Thermal creep continuum modeling

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Abstract. A thermal creep process is studied in quite wide rectangular micro channels. The inlet and outlet reservoirs are maintained at the same constant pressure. A constant temperature gradient exists along the walls of the channel joining the two tanks. Thus a gas flow is induced and thermally sustained until steady conditions are reached. A complete analytical solution is derived in slip regime, yielding all the flow parameters, for Knudsen numbers smaller than 0.25. The analytical results are in good agreement with the numerical "exact" solution of the continuum equation system. Furthermore our continuum approach data are compared to those deduced from approaches based on Boltzmann equation model treatments: these various methods lead generally to a satisfactory agreement between their respective mean parameters. Nevertheless significant differences appear on the transversal velocity profiles and are further discussed.

Keywords: micro fluidics, thermal creep, analytical solution, numerical simulation
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INTRODUCTION

The objective of this study is to deepen the fundamental understanding of the emerging field of microfluidic gas flows, especially in channels where tangential temperature gradients exist on the solid surfaces. It is possible to generate rarefied gas flows by means of tangential temperature gradients along the channel walls: then the fluid starts creeping from the cold towards the hot regions. Since, O.Reynolds introduces in 1879 the term "thermal transpiration", many authors have analyzed thermal creep flows by using kinetic models (BGK [1] and S-model [2]) or by solving the linearized Boltzmann equation [3]. The gas velocity and the heat flow profiles and the mass fluxes have so been numerically obtained over a large Knudsen number range. Velocity and temperature profiles have also been derived from the Navier-Stokes equations, assuming small compressible effects [4].

In this article we analyze the thermal creep phenomenon in rectangular micro channels for a fully compressible gas. We suppose that the temperature of the walls varies as a function of the *x*-streamwise direction and that the pressures in the tanks, located at the channel entry and exit sections, are maintained equal: thus we focus our interest on the stationary flows in slip regime. Then we estimate the magnitude of the non-dimensional macroscopic parameters and those of the non-dimensional gradients by using simplified thermal and dynamic streamwise balances. Thus the analytical expressions of temperature, velocity and pressure distributions are derived from the full compressible Navier-Stokes equations by applying a perturbation method according to the small aspect ratio of the channel. Analytical expressions are also obtained for the mass flow rate driven by the temperature gradient as well as for the corresponding heat fluxes.

Numerical calculations are carried out for different micro channels sizes, wall temperature gradients, pressures and gases. The Knudsen numbers, calculated at the exit of the channel and based on the channel heights, vary from 0.01 to 0.25. The comparisons between the analytical and numerical solutions confirm the validity of the analytical approach. A comparison with the results obtained by other authors applying the kinetic model equations is proposed.

EQUATION SYSTEM AND BOUNDARY CONDITIONS

Equation system. We consider the flow in rectangular micro channels connecting two reservoirs maintained by the same pressure. The temperature in the inlet and outlet reservoir is equal to T_{in} and to T_{out} respectively. We suppose that the temperature of the walls varies as a linear function of the *x*-streamwise direction from $T_{w_{in}}$ to $T_{w_{out}}$. Under these conditions the gas begins to flow from the cold to the hot tank. This is called the thermal creep effect. In this study we analyze this thermal creep phenomenon in channels where the value of the height H is bigger than that of the mean free path and much smaller than that of the channel length or width w, which means that it is possible to consider this configuration as two infinite parallel plates. According to the geometry the physical parameters depend only on the (x,y) spatial coordinates.

Then, the Navier-Stokes (NS) equations are used to describe the stationary flows supplemented with the gas state equation involving the specific gas constant $\mathscr{R}$. Finally the viscosity is treated within the variable hard sphere (VHS) model [5].

Boundary conditions. The boundary conditions for the NS equation system are the symmetry conditions on the axis and the slip velocity and the temperature jump conditions on the solid wall. Considering Knudsen number first order conditions only, the complete slip boundary condition on the upper solid wall reads [6]

$$u_s = -\sigma_p \frac{\mu}{p} v_m \left(\frac{\partial u}{\partial y}\right)_w + \sigma_T \frac{\mu}{\rho} \left(\frac{\partial \ln T}{\partial x}\right)_w, \tag{1}$$

where $v_m = \sqrt{2\mathscr{R}T_w(x)}$ is the most probable molecular velocity at the surface temperature T_w; σ_p is the slip velocity coefficient and σ_T is the thermal slip coefficient. In this article we use the velocity slip coefficient $\sigma_p^K = 1.012$ given by Kogan in [6], under the full accommodation assumption of the molecules at the wall. The well known value of σ_T, suggested by Kogan in [6] and equal to 0.84, the calculated helium value from [8], and also the measured air value from [9], are used in the present work. Finally a boundary condition proposed by [6] is also chosen to describe the temperature jump at the wall. Furthermore the mean free path is usually written as a function of macroscopic parameters

