Numerical analysis of thermal creep flow in curved channels for designing a prototype of Knudsen micropump

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Abstract. The possibility to generate a gas flow inside a channel just by imposing a tangential temperature gradient along the walls without the existence of an initial pressure difference is well known. The gas must be under rarefied conditions, meaning that the system must operate between the slip and the free molecular flow regimes, either at low pressure or/and at micro/nano-scale dimensions. This phenomenon is at the basis of the operation principle of Knudsen pumps, which are actually compressors without any moving parts. Nowadays, gas flows in the slip flow regime through microchannels can be modeled using commercial Computational Fluid Dynamics softwares, because in this regime the compressible Navier-Stokes equations with appropriate boundary conditions are still valid. A simulation procedure has been developed for the modeling of thermal creep flow using ANSYS Fluent®. The implementation of the boundary conditions is achieved by developing User Defined Functions (UDFs) by means of C++ routines. The complete first order velocity slip boundary condition, including the thermal creep effects due to the axial temperature gradient and the effect of the wall curvature, and the temperature jump boundary condition are applied. The developed simulation tool is used for the preliminary design of Knudsen micropumps consisting of a sequence of curved and straight channels.

1. Introduction
The increasing demand on microdevices over the last years led to the development of new fabrication techniques for manufacturing micro-electro-mechanical systems (MEMS), such as micro-heat exchangers, pressure gauges, micro-sensors for mass flow and temperature measurements and micropumps. The need to manipulate very small fluid volumes for example for medical, biological, or electronics cooling purposes led to the development of various micropumps, but even today in most microfluidic applications the pumping system remains the largest in size and the most expensive (mainly due to power consumption) part of a fluidic microsystem [1-4]. Miniaturization of these pumps would lead to minimization of the total size and cost and enable the portability (for example in chemical analysis systems). At the same time the necessity of simulation tools is equally important and crucial, especially in the case of gaseous fluids. For that reason various analytical and numerical approaches have been developed for the simulation of rarefied gas flows (continuum and kinetic models, Direct Simulation Monte Carlo method…) [5-6].
Rarefied gas flows can be encountered under low pressure and/or in micro/nano-scale dimensions. The degree of rarefaction of a gas is determined by the Knudsen number:

\[ Kn = \frac{\lambda}{D_h} \]  

defined as the ratio of the mean free path \( \lambda \) of the gas molecules over a characteristic length, for example the hydraulic diameter \( D_h \) of the microchannel. The Knudsen number encountered in classic microsystems (micropumps, microvalves, micronozzles, microflow sensors) is frequently between \( 10^{-3} \) and \( 10^{-1} \), which is the typical range of the well-known slip flow regime [7]. In this regime, even if the Navier-Stokes equations are still valid in the bulk flow, the gas is no longer in local thermodynamic equilibrium near the wall (Knudsen layer). In this region, a variety of rarefaction effects are exhibited, including the presence of non-negligible velocity slip and temperature jump at the walls [8, 9]. The slip flow regime is quite convenient from a theoretical point of view because it generally leads to analytical or semi-analytical solutions. In the literature, however, various forms of the boundary conditions can be found for the velocity slip and the temperature jump boundary conditions [10].

In rarefied gas flows, it is possible to generate a flow just by imposing a tangential temperature gradient along the walls without the existence of an initial pressure difference. This phenomenon is called thermal transpiration or thermal creep. In figure 1 a schematic representation of thermal driven gas flow in a narrow channel connecting two reservoirs at different temperatures is given. The phenomenon is well known since 1878 when Reynolds [11] experimentally observed it for the first time, namely in a tube connected to two reservoirs at different temperatures. Actually, the gas molecules move from the lower to the higher temperature zones, which eventually will cause a pressure difference and a reversed Poiseuille flow due to this pressure gradient. In addition, Reynolds showed that at the equilibrium the pressures are related to the temperatures according to the law:

\[ \frac{P_2}{P_1} = \left(\frac{T_2}{T_1}\right)^{1/2} \]  

where \( P \) and \( T \) are the pressure and the temperature, in the case of molecular flow regime in the microchannel. The subscript 1 corresponds to the cold side and 2 to the hot reservoir.

