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IDEAL GAS FLOWS THROUGH MICRO CHANNELS: REVISITED

F. DURST,[1] R. SAMBASIVAM,[2] and D.FILIMONOV[3]

FMP TECHNOLOGY GMBH, Germany, [1,3]
TATA Steel Limited Inc., India,[2]

f.durst@fmp-technology.com, rsambasivam@yahoo.com; d.filimonov@fmp-technology.com

Abstract

Over the last few years, the authors have carried out extensive work in the field of micro-channel flows using the extended Navier-Stokes equations, taking the diffusive mass transport into account. Through this previous work, a detailed insight into the physics of micro-channel flows was obtained. This insight was utilized in the authors' most recent work to provide the basis for analytical treatments of micro- channel flows. The work is summarized in this paper and the results are presented. These are compared with experimental results available in the literature. Finally, the authors suggest the utilization of their analytical results as a basis for further experimental studies. The results of the present work can be taken as the basis of detailed experimental and numerical investigations of micro-channel flows.

Keywords: Navier-Stokes-Equations, Micro-Channel, Analytical Solution, Diffusion Transport

INTRODUCTION AND AIM OF WORK

Micro-channel flows are nowadays treated by the assumptions that Maxwell slip velocities occur at the channel walls. The literature regarding theoretical treatments of these kinds of flows, by using the mentioned slip velocities, is diverse and a good summary of the work can be found in the book by[5]. This book also refers to the literature on the experimental and theoretical findings in this special field of fluid mechanics. It can be observed from the literature that in gaseous flows through micro-channels and micro-capillaries, under some conditions[1–3,6,7] the measured mass flow rates can be higher than those obtained from the classical theory, i.e. by solving the Navier-Stokes equations, with no-slip boundary condi- tions at the wall, for the same given inlet and outlet pressure conditions. This increase in mass flow rate is one of the many strange phenomena which have puzzled fluid flow re- searchers active in micro-channel flows. In order to bridge the gap between the experimental results and the theoretical predictions, first- or second-order Maxwellian slip velocity models have been introduced at the walls as boundary conditions.

In recent publications of the lead author and his collaborators, the physical assumptions of the Maxwell type of slip velocities at the walls of micro-channel flows were questioned and it was argued that the difference between experimentally and theoretically obtained results of flow rates occurred due to imperfections in the Navier-Stokes equations. It was claimed that these equations were strictly valid only for flow fields that did not contain strong gradients of density and temperature or strong temperature and pressure gradients. For this reason, the extended Navier-Stokes equations were derived, taking thermodynamic fluid property gradients into account and their related mass, momentum and heat transport properties caused by diffusion. The resultant equations for mass diffusion are summarized in Appendix A of this work, as they are needed in this paper. It is shown there that the Navier-Stokes equations should be written in terms of total velocity, made up of the convective velocity and the diffusive velocity terms.

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Some recent papers (e.g.[8,9]) have reported studies of micro-channel flows on the basis of the extended Navier-Stokes equations. Although these treatments demonstrated the ad- vantages of the extended basic fluid mechanics equations, the analytical handling of the flow equations still showed features of the conventional way of treating micro-channel flows. Numerical treatments of micro-channel flows using the extended Navier-Stokes equations have also been carried out and the results were published in a recent summary paper[10] where it was shown that the numerical computations required no assumption regarding the wall slip velocity.

The satisfactory agreement obtained by[10] by using numerical treatments of micro-channel flows, can be taken as solid proof that the extended Navier-Stokes equations need to be ap- plied to theoretical treatments of micro-channel flows. This suggests that it is the additional mass flow driven by the pressure gradient in micro-conduits which yields the additional mass flow rate that leads to the difference between experimental and theoretical findings.

The above summary of the existing theoretical work indicates that currently there is no analytical treatment available for micro-channel flows that shows good agreement with ex- perimental results. To remedy this situation, the present authors have carried out analytical studies of micro-channel flows based on the extended Navier-Stokes equations, including the mass diffusion term, given in Appendix A.

From these extended equations, in a manner described in many text books, the following equations are derived for two-dimensional and fully developed flow situations in micro-channels and micro-capillaries:

$$0 = -\frac{\mathrm{d}P}{\mathrm{d}x} + \mu\frac{\mathrm{d}^2 U^T}{\mathrm{d}y^2}\,, \tag{1}$$

where x and y are the components of rectangular coordinates, U^T is the total fluid velocity in the x-direction and P is the pressure. This equation can be split up into two sets of equations that yield the convective and the diffusive parts of the velocity profile. It is the same pressure gradient in the channel flows that drives the convective velocity and the diffusive velocity. Taking this into account, a complete analytical treatment of micro-channel flows is possible. This treatment is presented in this paper, providing theoretical results on the convective and diffusive mass flow rates. Relationships for the ratios of pressures and mass flow rates are given and final normalized results are plotted, which the fluid flow physics for micro-conduits must follow.