$$\lambda = k_\lambda \frac{\mu}{p}\sqrt{\mathscr{R}T}.$$

In the equation above the coefficient k_λ depends on the molecular interaction model. In the present study we use $k_\lambda = A(\omega) = \frac{2(7-2\omega)(5-2\omega)}{15\sqrt{2\pi}}$, the expression deduced by Bird in [5] for the variable hard sphere model (VHS) more general than the HS model, where the coefficient $A(\omega)$ depends only on the type of gas via ω $(0.5 \le \omega \le 1)$ viscosity index.

DIMENSIONAL ANALYSIS

A steady state flow is studied now, therefore the time derivatives are not taken into account in the following analysis. The variables are non-dimensioned in the following manner: the streamwise coordinate x by the channel length L, and the wall normal coordinate y by the channel height H. The channel height-to-length ratio ε will be small compared to unity:

$$\varepsilon = H/L, \qquad \varepsilon \ll 1.$$

The streamwise velocity u is normalized using the velocity u_R that is of the same order as the velocity at the channel exit and also of the same order as the characteristic velocity of the mass flow rate. Then the velocity v is normalized by εu_R. The pressure is normalized by using the pressure value at the channel exit p_{out} (where the subscript "out" refers to the outlet conditions). The temperature is normalized using the known value of the wall temperature at the channel outlet $T_{w_{out}}$; finally the density is normalized by using the appropriate outlet value $\rho_{w_{out}}$, and the viscosity coefficient by the value $\mu_{w_{out}}$ corresponding to the outlet wall temperature $T_{w_{out}}$. Let us now introduce a second non-dimensional variable θ, referring to the temperature, to be used in the dimensional analysis of the equation system:

$$\tilde{\theta} = \frac{T - T_{axe}(x)}{T_w(x) - T_{axe}(x)},$$

where T_{axe} is the temperature on the symmetry axis. This last form of the non-dimensional temperature was chosen in order to obtain θ and the derivative of θ along the y-axis, both of zero order, i.e. of the same order as 1. Furthermore, in this work we consider temperature gradient driven flows where the pressure keeps, anywhere in the channel, a value close to its value p_{out}, in the reservoirs. Therefore, like for the temperature and for similar reasons, we introduce a second non-dimensional variable $\tilde{\Pi}$ to represent the pressure:

$$\tilde{\Pi} = \frac{p - p_{out}}{p_M - p_{out}}, \tag{2}$$

where p_M represents the maximum pressure value in the channel. Thus choosing this $\tilde{\Pi}$ form, we obtain $\tilde{\Pi}$ derivatives along the x-axis of zero order, i.e. of the same order as $\tilde{\Pi}$ itself. We can also calculate the derivative of the $\tilde{\Pi}$ function in x-direction as a function of the non-dimensional pressure

$$\frac{\partial \tilde{\Pi}}{\partial \tilde{x}} = \frac{\partial}{\partial \tilde{x}}\left(\frac{p - p_{out}}{p_M - p_{out}}\right) = \frac{1}{p_M - p_{out}}\frac{\partial p}{\partial \tilde{x}} = \frac{p_{out}}{\Delta p_M}\frac{\partial \tilde{p}}{\partial \tilde{x}},$$

and the derivative in the y-direction has the same form. Then, defining the Knudsen, Reynolds and Mach numbers based on the normalizing constant parameters retained above, we obtain:

$$Re = \frac{\rho_{w_{out}} u_R H}{\mu_{w_{out}}}, \qquad Kn = \frac{\lambda}{H} = \frac{k_\lambda}{H}\frac{\mu_{w_{out}}}{p_{out}}\sqrt{\mathscr{R} T_{w_{out}}}, \qquad Ma = \frac{u_R}{a_{w_{out}}}, \qquad Kn = k_\lambda \sqrt{\gamma}\frac{Ma}{Re}. \tag{3}$$

where $a_{w_{out}} = \sqrt{\gamma \mathscr{R} T_{w_{out}}}$ represents the velocity of the sound, based on the outlet wall temperature $T_{w_{out}}$. It is necessary to remember here that we have restricted our study to the slip flow regimes characterized by a Knudsen number below 0.3. Furthermore, owing to the boundary conditions of the system, it is obvious that the flows under consideration here will be rather low speed flows and that the typical values of their Reynolds number will be of zero order $(O(1))$ or of ε order $(O(\varepsilon))$.

