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# The effect of gaseous slip on microscale heat transfer: An extended Graetz problem

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#### **Abstract**

On the basis of Langmuir's theory of adsorption of gases on solids, the effect of temperature jump on microscale heat transfer is investigated. A mathematical model, extended from the classical Graetz problem, is developed to analyze convective heat transfer in a microtube in various slip-flow regimes. The surface slip corrections are made by employing the Langmuir model, as well as the conventional Maxwell model. The effects of axial heat conduction are also investigated by extending the finite integral transform technique to the slip-flow case. We show that the Langmuir model always predicts a reduction in heat transfer with increasing rarefaction, as does the Maxwell model, except when the energy accommodation coefficient is relatively much smaller than that for momentum accommodation. This implies that, for most physical applications, the Reynolds analogy between heat transfer and momentum transfer is preserved in slip-flow regimes with low Mach numbers.

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Keywords: Extended Graetz problem; Temperature jump; Langmuir adsorption; Reynolds analogy; Microfluidics; Rarefied gas dynamics; Slip flow

# 1. Introduction

The study of non-linear transport in gas flows associated with micro and nanodevices [1,2] has emerged as an important topic in recent years. Understanding the fundamental physical phenomena [3–5] in such devices is essential in predicting their performance and searching for an optimal design. Several international theoretical and experimental research programmes are aiming to identify the main physical features of microscale gas flow and heat transfer [1,2,6]. The results of such fundamental work will be critical in answering questions about the usefulness of micro or nanodevices: can overall performance be improved by dividing a

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system into large numbers of microscale components? and can the traditional fluids knowledge base be applied in a scaled-down fashion to microfluidics?

In the field of microscale heat transfer, convective heat transfer in slip-flow regimes in simple geometries like channels and tubes is a key problem. Constant-wall-temperature convective heat transfer in microscale tubes and channels has been studied recently using analytical solutions to an extended Graetz problem [7–10] and DSMC simulations [10,11]. Using the fact that the characteristic speed in micro and nanodevices is usually very small (i.e. low Mach number), previous theoretical work has used the linear Navier–Stokes–Fourier equations (which rely on quasi local thermal equilibrium) to model flow and heat transfer phenomena. Accommodation coefficients of diffusive reflection were employed to describe the molecular interaction between the gas particles and solid surface atoms. The initial result in Ref. [7], based on the eigenvalues with velocity