![Figure 1. Schematic representation of thermal transpiration flow.](image)

After Reynolds, several studies have been devoted both to experimental [12-14] and computational analyses [15-19] of thermal creep flows. The modeling of this kind of flows, however, goes back to 1879 when Maxwell [20] proposed a mathematical expression, based on the kinetic theory, of a flow induced by a temperature gradient. A few years later (1909), Knudsen proved Reynolds law and mentioned the existence of two counter-current flows, due to the temperature gradient in one direction and due to the developed pressure difference in the opposite direction. After a transient phase during which the flow engaged by the temperature difference initially dominates, the effect of the Poiseuille counter-flow increases and finally leads to an equilibrium state with zero net flow.

The above flow is at the origin of the basic operation principle of the Knudsen pumps. A Knudsen pump is actually a compressor without moving parts that works for a gas under rarefied conditions. The basic design of such a pump consists of a thin channel, in which the gas is at least in the slip flow regime, connecting a cold and a hot region. In order to increase the efficiency of the pump it is possible to use an array of parallel thin channels and/or a cascade system consisting of several units.
connected in series by intermediate thick channels or reservoirs (figure 2a). It is obvious that in order to operate a Knudsen pump at atmospheric pressure, the dimensions of the narrow channel must be in sub-micro or nano-scale. Until recently, it was difficult to fabricate such a channel, but this limitation was overcoming by operating the system at low pressures and with channels of some ten to hundreds of micrometers. Today, it is possible to manufacture channels with very small height and in addition to work in vacuum conditions. Since the work of Knudsen, several researchers have tried to developed micromachined pumps [21-25] or pumps using alternative materials for the narrow channels [26-29].

In parallel, there are also some theoretical approaches to describe the operation of a Knudsen pump, either with the Direct Simulation Monte Carlo method [15] or with the BGK model [18, 19, 30, 31]. Recently, an alternative configuration has been proposed and numerically studied [18, 19], in which the sequence of narrow-wide segments could be replaced with a sequence of curved-straight segments. The curved (semicircular) segments have the same width as the straight segments (figure 2b). In this case, there is a uniform temperature gradient along the walls of the straight part (the temperature decreases linearly from \( T_H \) to \( T_L \) along the channel), while an opposed temperature gradient is applied along the walls of the curved part. As a consequence, two opposed thermal creep flows will be generated in the two parts. Due to the different geometry, however, the transpiration effect is stronger in the curved segments and a global net flow is observed. In addition, it has been shown [18, 19] that a multi-stage Knudsen compressor consisting of curved and straight channels can actually operate between the slip and the free molecular flow regimes. More precisely, there is an optimum Knudsen number, depending on the curvature of the bend part and also on the number of the stages, for achieving the highest compression efficiency. Under certain circumstances, it is possible to have maximum compression ratio in the slip regime or in the early transition regime.

![Figure 2. Configurations of a) classic Knudsen pump and b) curved-channel Knudsen pump.](image)

Motivation of the present work is the development of a simulation tool which will help in the preliminary design of a Knudsen micro-pump with curved channels. A two-dimensional numerical model has been developed for implementing the correct first order boundary conditions in the case of the slip flow regime, taking into consideration the thermal creep flow due to the axial temperature gradient and the effect of the wall curvature. The modeling of the thermally driven flow of rarefied gases in microchannels is achieved using the commercial CFD software ANSYS Fluent®, while C++ routines have been developed in order to apply the boundary conditions at the walls of the channels.

### 2. Boundary conditions

As already pointed out, the rarefied gas flow in the slip flow regime can be modeled using the Navier-Stokes equations, but together with the appropriate boundary conditions describing the slip velocity
and the temperature jump at the solid walls. For the case of a 2-D flow with a curved wall or with significant roughness, the expression of slip velocity at the walls can be written as [10, 32, 33]:

\[ u_{fluid} - u_{wall} = \alpha \left( \frac{2 - \sigma_t}{\sigma_t} \right) \lambda \left( \frac{\partial u}{\partial n} + \frac{\partial v}{\partial s} \right)_{wall} + \frac{3}{4} \mu R \frac{\partial T}{\partial s}_{wall} \]  

(3)

where \( \alpha \) and \( \sigma_t \) are a corrective coefficient and the tangential momentum accommodation coefficient, \( u \) and \( v \) are the tangential and the normal velocities, \( n \) and \( s \) the normal and the tangential coordinates, \( \mu \) and \( R \) the dynamic viscosity and the specific gas constant, \( P \) and \( T \) the pressure and the temperature. The first term of the right hand side is the first order isothermal slip velocity which derives from the tangential shear stress at the wall and the second term is the thermal creep due to the tangential temperature gradient. It is important to note that the additional derivative \( \partial v/\partial s \) must be taken into account in the case of curved channels, although in most published works this term is neglected or has been sometimes erroneously replaced with the derivative \( \partial u/\partial s \).