THERMAL BOUNDARY CONDITIONS, ENERGY BALANCES AND FINAL ANALYTICAL EXPRESSIONS.

The different steps to obtain the analytical approximate equation system are the following:

- In the NS system we use the general expression linking Kn, Re and Ma numbers (3).
- Assuming that usually in micro channel $Re \sim 1$ or $Re \sim \varepsilon$, we can eliminate some non-dimensional terms.
- Finally we estimate the order of magnitude of the remaining terms using energy balances in the channel: first a thermal balance concerning the gas macroscopically in the rest; then a balance involving the real gas flow.

Two main features are utilized to simplified the system even more:

- we specify our choice concerning the "driver" inlet/outlet temperature difference

$$T_{out} - T_{in} \sim T_{out} \sim T_{in}, \qquad \tilde{T} \sim 1 \qquad \text{and} \qquad \frac{\partial \tilde{T}}{\partial \tilde{x}} \sim 1.$$

- we estimate the respective magnitude orders of the thermal quantities characterizing respectively the transversal transfer and the streamwise transfer. In fact we assume that the fluid motion does not change the relative magnitude order of these conductive transfers. This assumption is based on the very small magnitude of the mass flow rate.

We obtain so u_R, of the same order as the outlet velocity ($u_R \sim u_{out}$), as the characteristic value used to normalize the two velocity components u and v, and thus explicit Re is deduced

$$u_R = \frac{\varepsilon}{2p_{out}}\frac{\mathscr{R}}{Pr}\mu_{w_{out}}\frac{T_{w_{out}}}{H} = \frac{1}{2p_{out}}\frac{\mathscr{R}}{Pr}\mu_{w_{out}}\frac{T_{w_{out}}}{L}, \qquad Re = \frac{\rho_{w_{out}} u_R H}{\mu_{w_{out}}} = \frac{\varepsilon}{2Pr},$$

here Pr is the Prandtl number. Following the way described above, we obtain the analytical expression of the transversal velocity profile:

$$\tilde{u}(\tilde{y}) = \left(\frac{3}{2}\left(4\tilde{y}^2 - 1\right) - 6Kn_* \tilde{T}^{\omega+0.5}\right)\frac{2\sigma_T K_w Pr \tilde{T}^{\omega} - \tilde{T}\tilde{Q}}{1 + 6Kn_* \tilde{T}^{\omega+0.5}} + 2\sigma_T Pr K_w \tilde{T}^{\omega}, \tag{4}$$

where the following notations are used

$$Kn_* = K_{slip} Kn_{out}, \qquad \partial \tilde{T}/\partial \tilde{x} = K_w, \qquad K_{slip} = \sigma_p \frac{\sqrt{2}}{k_\lambda}$$

and where $\tilde{Q}$ is the non-dimensional mass flow rate, non-dimensioned in the following manner:

$$Q = \tilde{Q}\mu_{out}H/2PrL.$$

The analytical expression of the pressure distribution is obtained in form of the second non-dimensional pressure variable $\tilde{\Pi}$ (2):

$$\tilde{\Pi} = \int_0^{\tilde{x}} Ad\tilde{x} - \tilde{Q}\int_0^{\tilde{x}} Bd\tilde{x} = \tilde{\Pi}_A - \tilde{Q}\tilde{\Pi}_B.$$

$$\tilde{\Pi}_A = \frac{2\sigma_T Pr}{Kn_*}\left(D_{\omega+0.5}(\tilde{x}) + \frac{1}{6Kn_*(\omega+0.5)}\ln\frac{1+6Kn_*\tilde{T}_{w_{in}}^{\omega+0.5}}{1+6Kn_*\tilde{T}^{\omega+0.5}}\right),$$

where we use D_υ defined as

$$D_\upsilon(\tilde{x}) = (\tilde{T}^\upsilon(\tilde{x}) - \tilde{T}_{w_{in}}^\upsilon)/\upsilon.$$

$$\tilde{\Pi}_B = \frac{c}{K_w}\left(\left(1+\frac{1}{2}cKn_* + \frac{1}{4}c^2Kn_*^2\right)D_{\omega+2}(\tilde{x}) - cKn_*\left(1+cKn_*\right)D_{2\omega+2.5}(\tilde{x}) + c^2Kn_*^2 D_{3\omega+3}(\tilde{x})\right), \quad c = \frac{6}{1+3Kn_*}.$$

Non-dimensional mass flow rate may be found according the following expression:

$$\tilde{Q} = \frac{\frac{2\sigma_T Pr}{Kn_*}\left(D_{\omega+0.5} + \frac{1}{6Kn_*(\omega+0.5)}\ln\frac{1+6Kn_*\tilde{T}_{w_{in}}^{\omega+0.5}}{1+6Kn_*}\right)}{\frac{c}{K_w}\left(\left(1+\frac{1}{2}cKn_*+\frac{1}{4}c^2Kn_*^2\right)D_{\omega+2} - cKn_*\left(1+cKn_*\right)D_{2\omega+2.5} + c^2Kn_*^2D_{3\omega+3}\right)}, \tag{5}$$

where $D_\upsilon(\tilde{x})|_{\tilde{x}=1} = D_\upsilon$.