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$A_2$	a coefficient depending on the exponent of the	X	a variable
=	inverse power potential in Eq. (4)	$\hat{z}$	axial coordinate
$\mathscr{A}_{jn}$	coefficients defined in Eq. (66)	Z	dimensionless axial coordinate $(\hat{z}\alpha(2-\alpha)/$
a	speed of sound		(RPe)
C	constant	$z^+$	dimensionless axial coordinate $(\hat{z}/(RPe))$
$C_{ m c}$	concentration of the complex		
$C_{ m m}$	concentration of the gas molecule	Greek	symbols
$C_n$	coefficients defined in Eq. (43)	α	fraction of surface covered at equilibrium
$C_{ m s}$	concentration of the site	$\sqrt{\alpha}$	slip radius
$c_p$	specific heat	β	a parameter in the Langmuir slip model
$\hat{D}_{ m e}$	potential parameter in the Langmuir slip model		$(K/(k_{\rm B}T))$
F	eigenfunctions	$ar{eta}$	a coefficient in the Langmuir slip model
$\mathscr{F}$	coefficients defined in Eq. (41)		$(1/(4\omega Kn))$
$_1F_1$	confluent hypergeometric function of the first	γ	specific heat ratio
	kind (Kummer function)	$\Gamma$	gamma function
h	heat transfer coefficient	$\Delta_n$	coefficients defined in Eq. (61)
K	equilibrium constant	$\theta$	dimensionless temperature $((T - T_w)/(T_0 - T_w))$
k	Chapman–Enskog thermal conductivity	$ ilde{ heta}$	a component of the dimensionless temperature
Kn	Knudsen number $(l/L)$		$(\theta(r,z) = \hat{\theta}(r,z) + \theta_0 \theta(0,z))$
$k_{\mathrm{B}}$	Boltzmann constant	$\theta_0$	downstream limit of the dimensionless tempera-
L	characteristic length $(2R)$		ture $(\theta_0=1-\alpha)$
l	mean free path	$\theta_{ m m}$	dimensionless bulk-average temperature
M	Mach number $(U/a)$	$oldsymbol{arTheta}_j$	transformed variables of the temperature $\hat{\theta}$
N	number of sites	$\lambda_n$	eigenvalue
N	coefficient defined in Eq. (42)	$\Lambda_n$	coefficients defined in Eqs. (57), (68) and (79)
m	molecular mass	$\mu$	Chapman–Enskog viscosity
$N_{\delta}$	composite number $(\mu U_{\text{ave}}/(pL))$	v	exponent of the inverse power laws
Nu	Nusselt number $(Lh/k)$	ho	density
Pe	Peclet number $(Re \cdot Pr)$	$ar{\sigma}$	ratio of energy accommodation to momentum
Pr	Prandtl number $(\mu c_p/k)$		accommodation $(\sigma_{\rm T}/\sigma_{\rm v})$
p	pressure	$\sigma_{ m v}$	a coefficient of momentum accommodation
R	pipe radius		$[(2-\phi_{\rm v})/\phi_{\rm v}]$
$R_n$	coefficients defined in Eq. (43)	$\sigma_{ m T}$	a coefficient of energy accommodation
Re	Reynolds number $(\rho U_{\text{ave}}(2R)/\mu)$	,	$[(2-\phi_T)/\phi_T \cdot 2\gamma/(\gamma+1) \cdot 1/Pr]$
$\hat{r}$	dimensional radial coordinate	$\phi_{ m v}$	momentum accommodation coefficient
r	dimensionless radial coordinate $(\sqrt{\alpha}\hat{r}/R)$	$\phi_{ m T}$	thermal accommodation coefficient
T	temperature	$\omega$	an accommodation coefficient in the Langmuir
$T_{\rm m}$	bulk-average temperature	63	slip model defined in Eq. (4)
$T_{\mathrm{w}}$	wall temperature	$\omega_0$	coefficient in the Langmuir slip model defined in
$T_0$	inlet temperature		Eq. (4)
U	gas velocity  gas flux average velocity $(U_1 - U_2 - v_1)/2$	Cark a =	ninta
$U_{ m ave}$	gas flux-average velocity ( $U_{\text{ave}} = U_{\text{max}}(2 - \alpha)/2$ ) gas maximum velocity (at the tube centerline)	Subsci	reference condition
$U_{\rm max}$	dimensionless gas velocity ( $U/U_{\text{max}}$ )	r n i	
и	unitensioniess gas velocity (U/Umax)	n,j	n, jth eigenvalue

slip only [12], indicated that heat transfer increases as the degree of rarefaction increases. This seemed doubtful, physically, as the famous experimental observations of Millikan [13] indicated that the drag coefficient decreases with increasing rarefaction. As a result, the so-called Reynolds analogy between heat transfer and momentum transfer was not preserved in this previous work [7]. At the same

time, a careful investigation [8] in which the temperature slip is taken into account revealed a more complicated picture: that heat transfer can increase or decrease with increasing rarefaction, depending on the ratio of energy accommodation to momentum accommodation. Even though this result is very instructive in its own right, a conceptual problem remains. The core result depends on the

ratio of two free parameters (the accommodation coefficients) which must be chosen by other means, for example, from experimental data.

Recently some new developments have been reported on modelling gaseous slip phenomena from the viewpoint of the gas-surface molecular interaction [14–18]. This may provide useful information which could help solve the aforementioned problem. An important result obtained from this work is that a physical slip model can be derived from Langmuir's theory of gaseous adsorption on solids (gas molecules can be adsorbed onto a surface owing to long range forces between the gas particles and the surface atoms). As a result, it has been shown that a physical meaning (heat adsorption) can be assigned to the accommodation coefficient in the Maxwell model; otherwise it is a free parameter to be determined by other means. It is therefore interesting to examine whether the Reynolds analogy is preserved in this Langmuir model.

The objective of our present work is to investigate microscale heat transfer where the gaseous slips at the solid surface, in particular the temperature jump, are the dominant phenomena. Slip corrections will be made by employing the new Langmuir model as well as the conventional Maxwell model. Our emphasis will be on the qualitative features of microscale heat transfer, for example, enhancement or reduction of heat transfer in microscale geometries. For the purpose of avoiding numerical uncertainty in these low-speed gas flows, we adopt an analytical solution approach and all our calculations are done with the help of a high-accuracy numerical program.