In a similar way, the first order temperature jump boundary condition is:

\[ T_{fluid} - T_{wall} = \beta \left( \frac{2 - \sigma_t}{\sigma_t} \right) \frac{2 \gamma}{\gamma + 1} \frac{\lambda}{Pr} \frac{\partial T}{\partial n}_{wall} \]  

(4)

where \( \beta \) and \( \sigma_t \) are a corrective coefficient and the thermal accommodation coefficient, \( \gamma \) and \( Pr \) the ratio of the specific heats and the Prandtl number. Both corrective coefficients in equations (3) and (4) have been added to the initial Maxwell-Smolukowski boundary conditions, derived from numerical simulations [34].

3. Numerical Model

The numerical modeling has been carried out using the commercial CFD code ANSYS Fluent® 12.1, which implements the finite element method. The velocity slip boundary condition is imposed as the velocity of a moving wall, and the temperature jump as a modified temperature of the wall, both of them applied cell by cell at the wall. For that reason User Defined Functions (UDFs) have been developed by means of C++ routines and compiled in the solver. Through the UDFs the derivatives of the velocities and the temperature are extracted from the solver and the slip velocity and temperature jump are calculated based on equations (3) and (4). In addition, the temperature of the walls is imposed with the UDFs, either as a constant temperature or as a temperature gradient when needed.

Due to the surface curvature, the local wall coordinate system is in general not aligned with the solver’s coordinate system. This makes a transformation of coordinate system necessary. The velocity vectors and all derivatives can be extracted from the solver, but are expressed in the solver coordinate system (x, y). In the case of straight channels, the normal (y direction) and tangential (x direction) derivatives of the velocity and the temperature, which are included in equations (3) and (4), are aligned with the solver coordinate system and can be replaced with the terms \( \partial u/\partial y \), \( \partial v/\partial x \), \( \partial T/\partial y \) and \( \partial T/\partial x \) , respectively. In curved channels, the derivatives \( \partial u/\partial n \), \( \partial v/\partial s \), \( \partial T/\partial n \) and \( \partial T/\partial s \) must be expressed as functions of the known \( \partial u/\partial x \), \( \partial u/\partial y \), \( \partial v/\partial x \), \( \partial v/\partial y \), \( \partial T/\partial x \) and \( \partial T/\partial y \).

All calculations are performed with the two-dimensional segregated solver assuming steady state laminar flows. A second order upwind spatial discretization scheme is applied. The dilute gas is considered as an ideal compressible gas, while the temperature-dependent viscosity is calculated from the power law:

\[ \mu = \mu_{ref} \left( \frac{T}{T_{ref}} \right)^{\omega} \]  

(5)

where \( \mu_{ref} \) is the dynamic viscosity of the gas at the reference temperature \( T_{ref} \) and \( \omega \) is a power law coefficient. The values of these coefficients are available in the literature for various gases [35]. The corrective coefficients \( \alpha \) and \( \beta \) and the accommodation coefficients \( \sigma \) and \( \sigma_t \) of equations (3) and (4) have been kept equal to unity throughout the numerical simulations presented here. Assuming a dilute gas, the Prandtl number is set to 2/3 for a monatomic and to 0.72 for a diatomic gas, whereas the ratio...
\( \gamma \) is equal to 5/3 for a monatomic and to 7/5 for a diatomic gas. The specific gas constant \( R \) is the ratio of the gas constant \( R = 8.314 \text{ J mol}^{-1} \text{K}^{-1} \) to the molar mass \( M \) of the gas.

