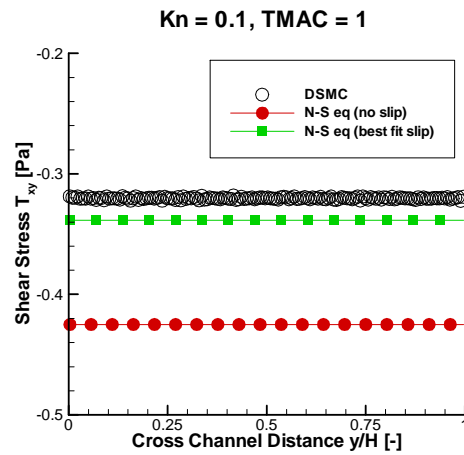
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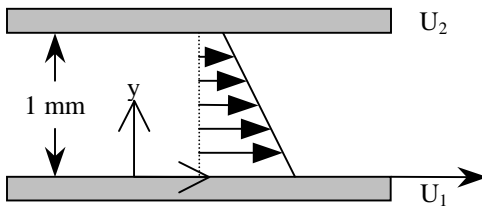
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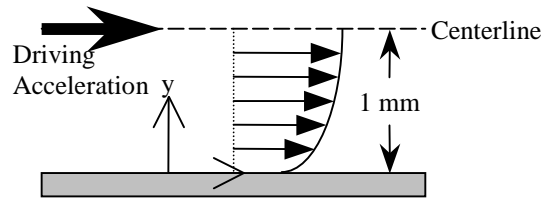
**Figure 1.** A representative DSMC velocity profile illustrates the violation of the no-slip boundary condition for  $Kn = 0.1$  because the gas has deviated from local thermodynamic equilibrium.



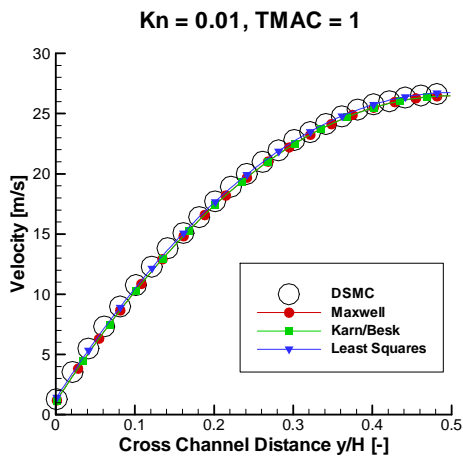
**Figure 2.** The DSMC solution for  $Kn = 0.1$  illustrates that the Newtonian shear stress closure no longer is accurate because the gas has deviated from local thermodynamic equilibrium.



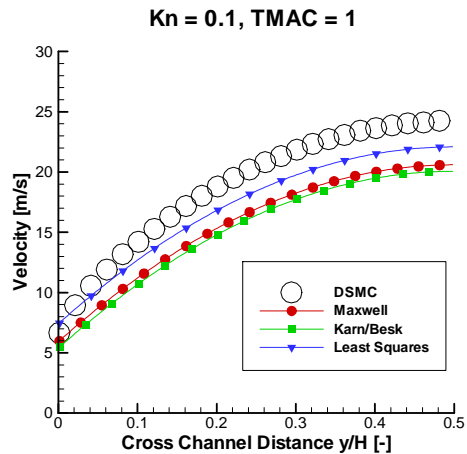
**Figure 3.** Illustration of the Couette flow geometry, the upper wall is stationary while the lower wall moves at 20 m/s. The dimensions are fixed for all cases, only the number density is changed for different flow conditions.



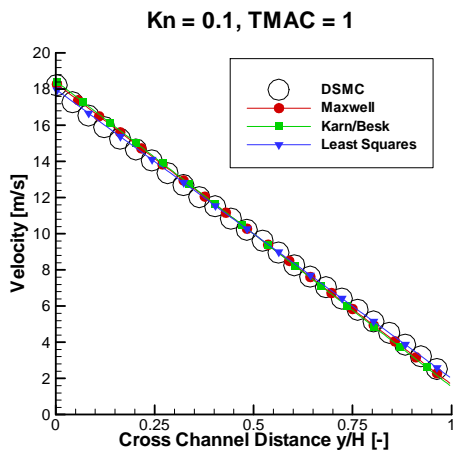
**Figure 4.** Illustration of the Poiseuille flow geometry, the wall is stationary while the driving acceleration and number density are changed to yield different flow conditions.



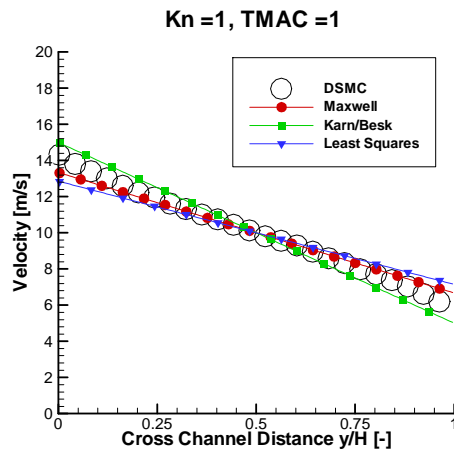
**Figure 5.** Absolute velocity profiles for Poiseuille flow near the incompressible limit for  $Kn = 0.01$ , all the slip models are in close agreement with each other, and have a maximum error within 4%.