### 2. Temperature slip based on Langmuir adsorption

## 2.1. Langmuir's slip model

A physical approach to describing the slip can be developed by taking into account the interfacial interaction between the gas molecules and the surface molecules. In this approach the gas molecules are assumed to interact with the surface of the solid via a long range attractive force. Consequently the gas molecules can be adsorbed onto the surface, and then desorbed after some time lag. This mechanism of the deposition of a layer with a thickness of one or more molecules onto the surface is known as adsorption in the literature of surface chemistry [19,20]. If we model this interaction as a chemical reaction in which the gas molecule, m, and the site, s, form the complex, c, we may obtain an expression for the fraction of the surface covered by adsorbed atoms at thermal equilibrium,  $\alpha$ :

$$\alpha = (1 - \alpha)\beta p$$
 or  $\alpha = \frac{\beta p}{1 + \beta p}$ , where 
$$\beta = \frac{K}{k_{\rm B}T_{\rm w}} \quad \text{and} \quad K = \frac{C_{\rm c}}{C_{\rm m}C_{\rm s}}.$$
 (1)

The fraction  $\alpha$  is a function of the pressure, p, and the equilibrium constant, K, which are functions of the concentra-

tions  $C_{m,s,c}$ , and the surface temperature,  $T_w$ . As the pressure increases, its value approaches unity, implying that most of the molecules are at thermal equilibrium.

With information about the fraction of the surface covered at equilibrium determined by this Langmuir adsorption isotherm, it is possible to develop a slip model for the gas-surface molecular interaction. The velocity and temperature slip can be expressed, in dimensional form, as [14–16]

$$u = \alpha u_{\mathbf{w}} + (1 - \alpha)u_{\sigma}, \quad T = \alpha T_{\mathbf{w}} + (1 - \alpha)T_{\sigma}, \tag{2}$$

where subscript g denotes a local value adjacent to the wall, for example, a mean free path away from the wall, or a reference value such as the free-stream condition. The only parameter requiring further investigation is  $\beta$  (or the equilibrium constant K). A previous study [16] showed that the parameter  $\beta$  takes the form

$$\beta = \frac{1}{4\omega Kn} \frac{1}{p_r},\tag{3}$$

where

$$\omega = \omega_0(v) \left(\frac{T_{\rm w}}{T_{\rm r}}\right)^{1+2/(v-1)} \exp\left(-\frac{D_{\rm e}}{k_{\rm B}T_{\rm w}}\right),$$

$$\omega_0(v) = \frac{8\sqrt{2}}{5\pi} A_2(v) \Gamma\left[4 - \frac{2}{v-1}\right].$$
(4)

Then Eq. (1) reduces to (in dimensionless form),

$$\alpha = \frac{\bar{\beta}p}{1 + \bar{\beta}p}, \quad \text{where } \bar{\beta} = \frac{1}{4\omega Kn}.$$
 (5)

Tabulated values of  $A_2(v)$  and  $\omega_0(v)$  are given in Table 1 for exponents v > 2 [3,21]. The coefficient  $\omega_0$  has a value between 1.02806 (for v = 6) and 1.52001 (for v = 3) and becomes 1.44051 (for  $v \to \infty$ ) for rigid elastic sphere molecules. The role of the coefficient  $\omega$ , which is a function of v,  $T_{\rm w}$ , and  $D_{\rm e}$ , is very similar to the slip coefficient,  $\sigma$ , in the Maxwell model. For most molecular interaction models,

Table 1 Tabulated values of  $A_2(v)$  and  $\omega_0(v)$  for an inverse power-law molecular force

v	$A_2(v)$	$\omega_0(v)$
3	1.05519	1.52001
4	0.56081	1.12217
5	0.43619	1.04409
6	0.38401	1.02807
7	0.35675	1.03094
8	0.34066	1.04056
9	0.33040	1.05255
10	0.32352	1.06517
11	0.31873	1.07762
12	0.31530	1.08955
13	0.31282	1.10090
14	0.31099	1.11157
15	0.30964	1.12160
20	0.30674	1.16325
50	0.31113	1.27766
$\infty$	0.33333	1.44051

the value of the heat of adsorption,  $D_{\rm e}$ , falls within the range  $O(10^{-1}-10)$  kcal/mol. Its value may be inferred from theoretical predictions of intermolecular forces, or from experimental data.