NUMERICAL SIMULATION AND COMPARISON WITH THE ANALYTICAL APPROACH AND OTHER THEORIES

Numerical modeling

For the numerical simulation of the micro channel flows the NS equation system is solved. The computations are carried out for a two dimensional flow between the symmetry axis and the parallel plate at the distance $H/2$. The flow is sustained by a temperature gradient. The total pressure and temperature are fixed in the inlet and outlet reservoirs. It should be remembered that the pressures are the same in both reservoirs and that the temperatures are different. The other flow parameters at the inlet and outlet sections of the channel are deduced from the characteristic equations.

The computations are performed for different gases: helium, nitrogen and air. The calculations are carried out for a channel of H of $10\mu m$ in height and L of $1cm$ in length. We have compared the analytical and numerical profiles of the flow parameters in the channel under three different types of flow conditions:

- The pressure in both tanks is equal to the atmospheric pressure $p_{atm} = 1.013\cdot10^5 Pa$, the temperature in the inlet tank is equal to $295.6K$, the temperature difference between the tanks is equal to $277.4K$. The flows of helium and of air are considered.
- The pressure in both tanks is equal to the atmospheric pressure p_{atm}, the temperature in the inlet tank is equal to $295K$. The different values of the temperature difference between the tanks are considered (see Table 1) and its influence on the flow is studied. The flow of nitrogen is considered.
- The temperature in the inlet tank is equal to $295K$. Different values of the pressure (the same in the two tanks) are considered (see Table 1), which correspond to different values of the Knudsen number. The influence of the Knudsen number on the flow is studied. The flow of nitrogen is considered.

Comparisons and comments

The classical thermal transpiration phenomenon generally considered consists in the apparition and the development of an unsteady flow between two reservoirs. At the beginning of the experiment both reservoirs are kept at the same

TABLE 1. Dimensionless mass flow rate $Q*10^{12}kg/s$ for the nitrogen flow obtained according to (5).

$T_{out}-T_{in}$ (K)	140	300	600
Kn_{out}	0.008	0.0126	0.0209
Q NS (num.sol.)	1.318	2.665	4.887
Q NS (anal.sol.)	1.318	2.665	4.887
Q BE (S-model) [2]	1.252	2.408	4.102

p_{out}	p_{atm}	$0.1p_{atm}$	$0.05p_{atm}$
Kn_{out}	0.0126	0.126	0.253
Q NS (num.sol.)	2.665	2.675	2.678
Q NS (anal.sol.)	2.665	2.648	2.595
Q BE (S-model) [2]	2.408	2.720	2.266

pressure and at different temperatures, while the temperature difference is maintained during the experiment. If these two reservoirs are connected with a relatively small channel the gas starts to creep from the cold to the hot reservoir until to the establishment of a well known relation between the pressures and temperatures, while the mass flow rate in the channel completely vanishes. In our investigation the temperature difference between the two reservoir is maintained, while the pressures are kept equal. As results, we obtain a steady flow from the cold to the hot reservoir. A non-linear pressure profile forms along the channel and the mass flow rate does not vanish.

The mass flow rate through the channel calculated numerically and analytically is compared in Table 1 for the different flow conditions. The analytical and numerical values of mass flow rate coincide practically for the small Knudsen numbers and start to differ from $\sim 3\%$ for a Knudsen number greater than 0.25. The comparison with the results obtained in [2] applying the S-model kinetic equation are also carried out. The difference in the mass flow rate between the proposed analytical approach and the method used in [2] is about $10-15\%$. It is necessary to note at this point that the author of [2] models the collision integral in the Boltzmann equation using the linearized S-model which gives a correct Prandtl number but which is valid only for monatomic gases.

It is interesting to note that in the first half of the channel the maximum of the velocity is found on the wall and the gas flows increase the pressure, while in the second part the maximal velocity is on the axis, and the velocity profile has a typical form similar to that of the Poiseuille flow and the gas pressure decreases along the streamwise direction see Fig. 1).