It is worth mentioning that the commercial CFD code ANSYS Fluent® gives the possibility of implementing the first-order slip and temperature jump boundary conditions, with the so-called Low Pressure Boundary Slip (LPBS) method. The choice of velocity slip boundary condition is, however, limited to Maxwell’s first-order condition, without taking into account the effect of the curvature of the wall and the thermal creep. In addition, the mean free path can be adjusted only through the Lennard-Jones length. The validity of the LPBS method was tested for the simplest case of pressure driven gas flows in straight microchannels, and comparison with analytical solutions, which can be found in literature [35], showed a very good agreement. It has been shown [36], however, that the obtained results are not always very accurate, especially in three-dimensional flows with cross-sections involving acute angles. To overcome these drawbacks and also to implement, if needed, higher-order boundary conditions, specific UDFs have been developed in the present work.

4. Validation of the numerical model

Several benchmark cases for gas flows in the slip flow regime are simulated in order to test the validity of the developed numerical procedure used for implementing the boundary conditions, e.g. pressure and/or temperature driven gas flows in straight and curved microchannels of rectangular and circular cross sections. The results of the model are compared either with analytical or numerical results when possible.

Initially, the numerical model (UDF method) has been validated for the simplest case of pressure driven gas flows for the below cases:

- isothermal flow in a plane microchannel limited by parallel plates compared with an analytical solution [35],
- isothermal and non-isothermal flows (without taking under consideration the thermal creep and the effect of the curved wall) in rectangular and circular straight channels compared with the numerical results of ANSYS Fluent® using the LPBS boundary condition method and
- isothermal and non-isothermal flows (without taking under consideration the thermal creep and the effect of the curved wall) in a sequence of straight and curved rectangular microchannels compared with the LPBS method.

Next, the UDF method is validated for the case of temperature driven flows in a straight rectangular microchannel and a sequence of straight and curved rectangular channel, taking into account the curvature of the bent channels and thermal creep effect.

4.1. Pressure driven flows in bent microchannels

The isothermal and non-isothermal flow in a straight and curved rectangular microchannel connecting two reservoirs maintained at different pressures is considered (see figure 6a). In the isothermal case the whole system is at constant temperature \( T = 300 \text{ K} \) and neither the temperature jump nor the thermal creep terms are taken into account. On the other hand, in the non-isothermal case the wall temperature \( T_L = 300 \text{ K} \) is imposed at the inlet and outlet sections A and C, and, the wall temperature \( T_H = 900 \text{ K} \) is imposed at the intermediate section B; between these sections, the temperature of the wall varies linearly. In that case both the velocity slip and temperature jump at the walls are taken into account, while the thermal creep effect is still not considered. In both cases, the effect of the wall curvature expressed by the additional derivative of the normal velocity \( (\partial v/\partial s) \) in equation (3) is not taken into account. The results of the simulations using the UDF method are compared with those obtained imposing the LPBSC provided by ANSYS Fluent®.

The width of the microchannel is \( D = 100 \mu \text{m} \), the length of the straight part is \( L_s = 314 \mu \text{m} \), while the radius of the centerline of the curved part is \( R_C = 100 \mu \text{m} \). A pressure drop \( \Delta P = P_A - P_C = 100 \text{ Pa} \) is imposed between the inlet and the outlet of the whole microchannel. The gas is argon, considered as an ideal gas. Under these conditions the gas is in rarefied conditions and the Knudsen number at the
inlet is $Kn_A = 0.012$. The grid used in the simulations contains $200 \times 50$ cells. It has been checked that a finer grid leads to identical results, which means that the mesh is fine enough.

In figure 3 the pressure distributions along the centerline are presented ($s$ represents the curvilinear abscissa, with $s = 0$ corresponding to the inlet A of the curved channel) for both the isothermal (in black) and non-isothermal flow (in red). The pressure distribution along a microchannel should be a 2$\text{nd}$ order polynomial, as shown in [35, 37-39], with opposite effects of rarefaction and compressibility on the curvature of the polynomial distribution. The main effect is due to compressibility and rarefaction effects (characterized by $Kn$) tend to reduce the curvature of the pressure distribution. In the isothermal case of figure 3, however, the pressure distribution is very close to a linear one due to the small imposed pressure drop which results in negligible compressibility effects. On the other hand, for the non-isothermal case, compressibility effects induced by temperature variations —density is strongly temperature dependent— cause the curvature on the pressure distribution between the two cold ends of the microchannel and the hot junction of the straight and bent part.