A few comments should be added with regard to the characteristics of this slip model, and their implications. First, in the present model there are no terms related to high-order effects, such as thermal creep and viscous heat dissipation. This is in contrast to the common practice of including them in the original formulation but later ignoring them by assuming a low Mach number flow. The same spirit is taken in the development of our model, but it is implemented differently. The composite number,  $N_{\delta}$ , defined as the ratio of viscous forces to the hydrostatic pressure, is a parameter which indicates the degree of thermal non-equilibrium in macroscopic thermodynamic space. It can be shown that the nature of the constitutive equations in either the moment method [5] or the Chapman-Enskog method [3] depends primarily on this parameter. Consequently, the slip phenomenon consists largely of two components: one being the non-Newtonian effect in the bulk flow region measured by the composite number,  $N_{\delta}$ , and the other being the gassurface molecular interaction measured by the Knudsen number, Kn. The former is of purely hydrodynamic origin, and has nothing to do with the gas-surface molecular interaction. It is responsible for non-linear coupling effects, including the aforementioned high-order effects. Since  $N_{\delta} \approx Kn \cdot M$ , these non-linear effects are usually negligible for small Mach number, meaning that the linear Navier-Stokes-Fourier equations can still be valid in most lowspeed microscale gas flows. However, coupling between the normal and shear stresses may be non-negligible even when  $N_{\delta}$  is small, and this may produce a Knudsen-layer effect even at low speeds. While this remains to be investigated, in any case, it is of lesser importance than the slip effect due to the gas-surface molecular interaction and consequently it is ignored in our present study. Non-negligible Knudsen numbers in microscale gas flows require some kind of model capable of describing the slip phenomenon.

The second comment we make here is that, within this new framework, there is no distinction between momentum and energy accommodation: they are represented by a single parameter  $\alpha$  (0  $\leq \alpha \leq 1$ ), the fraction of the surface covered by adsorbed atoms at thermal equilibrium. This feature is in some sense equivalent to the case of equal momentum and energy accommodation in the Maxwell model. Since the ratio of momentum and energy accommodation plays a crucial role in determining the qualitative features of microscale heat transfer, enhancing or reducing heat transfer [7,8,10,22], this difference may have important implications. This will be discussed in detail in Section 3. However, when we consider the fact that the accommodation coefficients in the Maxwell model do not depend explicitly on the wall temperature, while the parameter  $\alpha$ in the Langmuir model is a function of the wall temperature, the difference is largely related to how one implements the wall temperature dependence. Therefore, it can be said that there is no prior theoretical justification in favor of one model or the other, except that the Langmuir model is simpler (involving only one parameter, instead of two in the case of the Maxwell model).

# 2.2. The extended Graetz problem

The low-speed microscale (creeping) regime, typical of gas flows in microsystems at atmospheric conditions, generally falls within the non-equilibrium parameter ranges

$$Kn = O(10^{-2} - 1), N_{\delta} = O(10^{-5} - 10^{-2}).$$

In this range of small values of  $N_{\delta}$ , the Newtonian (Navier–Stokes–Fourier) constitutive equations are assumed to be valid. On the other hand, non-negligible Knudsen numbers require a slip model for the gas-surface molecular interaction. If we consider monatomic gas flow and heat transfer in forced laminar flow through a circular tube with constant-wall temperature with the usual assumptions of the classical Graetz problem, i.e. fully developed flow, incompressible, constant-properties gas, and high Peclet number [23], the momentum and energy equations may be expressed as

$$\frac{1}{\hat{r}}\frac{\mathrm{d}}{\mathrm{d}\hat{r}}\left(\hat{r}\frac{\mathrm{d}U}{\mathrm{d}\hat{r}}\right) = C,\tag{6}$$

$$\rho c_p U \frac{\partial T}{\partial \hat{z}} = k \frac{1}{\hat{r}} \frac{\partial}{\partial \hat{r}} \left( \hat{r} \frac{\partial T}{\partial \hat{r}} \right), \tag{7}$$

with the Langmuir slip boundary conditions at the stationary wall

$$U(\hat{r} = R) = (1 - \alpha)U_{\text{max}},\tag{8}$$

$$T(\hat{r} = R, \hat{z}) = \alpha T_{w} + (1 - \alpha)T(\hat{r} = 0, \hat{z}), \tag{9}$$

where the non-equilibrium parameter  $\alpha$  is related to  $\bar{\beta}$  by the relation

$$\alpha = \frac{\bar{\beta}}{1 + \bar{\beta}} \tag{10}$$

and other boundary conditions of

$$\left[\frac{\partial U}{\partial \hat{r}}\right]_{\hat{r}=0} = 0,\tag{11}$$

$$\left[\frac{\partial T}{\partial \hat{r}}\right]_{\hat{r}=0} = 0,\tag{12}$$

$$T(\hat{r}, \hat{z} = 0) = T_0. \tag{13}$$

In the temperature jump boundary condition (9), a local temperature at the tube centerline  $T(\hat{r}=0,\hat{z})$  is used as the reference temperature  $T_g$  so as to take into account the axial variation of the gas temperature adjacent to the tube wall. This is in the same spirit as the Maxwell model, where such variation is included through the radial gradient of local temperature near the wall.