The influence of the temperature gradient along the wall is studied in the second series of calculations. The mass flow rate increases with the streamwise temperature gradients (see Table 1). The outlet Knudsen number increases here only due to the temperature increase in the outlet reservoir since the pressure in the reservoir remains the same.

The influence of the reservoir pressures (i.e. of the Knudsen number, since the temperature difference remains the same when the pressure changes) is studied in a third series of calculations. It is to note that the dimensional mass flow rate depends weakly on the reservoir pressure for the pressure range under consideration (see Table 1), which is not surprising if considering analytical expressions (5). The pressure inside the channel increases when the Knudsen number increases. As was mentioned above, we can see that the velocity profiles have their maximal values at the wall in the first part of the channel and on the channel axis in the second part of the channel (see Fig. 1). When the Knudsen number increases the profiles become smoother and finally quasi-uniform.

Generally, it is clear, that the analytical and numerical profiles are in very good agreement.

When comparing our results with a kinetic approach [2] we obtain a reasonable agreement if we exclude a part of the transversal velocity profiles. Near the wall the kinetic and continuum profiles are different. This local difference may be partially due to the Knudsen layer effects.

CONCLUDING REMARKS

We have focused our interest on the non isothermal steady continuum approaches in slip regime (up to Knudsen numbers close to $0.25-0.30$) using the Navier Stokes equations. From this equation system, describing the case where the reservoir pressures are the same, we have derived a mass flow rate expression, the analytical profiles of pressures and velocities and the heat flux, using energy balance and small perturbation method. Globally in this Knudsen range our analytical profiles agree perfectly with the "exact" numerical results and they agree reasonably with the results of the numerical solution of the S-model kinetic equation (if we disregards the velocity profiles in the closest wall neighbouring where the discrepancies are more important). Such analytical expressions are original for compressible flows. They are obviously useful in the development of various micro devices using thermal creep effect to start and maintain gas motions in micro channels. Indeed explicit expressions of the gas physical quantities appears very easy to use; they especially minimize calculation time consumed to found the optimal values of sensitive parameters

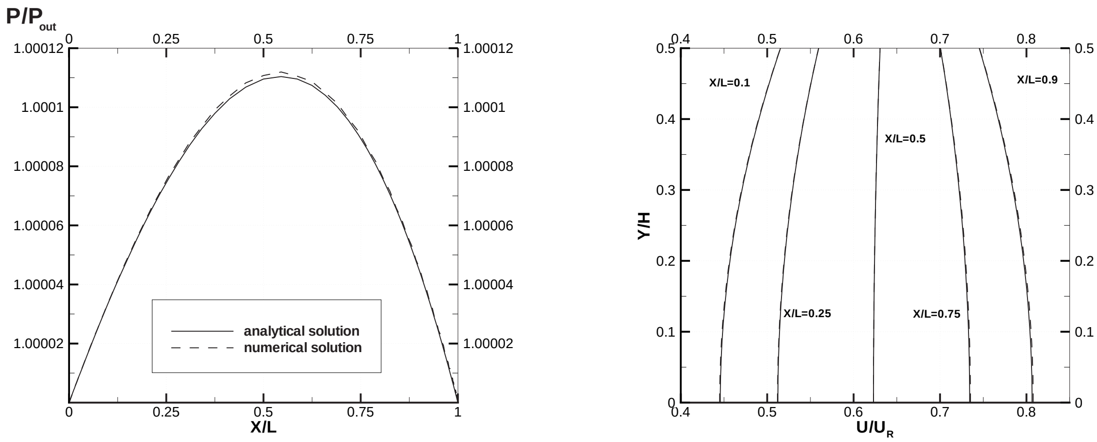

FIGURE 1. Pressure and velocity profiles for helium flow, $Kn_{out} = 0.036$. The solid curve is the analytical solution, the dashed line represent the numerical solution.

characteristic of any specific micro device. Finally the main noticeable physical features appearing from the previous analytical description of the thermally creeping flows may be summarized as follows:

- the mass flow rate depends very weakly on the reservoir pressure and increases regularly with the streamwise temperature gradient.
- the pressure variation along the streamwise direction (of second order magnitude according to the Knudsen number) is significantly non linear and presents a maximal value in a point x where the pressure itself is maximal.
- the curvature of the velocity transversal profiles changes at this x point. In the second part of the channel this curvature becomes similar to that of isothermal profiles; but the weight of the slip velocity remains everywhere more important than in the isothermal case.
- the non dimensional transversal heat flux is a second order quantity according to the aspect ratio, as do the relative transversal temperature differences. These thermal parameters are not uniform over each transversal section. In addition they very sensitively depend on the thermal slip coefficient σ_T.

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