It is shown that the presented analytical treatments yield very good agreements with ex- isting corresponding experimental results. The present analytical treatments are also taken a proof that the extended Navier-Stokes equations, as presented by[10] , allow flows to be treated that are dominated by diffusion. The classical Navier-Stokes equations do not allow correct treatment of diffusion-dominated flows.

In the final section, the authors suggest basing the layout of the experimental test rigs for studies of micro-channel flows on the analytically derived results. Strong ”micro-channel effects” are obtained if the pressure at the outlet of the channel is taken to lie below the √ characteristic pressure Pc = µ3RT /h, where µ is the viscosity of the fluid, T is the temperature, R is the gas constant and h is the half-height of the parallel plate micro-channel.

SELF-DIFFUSION IN IDEAL GAS FLOWS

In recent paper, (10) have published numerical results for micro-channel and micro-capillary flows based on the full set of the extended Navier-Stokes equations. The extended Navier- Stokes equations can be written, for example, in rectangular coordinates as follows:

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$$\frac{\partial \rho}{\partial t} + \frac{\partial (\rho U_i^T)}{\partial x_i} = 0, \tag{2}$$

$$\rho \left(\frac{\partial U_j^T}{\partial t} + U_i^T \frac{\partial U_j^T}{\partial x_i} \right) = -\frac{\partial P}{\partial x_j} - \frac{\partial \tau_{ij}^T}{\partial x_i} + \rho g_j \tag{3}$$

containing the following term:

$$\tau_{ij}^T = -\mu \left(\frac{\partial U_j^T}{\partial x_i} \right) + \frac{2}{3} \delta_{ij} \mu \frac{\partial U_k^T}{dx_k}$$

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where ρ is the density of the fluid, t is the time, δ_{ij} is the Kronecker delta and U_i^T is the total velocity in the x_i -, x_j -, x_k -direction, respectively. These equations contain the total velocity $U^T_{i,j,k}$ rather than the convective velocity in all corresponding terms as

$$U_i^T = U_i^C + U_i^D \tag{5}$$

where U_i^C is the convective velocity and U_i^D is the diffusive velocity. The authors claimed in their recent paper (see[10]) that the usually employed Navier-Stokes equations are valid only when the diffusive local mass flux is zero. In that case, the continuity and the Navier-Stokes equations contain the same terms as equations (2) - (4), but they contain the convective velocity rather than the total velocity.

Solving numerically the extended Navier-Stokes equations for micro-channel flows,[10] obtained very good agreement with the experimental findings of[2] . This encouraged the research carried out as the basis of the present paper, aimed at analytical solutions for fully developed micro-channel and micro-capillary flows. When self-diffusion in ideal gas flows occurs, density and temperature gradients yield local diffusive mass fluxes expressed as

$$M_i^D = \rho U_i^D = -\rho D \left(\frac{1}{\rho}\frac{\partial \rho}{\partial x_i} + \frac{1}{2T}\frac{\partial T}{\partial x_i} \right), \tag{6}$$

where D is the coefficient of mass diffusion and

$$(M_i^D)^F = -D\frac{\partial \rho}{\partial x_i} = \text{Fick's diffusion term,} \tag{7}$$

$$(M_i^D)^S = -\frac{\rho D}{2T}\frac{\partial T}{\partial x_i} = \text{Soret's diffusion term.} \tag{8}$$

Both of these mass fluxes are those for self-diffusion in ideal gases, driven by density and temperature gradients. Considering the ideal gas equation $P = \rho RT$, we obtain

$$\frac{1}{P}\frac{\partial P}{\partial x_i} = \frac{1}{\rho}\frac{\partial \rho}{\partial x_i} + \frac{1}{T}\frac{\partial T}{\partial x_i}. \tag{9}$$

Replacing the density term in equation (6) by the term in equation (9) yields

$$M_i^D \quad \left(\frac{1}{P}\frac{\partial P}{} \quad \frac{1}{}\frac{\partial T}{} \right)$$

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$$i \quad = -\rho D \quad P\, \partial x_i \ - \ 2T\, \partial x_i \qquad (10)$$

Hence the local mass flux for self-diffusion can also be expressed in terms of pressure and temperature gradients. For isothermal flows through micro-channels and micro-capillaries, the local diffusive mass flux is driven by a pressure gradient and can be written as follows,
since $\rho D = \mu$:

$$\rho U_1^D = -\frac{\mu \, \mathrm{d}P}{P \, \mathrm{d}x_1}. \qquad (11)$$

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For micro-channel flows, the imposed pressure gradient in the x_1-direction also results in a convective part of the flow, for which the following differential equation holds:

$$\frac{1}{\rho}\frac{\mathrm{d}P}{\mathrm{d}x_1} = \frac{\mu}{\rho}\frac{\mathrm{d}^2 U_1^C}{\mathrm{d}^2 x_2}. \tag{12}$$

The flow given by equation (12) is usually considered when plane channel flows are treated theoretically. The diffusive mass flux, expressed by equation (11), is neglected since it is small for Reynolds numbers $Re > 1$. For micro-channel flows, the diffusive mass flux needs to be taken into account, since it is not negligible.