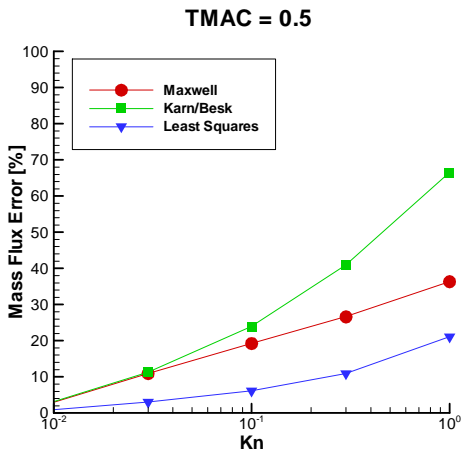
**Figure 6.** Absolute velocity profiles for Poiseuille flow near the incompressible limit for  $Kn = 0.1$ , the slip models begin to diverge from each other, and have a maximum error within 17%.



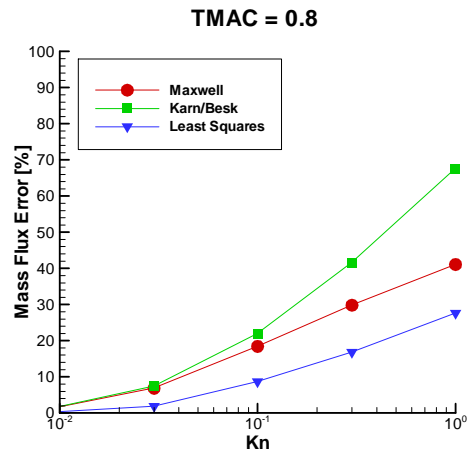
**Figure 7.** Absolute velocity profiles for Couette flow near the incompressible limit for  $Kn = 0.1$ , all the slip models are in close agreement with each other, and have a maximum error within 2%.



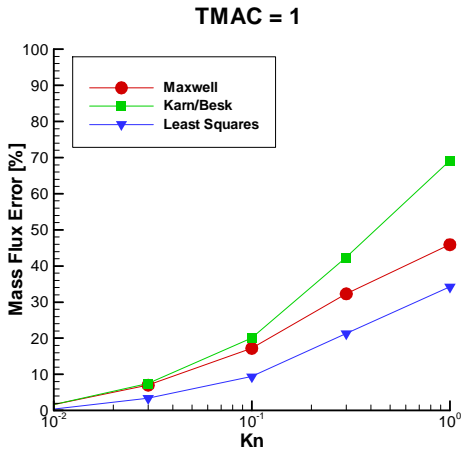
**Figure 8.** Absolute velocity profiles for Couette flow near the incompressible limit for  $Kn = 1$ , even though the thin Knudsen layer approximation is ungrounded, all models are within 10% of the DSMC data.



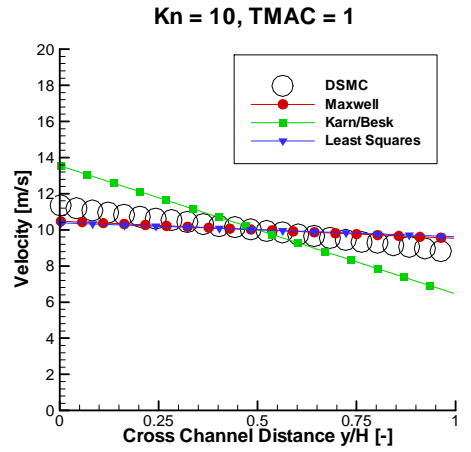
**Figure 9.** Mass flux error for  $TMAC = 0.5$ , the empirical least squares method performs the best for the largest range of Knudsen numbers.



**Figure 10.** Mass flux error for  $TMAC = 0.8$ , the empirical least squares method performs the best for the largest range of Knudsen numbers.

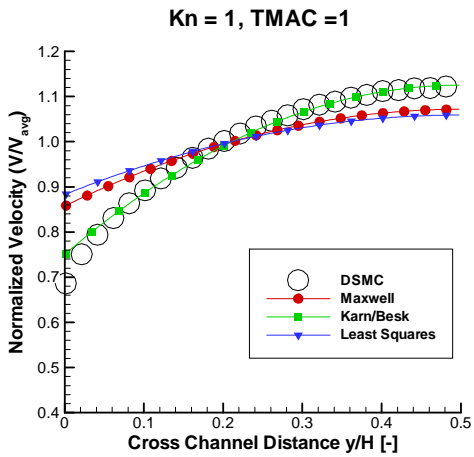


**Figure 11.** Mass flux error for  $TMAC = 1.0$ , the empirical least squares method performs the best for the largest range of Knudsen numbers.

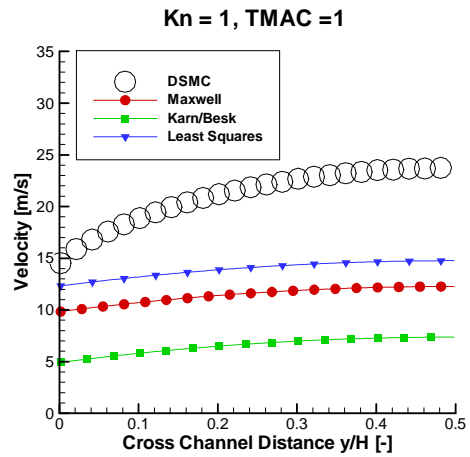


**Figure 12.** Absolute velocity profiles for Couette flow near the incompressible limit for  $Kn = 10$ , even though the thin Knudsen layer approximation is ungrounded, Maxwell's model, and the least squares empirical model are with 10% of the DSMC data.





**Figure 13.** Normalized velocity profiles for Poiseuille flow near the incompressible limit for  $Kn = 1$ , even though the thin Knudsen layer approximation is ungrounded, the K&B model has a maximum error less than 10%.



**Figure 14.** Absolute velocity profile for Poiseuille flow near the incompressible limit for  $Kn = 1$ , all models perform poorly with errors ranging from 40% to 75%.