It is worth mentioning that our present model can be easily extended to treat flow in a microchannel with a minor change accounting for the different geometry [9,10].

assumption of equal momentum and energy accommodation coefficients  $\phi_{\rm v}=\phi_{\rm T}$ , or  $\bar{\sigma}=15/8$ , for  $\gamma=\frac{5}{3}$  and  $Pr=\frac{2}{3}$  is used here. This figure shows that heat transfer reduces with increasing rarefaction in both models, even though the level of reduction is slightly more pronounced in the Langmuir models. This finding coincides with the conclusion of Ref. [8] that a heat transfer reduction is predicted for  $\bar{\sigma}>1$  in slip flow. Note also from Fig. 3 that there exists an asymptotic value of the Nusselt number in both the Maxwell and Langmuir models. (In comparison,  $Nu\approx 3.657$  for the continuum case, 3.446 in the Maxwell model and 3.355 in the Langmuir model, for Kn=0.02.)

Fig. 4 shows the axial variation of temperature, measured at the centerline of the tube,  $\theta(r=0,z^+)$ , for Knudsen numbers (0.0,0.02). The eigenfunctions necessary for determining the temperature profile are obtained by summation of the first 60 terms in the infinite series of the Kummer function. It can be seen that, due to the jump at the wall, the level of temperature reduction along the tube centerline decreases with increasing rarefaction. Note also that the Maxwell model and the Langmuir model yield almost the same temperature profile, even though, due to the numerical error associated with the lowest order treatment of the term  $\frac{\theta_0}{1-\theta_0}\frac{\mathrm{d}\theta(r=0,z)}{\mathrm{d}z}$  in Eq. (26), the profile of the Langmuir model near the tube inlet (small  $z^+$ ) deviates from the Maxwell model.

Finally, from the results presented in Figs. 1–4 it can be concluded that both models predict that the Reynolds analogy is preserved in low speed slip flow. In our opinion, the case with  $\bar{\sigma} > 1$  is more relevant physically since a large difference in momentum and energy coefficients is extreme rather than typical in the Maxwell model. In addition, by recalling that the reduction of drag coefficient in slip flow is directly related to the decrease of the tangential velocity gradient near the wall due to the velocity slip, one can expect that the same mechanism associated with the temper-

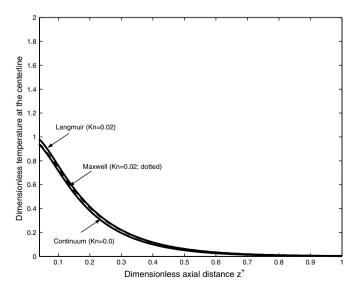


Fig. 4. Comparison of temperature variation at the centerline of the tube. (Langmuir and Maxwell models;  $Pe = 10.0, \gamma = \frac{5}{3}, Pr = \frac{2}{3}, \bar{\sigma} = 15/8$ ).

ature jump is responsible for the reduction of heat transfer in slip flow, implying the preservation of the Reynolds analogy in slip-flow regimes. An experimental validation study will be required to clarify this critical issue in the future.

#### 4. Conclusions

As a step towards answering a fundamental physical question in microscale heat transfer, convective heat transfer in a microtube in slip-flow regimes was investigated using a mathematical method extended from the classical Graetz problem. The slip corrections were made by employing a new Langmuir model based on the concept of adsorption of gases onto solids, as well as the conventional Maxwell model. The effects of axial heat conduction were included by extending a finite integral transform technique to the slip-flow case. We found that the Langmuir model always predicts the reduction of heat transfer with increasing gas rarefaction, and the Maxwell model predicts the same, except when the value of the energy accommodation is much smaller than that of the momentum accommodation. This implies that, for most physical applications, the Reynolds analogy between heat transfer and momentum transfer is preserved in slip-flow regimes with low Mach numbers.

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