THEORETICAL SOLUTION AND RESULTS FOR MICRO-CHANNEL FLOWS

To obtain an analytical solution for fully developed micro-channel flows, one can solve equa- tion (1), expressed in rectangular coordinates, with the boundary condition from equa- tion (11) at the wall as

$$\rho U = -\frac{\mu}{P}\frac{dP}{dx} \quad \text{at } y = \mp h. \tag{13}$$

Then the analytical solution in a micro-channel can be written as

$$\rho U = -\frac{\rho}{2\mu}(h^2 - y^2)\frac{dP}{dx} - \frac{\mu}{P}\frac{dP}{dx}. \tag{14}$$

It should be noted that the second term on the right-hand side arises from the diffusion influence, and the diffusive part of the mass flow rate will only make strong contributions to the velocity for low pressures P.

From equation (14), one can derive the relation between the total mass flow rate M^T, the diffusive mass flow rate M^D and the pressure. Therefore, one can derive the relation for the total mass flow rate by integrating equation (14), first in the cross-flow and second in the flow direction, yielding

$$M^T = w\int_{-h}^{h}(\rho U)dy = -w\int_{-h}^{h}\left\{\frac{\rho}{2\mu}(h^2 - y^2)\frac{dP}{dx} + \frac{\mu}{P}\frac{dP}{dx}\right\}dy$$

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$$= -2hw\left(\frac{h^2 P}{3\mu RT} + \frac{\mu}{P}\right)\frac{dP}{dx} \qquad (15)$$

where w is a width of the micro-channel. Integrating equation (15) from the inlet $(x = 0)$ to the outlet $(x = L)$, one can obtain

$$M^T = \frac{h^3 w P_{out}^2}{3\mu LRT}\left\{\left(\frac{P_{in}}{P_{out}}\right)^2 - 1\right\} + \frac{2\mu hw}{L}\ln\left(\frac{P_{in}}{P_{out}}\right). \qquad (16)$$

Therefore, the total mass flow rate M^T can be expressed as a function of the pressure ratio P_{in}/P_{out}.

Furthermore, one can proceed to obtain a universal relationship between the total mass flow rate and pressure. Therefore, equation (15) can be rewritten as

$$M^T = -2hw\frac{\mu}{P}\frac{dP}{dx}\left(\frac{h^2 P^2}{3\mu^2 RT} + 1\right). \qquad (17)$$

Since the pressure P is constant in the y-direction, the diffusive mass flow rate M^D can be expressed by integrating equation (13) over a cross-sectional area to obtain

$$M^D = -2hw\frac{\mu}{P}\frac{dP}{dx}. \qquad (18)$$

Substituting equation (18) into equation (17) yields

$$\frac{M^D}{M^T} = \frac{1}{\frac{h^2 P^2}{3\mu^2 RT} + 1}. \qquad (19)$$

Defining the characteristic pressure as $P_c = \mu\sqrt{3RT}/h$, one can rewrite equation (19) as follows:

$$\frac{M^D}{M^T} = \frac{1}{\left(\frac{P}{P_c}\right)^2 + 1}. \qquad (20)$$

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$$P_C \;) \;+$$
$$1$$

The above final equation is a universal relation between the local mass flow rate and the normalized local pressure.

Utilizing the above equations, one can calculate the total mass flow rates of a helium gas flow in a micro-channel with boundary conditions corresponding to the experiments of[2], which are tabulated in Table I. The total mass flow rates M^T for the outlet pressure P_{out}

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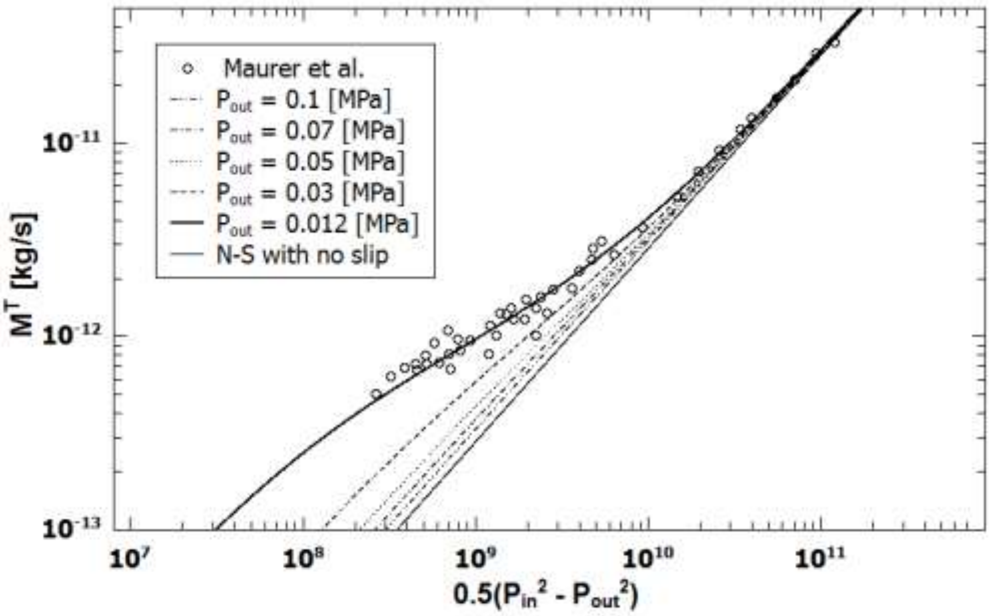

FIG. 1: THE TOTAL MASS FLOW RATE AS A FUNCTION OF THE DIFFERENCE OF SQUARES OF PRESSURE AT THE INLET AND OUTLET TOGETHER WITH EXPERIMENTAL DATA OF[2].

changing from 0.012 to 0.1 MPa are shown in Figure 1 together with experimental results of[2], where the abscissa is expressed as $0.5(P^2_{in} - P^2_{out})$ according to the notation of[2]. Figure 1 shows that the choice of the outlet pressure conditions is relevant to obtain the typical micro-channel effects on the gas flow. It can be seen that, as the outlet pressure is de- creased, the deviation of the total mass flow rate, obtained from the extended Navier-Stokes equations, increases with respect to the convective mass flow rate obtained from the com- pressible Navier-Stokes equations with no-slip boundary conditions. The total mass flow rate, especially for $P_{out} = 0.012$ MPa, shows considerable deviations from predictions based on the Navier-Stokes equations with no-slip conditions. The present analytical result of $P_{out} = 0.012$ MPa shows good agreement with the experimental results of[2] and the ana- lytically deduced solution follows the micro-channel effect that occurred in the experiment. This finding is good proof that the order of magnitude estimate, carried out in this study, yields the equation which describes physically well the flow in micro-channels.

Utilizing the derived analytical solutions, one can understand why the deviation between the mass flow rates obtained from the extended Navier-Stokes equations and the classical theory decreases as $(P^2_{in} - P^2_{out})$ is increased. This means that the increase in the pressure ratio P_{in}/P_{out} reduces the deviation between the mass flow rates. This behavior can be explained

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TABLE I: EXPERIMENTAL CONDITIONS OF[2] AND[3].

Experimental Parameters	2	3
Gas used	He	He
Temperature [K]	293	314
Outlet pressure P_{out} [MPa]	0.012 ~ 0.1	0.1
Dynamic viscosity [10^{-5} Pa · s]	1.99	2.066
Gas constant [J/kg·K]	2077	2077
Height h [μm]	0.57	0.665
Width w [μm]	200	52.25
Length L [μm]	10000	7500
Characteristic pressure P_c [MPa]	0.0477	0.0435

by equation (16). Namely, a significant deviation from the classical theory appears at lower pressure ratios for a given outlet pressure P_{out} , because the diffusion effect is proportional to the term $\ln(P_{in}/P_{out})$ and the order of this term is comparable to that of $(P_{in}/P_{out})^2$ only for smaller pressure ratios. This implies that the diffusion is effective for the micro-channel flow only if the pressure range P is absolutely small and the pressure ratio (P_{in}/P_{out}) between the inlet and outlet is also small.

In addition, the authors calculated the mass flow rates for the different pressure conditions corresponding to[3] and[4] given in Tables I and II. These comparisons of the analytical results with the experimental data are shown in Figures 2 and 3, where the abscissa is expressed as the pressure ratio. The results obtained from the extended Navier-Stokes equations (ENSE) are shown by solid lines and those given by the classical compressible Navier-Stokes equations (CNSE) with no-slip boundary conditions by dashed lines. It can be seen that the diffusion effects are present but they are small. This is mainly because the pressures in the experiments of[3] and[4] were larger and, therefore, did not show the micro-channel effect. In order to explain why the diffusion effect is small, the relation between the mass flow rate and the characteristic pressure defined by equation (20) is shown in Figure 4. One can see that the diffusive mass flow rate reaches 50% of the total mass flow rate for $P/P_c = 1$. This means that the convective and the diffusive mass flow rates are of the same order in the total mass flow rate. The characteristic pressure ratio P/P_c follows the order $P_{in}/P_c > P/P_c > P_{out}/P_c$.

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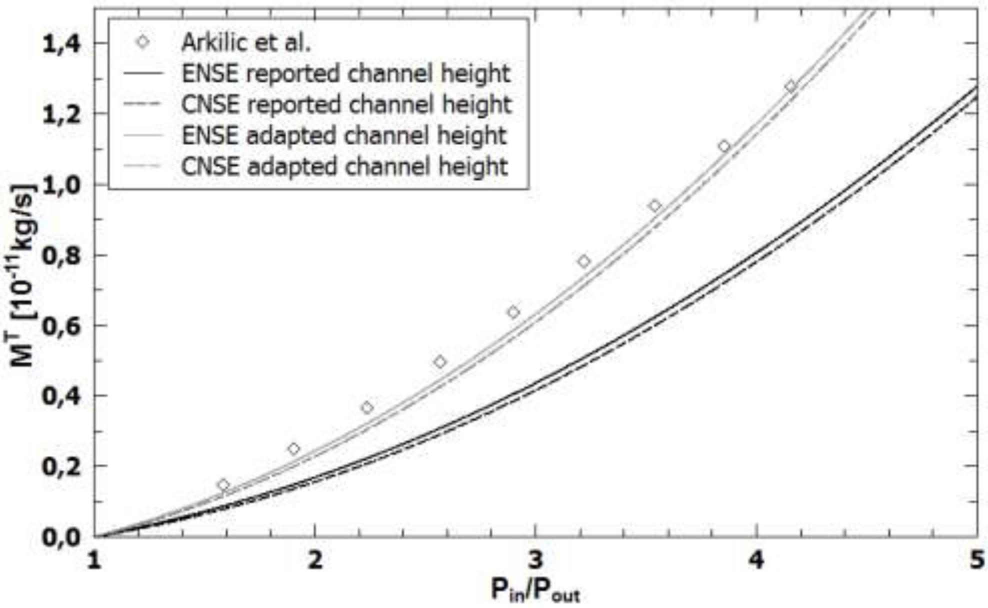

FIG. 2: *COMPARISON OF THE TOTAL MASS FLOW RATE AS A FUNCTION OF THE PRESSURE RATIO WITH EXPERIMENTAL DATA OF[3] FOR SOLUTIONS OF THE CLASSICAL (CNSE) AND THE EXTENDED (ENSE) NAVIER-STOKES EQUATIONS USING THE REPORTED AND ADAPTED (10 % HIGHER) CHANNEL HEIGHTS.*

With decrease in the pressure from Pin to Pout , the diffusive effect starts to increase in importance, since the characteristic pressure ratio P/P_C is decreased. If the inlet and outlet pressures are chosen to lie close to the characteristic pressure, the total mass flow rate increases due to the strong effect of the self-diffusion, and this yields the considerable deviation from the predictions based on the classical Navier-Stokes equations.

Figure 4 includes the pressure ranges of the experimental data of[2] ,[3] and[4]. As previously mentioned, the strong diffusion effect was obtained analytically for the experimental condi- tions of[2] . Their strong "micro-channel effects" can now be explained with the help of the characteristic pressure, since the pressure ratios are small and the pressure range is close to the characteristic pressure P_C of the experimental setup. On the other hand, for the experimental conditions of[3] and[4], the chosen pressures in the experiments are larger com- pared with their characteristic pressures. Therefore, only small diffusion effects are present. Knowing that the diffusive effect is significant for low pressures (or for high temperatures), the outlet pressure at the exit of the micro-channel should be taken as very small to show experimentally the typical "micro-channel effect" at room temperature.

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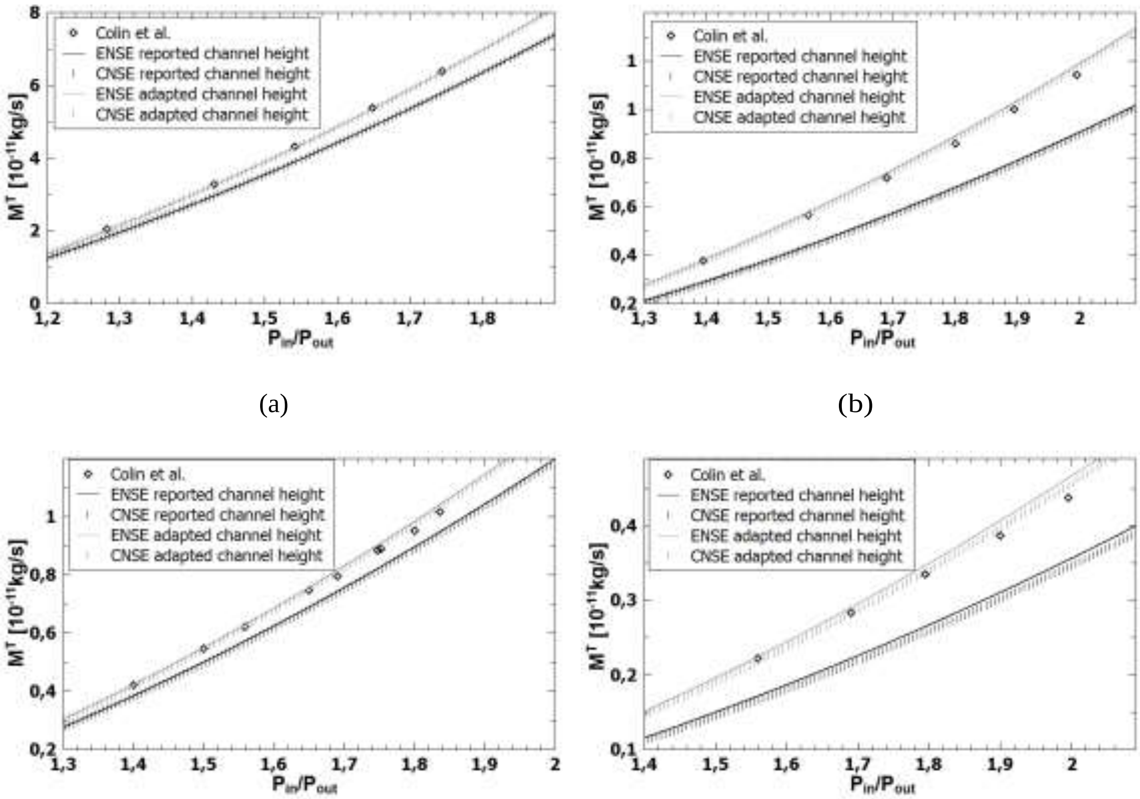

(a) (b)

(c) (d)

FIG. 3: *COMPARISON OF THE TOTAL MASS FLOW RATE AS A FUNCTION OF THE PRESSURE RATIO WITH EXPERIMENTAL DATA OF*[4] *FOR SOLUTION OF THE CLASSICAL (CNSE) AND THE EXTENDED (ENSE) NAVIER-STOKES EQUATIONS USING THE REPORTED AND ADAPTED (3 - 10 % HIGHER) CHANNEL THICKNESSES. THE DETAILS OF EACH CASE ARE REPORTED IN TABLE II.*

TABLE II: *EXPERIMENTAL PARAMETERS OF*[4]

Experimental Parameters	a	b	c	d
Gas used	N	N	He	He
Temperature [K]	294.2	294.2	294.2	294.2
Outlet pressure [10^5 Pa]	2	0.65	1.9	1.026
μ [10^{-6} Pa·s]	19.0	19.0	17.5	17.5
Gas constant [J/kg·K]	296.9	296.9	2077	2077
Channel length [μm]	5000	5000	5000	5000
Channel width [μm]	21.2	21.2	21.2	21.2
Reported h [μm]	1.88	1.88	1.88	1.88
Adapted h [μm]	1.94	2.06	1.94	2.06

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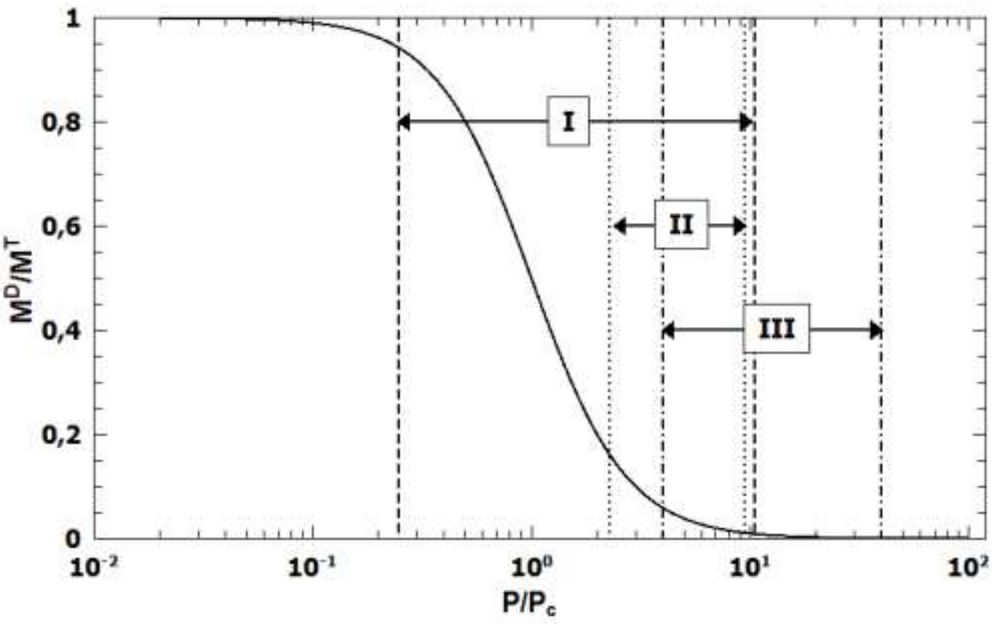

FIG. 4: *RATIO OF THE DIFFUSIVE MASS FLOW RATE TO THE TOTAL MASS FLOW RATE VS. RATIO OF THE PRESSURE TO THE CHARACTERISTIC PRESSURE WITH RANGES OF THE EXPERIMENTAL DATA OF (I)*[2], *(II)*[3] *AND (III)*[4] .

Although the choice of the pressure range for the experiments has been shown to be the reason why the diffusion effect is small under the conditions of[3]] and[4], a considerable dis- crepancy between the present analytical predictions and the corresponding experimental results still exists. The discrepancy can be attributed either to incorrect pressure distribu- tions or to the measurement errors of the flow rate in the mentioned experiments. As shown previously, the experiments conducted by[3] and[4] lay in the convection-dominated region, i.e. in the pressure region where the diffusion effect is small.

Therefore, the main reason for the discrepancy may be measurement errors during their experiments.[4] reported an uncertainty of about 10% for the measurement of the channel height. Such an uncertainty of the mea- surement of the channel height can cause the discrepancy between the experimental data and theoretical prediction . In order to examine the possibility of the uncertainty effect on the discrepancy between the present analytical solution and the corresponding experimental results, we attempted to calculate the mass flow rate for the slightly different conditions of the experiments of[3] and[4]]. Using a 10% greater channel height to calculate the total mass flow rates in case of[3] and a 3 - 10% greater channel height in the four cases of[4] (see Table II), one can obtain very good agreement between the present analytical results and the mentioned experimental data, as shown in Figures 2 and 3. The adapted channel height for each case of[4] is also reported in Table II.

It is obvious from the above suggested corrections of the channel height that small property changes are affecting the total mass flow rate through the channel and bring the theoretical results closer to the experiments. The above suggested corrections yield different channel heights for the different gases, although the same channel was employed for properties to be that of an ideal gas need to be questioned. Up to the conference, the authors will investi- gate deviations of the thermal capacitance c_p will affect the mass transfer rates through the channel. It has been shown by[E.H. Kennard] that for self-diffusion, the appropriate diffusion coefficient can vary between 1.2 d and 1.4 for 3d, depending on the type of molecule one assumes for the various gases. Choosing $d = \mu/\rho$

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is likely to be the cause of the gas influ- ence on the discrepancies between the experimental results. The authors will investigate this further and will report at the conference about their findings.

Concluding this section, we point out that the measurement accuracy can be seen as one of the prime factors of the discrepancy between the present analytical results and the experimental data. It should be noted that there was no difference in the experimental conditions of[3] and[4] between the mass flow rates obtained by the extended Navier-Stokes equations (ENSE) and the classical Navier-Stokes equations (CNSE) with no-slip conditions, because the pressures chosen in their experiments were in the convection-dominated range. To measure typical ”micro-channel effects”, the pressure range of experiments should be chosen to lie close to the characteristic pressure of the experimental setup and the chosen fluid.

CONCLUSIONS, FINAL REMARKS AND OUTLOOK

In recent years, the present authors have carried out extensive work in the field of micro- conduit flows using the extended Navier-Stokes equations, taking the diffusive mass transport into account. Applying the extended equations, a detailed insight into the physics of micro- channel flows was obtained.The present paper summarizes their numerical investigations and validates their results by comparison of the numerical prediction with the experimental data available in the literature.

The full set of the extended Navier-Stokes equations, which was used for numerical simu- lations, can be reduced by applying order of magnitude considerations for different terms. A set of equations results that can be solved analytically, as is shown here together with analytical results for micro-channel flows. The analytical solutions are also compared with experimental results from the literature, showing good agreement.

Using the extended Navier-Stokes equations, the authors can explain the physics behind the typical ”micro-channel effects”. It is shown that for certain experimental conditions the diffusive effects in the micro-conduit flows become significant and the total mass flow rate shows considerable deviations from the classical theory. This is also found to be the reason for the ”Knudsen paradox”, which describes the relation between the conductance of the micro-channel and the average Knudsen number.

A characteristic pressure for micro-channel and micro-capillary flows has been introduced. At such a characteristic pressure, the flow in a micro-conduit starts to behave differently, namely, for pressure values less than the characteristic pressure the flow is dominated by diffusion. If the local pressure is higher than the characteristic pressure, the flow is dom- inated by convection. As already mentioned, the diffusive mass flow causes the difference between the classical and the extended Navier-Stokes equations and is also the reason for the deviations of the experimental results from predictions of the classical theory. To show the typical ”micro-conduit effect” in experiments, the inlet and outlet pressures should be chosen to lie close to the characteristic pressure of th experimental setup.

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DIFFUSIVE MASS TRANSPORT EQUATIONS

When considerations of kinetic gas theory are applied, the molecular transport of mass can be given as $M^+_x = \rho\overline{U}_x/6$ in the positive x-direction and $M^-_x = -\rho\overline{U}_x/6$ in the negative x-direction, yielding a diffusive mean mass flux $M^D = 0$ if no spatial density and temperature gradients exist in a flow. In the presence of thermodynamic property gradients of the fluid, a net diffusive mass flux results that can be expressed as

$$M^D_i = \frac{1}{6}\left[\rho(x_i - \lambda)\overline{U}_i(x_i - \lambda) - \rho(x_i + \lambda)\overline{U}_i(x_i + \lambda)\right], \tag{21}$$

where $\overline{U}_i$ is the molecular mean velocity in the i-direction, which can be given as

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$$\overline{U}_i = \overline{U}_M = \sqrt{\frac{8kT}{\pi m_M}}, \tag{22}$$

where T is the temperature, k is the Boltzmann constant, m_M is the molecular mass and λ is the molecular mean free path of a considered ideal gas. The conditions for M_i^D to exist are sketched in Figure 5.

Series expansions of the ρ and $\overline{U}_i$ terms in the square brackets of equation (21) yield, after truncation of the series after the linear terms,

$$M_i^D = \frac{1}{6}\left[\left(\rho(x_i) + \frac{\partial \rho}{\partial x_i}(-\lambda)\right)\left(\overline{U}_i(x_i) + \frac{\partial \overline{U}_i}{\partial x_i}(-\lambda)\right) - \left(\rho(x_i) + \frac{\partial \rho}{\partial x_i}(-\lambda)\right)\left(\overline{U}_i(x_i) + \frac{\partial \overline{U}_i}{\partial x_i}(-\lambda)\right)\right]. \tag{23}$$

This equation can be rewritten to yield for the diffusive mass transport in the x_i-direction if only those product terms are considered that contain first-order derivatives, also considering the isotropy of the molecular motion yielding $\overline{U}_i(x_i) = \overline{U}_M$:

$$M_i^D = -\frac{1}{3}\lambda\left[\overline{U}_M \frac{\partial \rho}{\partial x_i} + \rho \frac{\partial \overline{U}_M}{\partial x_i}\right]. \tag{24}$$

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Taking into account that the diffusion coefficient D can be written as $D = -1/3(\lambda \overline{U}_M)$

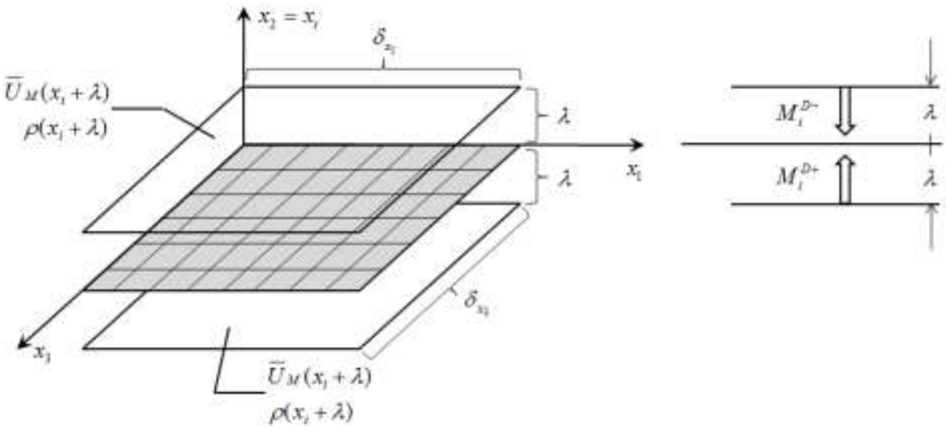

FIG. 5: *MASS TRANSPORT DUE TO DENSITY AND TEMPERATURE GRADIENTS IN A FLUID FLOW.*

results in

$$M_i^D = -D\left[\frac{\partial \rho}{\partial x_i} + \frac{\rho}{\overline{U}_M}\frac{\partial \overline{U}_M}{\partial x_i}\right]. \tag{25}$$

Taking $\mu = D\rho$ into account yields

$$M_i^D = -D\left[\frac{\partial \rho}{\partial x_i} + \frac{\rho}{2T}\frac{\partial T}{\partial x_i}\right] = -\underbrace{D\rho}_{\mu}\left[\frac{1}{\rho}\frac{\partial \rho}{\partial x_i} + \frac{1}{2T}\frac{\partial T}{\partial x_i}\right] \tag{26}$$

Hence diffusive transports of mass are driven by local density and temperature gradients.

Assuming a local thermodynamic equilibrium to exist, the ideal gas law can be employed to derive for the term in equation (26) containing the density

$$P = \rho R T \quad \rightarrow \quad \frac{1}{\rho}\frac{\partial \rho}{\partial x_i} = \frac{1}{P}\frac{\partial P}{\partial x_i} - \frac{1}{T}\frac{\partial T}{\partial x_i}. \tag{27}$$

Hence equation (26) can be rewritten as

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$$M_i^D = -(D\rho)\left[\frac{1}{P}\frac{\partial P}{\partial x_i} - \frac{1}{2T}\frac{\partial T}{\partial x_i}\right] = -\mu\left[\frac{1}{P}\frac{\partial P}{\partial x_i} - \frac{1}{2T}\frac{\partial T}{\partial x_i}\right] \tag{28}$$

The results of the above derivations are well known. They yield in equation (26)

$$M_i^F = -D\frac{\partial \rho}{\partial x_i} \quad \text{Fick's mass diffusion term,} \tag{29}$$

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$$M_i^F = -\frac{(D\rho)}{2T}\frac{\partial T}{\partial x_i} \quad \text{Soret's mass diffusion term,} \tag{30}$$

where $D^S = -\mu/2T$ is the Soret diffusion coefficient.

The terms in equations (29) and (30) are not taken into account in most research work when fluid flows with heat and mass transport are computed numerically, i.e. they are neglected as being small with respect to the convective mass transport terms.