Moreover, it is observed in figure 3 that the agreement between the two simulation procedures is good and the results are very close. For the isothermal flow the deviation between the mass flow rates per unit of depth calculated with both methods is about 1.2 %, the LPBS method giving $4.74 \times 10^5$ kg s$^{-1}$ m$^{-1}$ and the UDF $4.68 \times 10^5$ kg s$^{-1}$ m$^{-1}$. For the non-isothermal flow, the mass flow rate calculated with the LPBS method is equal to $1.43 \times 10^5$ kg s$^{-1}$ m$^{-1}$ and to $1.41 \times 10^5$ kg s$^{-1}$m$^{-1}$ with the UDF method.

![Figure 3](image_url)

**Figure 3.** Pressure profiles along the centerline for pressure driven isothermal and non-isothermal gas flows - Comparison between UDF and LPBS methods.

4.2. Thermal creep flows in straight microchannels

The temperature driven fully developed flow of rarefied gas between parallel plates is simulated taking under consideration the thermal creep in this test case. The computations are carried out for a two-dimensional flow limited by the symmetry plane and the upper plate (figure 4). The temperatures at the inlet and the outlet are noted $T_L$ and $T_H$, respectively, with $T_L < T_H$ and the wall temperature is varying as a linear function of the streamwise coordinate $x$. The pressures at the inlet and outlet are always the same. The channel has a width of $D = 10$ µm and a length of $L = 1$ cm. The grid has $100 \times 25$ cells. The gases are helium or nitrogen, considered as ideal monatomic or diatomic gases. The data used in the simulations are presented in table 1.

The results are compared with the numerical solution of the Navier-Stokes equations with the appropriate boundary conditions calculated by Méolans & Graur [17]. The model developed by these
authors is based on the exact numerical solution of the compressible Navier-Stokes equations associated with similar boundary conditions as those described by equations (3) and (4). In addition, Méolans & Graur derived a simplified analytical model using a perturbation method according to a small geometric parameter. The boundary conditions used in the UDF model have been modified for the present comparisons, in order to be applied to the equations proposed by the above authors.

**Figure 4.** Straight channel parameters for thermal creep simulation.

**Table 1.** Simulation parameters of the thermal creep flow in a straight microchannel and mass flow rates calculated by the present UDF method and the numerical simulation of Méolans & Graur [17].

| Case | Gas | \( T_{in} \) (K) | \( T_{out} \) (K) | \( P \) (Pa) | \( Kn_{out} \) | Mass flow rate \( (10^{-8} \text{ kg s}^{-1} \text{ m}^{-1}) \) | Deviation (%) |
|------|-----|----------------|----------------|--------------|-------------|----------------|---------------|
|      |     | 295.6          | 295            | 101325       | 0.036       | 1.884          | 0.263         |
|      | He  | 295            | 435            | 101325       | 0.009       | 1.792          | 0.143         |
| 2    | N\(_2\) | 295           | 595            | 101325       | 0.0126      | 1.408          | 0.161         |
| 3    | N\(_2\) | 295           | 895            | 101325       | 0.021       | 1.280          | 0.281         |
| 4    | N\(_2\) | 295           | 895            | 101325       | 0.126       | 1.169          | 0.462         |
| 5    | N\(_2\) | 295           | 895            | 5066.25      | 0.253       | 0.871          | 0.342         |
| 6    | N\(_2\) | 295           | 595            | 5066.25      | 0.253       | 0.871          | 0.342         |

The mass flow rates are calculated per unit of depth of the channel and are compared in table 1. It is obvious from this table that the constant pressure level in the reservoirs connected to the inlet and outlet of the microchannel has little influence on the mass flow rate (see cases 3, 4 and 6). This result is expected, as the flow is not pressure driven and the relative pressure variation along the microchannel is small (see figure 5b), and the thermal creep term in equation (3) is inversely proportional to the pressure. This term is the major contribution of the velocity slip, as can been proved by comparing the order of magnitude of the two terms of the RHS of equation (3): the ratio of the first over the second term of the RHS is of the order of \( 10^{-4} \). As a result, the velocity slip and the local velocity are also roughly inversely proportional to the pressure and the mass flow rate defined as:

\[
\dot{m} = \int_{S} \rho u dS = \frac{P}{R} \int_{S} T u dS
\]

is almost not pressure dependent. On the other hand, the temperature gradient across the microchannel strongly affects the flow rate (see cases 2, 3 and 4). An increase in the temperature of the hot reservoir causes an increase in the flow rate. The deviation in the calculated mass flow rate between the two specific approaches is very small, less than 0.5 %, for all the studied cases. Méolans & Graur [17] compared their results with a numerical solution of the Boltzmann equations (S-model) and they found that for small Knudsen numbers there is a very good agreement, but for large Knudsen numbers there
is a significant deviation (15 %). This deviation, however, is expected as the regime deviates from the slip flow regime.

The velocity profiles in various cross-sections of the channel are presented in figure 5a. The streamwise velocity $u$ has been normalized with the velocity:

$$u_R = \frac{R \mu_{out} T_{w, out}}{2 P_{out} \Pr L}$$

and the normal coordinate $y$ with the width $D$ of the channel. In the first half of the channel, where the pressure increases, the maximum of the velocity is observed at the wall, while on the other half the maximum is on the centerline.

Figure 5b shows the pressure profiles along the streamwise direction on the centerline for two values of the Knudsen number. In that case the pressure is normalized with the outlet pressure and the streamwise position $x$ with the length $L$ of the microchannel. It can be seen that the pressure distribution along the channel is non-linear with a non-symmetric distribution and a maximum value downstream from the mid-section of the channel.

**Figure 5.** a) Velocity profiles in various cross-sections (He, $Kn = 0.036$). The red curves correspond to the present UDF model and the black ones to the numerical solution of Méolans & Graur [17]. b) Pressure profiles calculated by the UDF model for two Knudsen numbers. Flow of nitrogen.

4.3. Temperature driven flows in ringed shaped channels

In this section, the layout proposed by Aoki et al. [18, 19] is considered. The complete expressions of the boundary conditions, as described by the equations (3) and (4), are used. The basic unit of this device consists of a straight channel with length $L_s$ connected to a semi-circular part with radius of the centerline $R_c$ (figure 6a). The height of the straight and bent channel is $D$. A linear temperature gradient is applied in the straight part and the temperature is increasing from $T_L$ to $T_H$. An opposed temperature gradient is applied to the curved part. By completing this configuration with a symmetrical part, a close ring can be formed (figure 6b). It has been proved with theoretical approaches by Aoki and co-workers that a circulating flow is generated inside the ring. Using the Boltzmann-BGK model as the governing equation for the gas flow, Aoki et al. have developed numerical methods based either on the asymptotic technique of the diffusion approximation [18] or on the deterministic finite volume scheme [19].

The geometry of the ring is symmetric with reference to the centre of the ring and so the configuration of figure 6a is simulated with the present method. Periodic boundary conditions are applied at the inlet and outlet sections A and C, expressed as $T_A = T_C$ and $P_A = P_C$. The steady state 2-
D compressible flow of an ideal gas (argon) is simulated and the results are compared with the numerical simulation of Aoki et al. [19].

Three different layouts are tested, the parameters of which are presented in table 2. The pressure in the inlet is $P_A = 0.15$ Pa and the hot and cold temperatures are $T_H = 900$ K and $T_L = 300$ K, respectively. The Knudsen number defined for the global average density in the channel and given by Aoki et al. [19] is $Kn = 0.1$, but when calculated for the entrance conditions, its value is $Kn_A = 0.04$. Due to the pressure level, the system is not in micro-scale, but a device with macro dimensions working under very low pressures, which ensures that the gas is in rarefied conditions.

The channel is discretized with a number of cells depending on its size: the mesh contains 200x200 cells for case 1, 200x100 cells for case 2 and 400x100 cells for case 3. In all cases the grid is non-uniform in the spanwise direction with an increased density near the walls. Coarse and fine meshes either uniform or non-uniform have been tested and the specific grids were chosen by comparing the results obtained with the different meshes and also with the numerical simulations of Aoki et al. [19].

Table 2. Simulation parameters of thermal creep flow in a curved channel and mass flow rates calculated by the present UDF method and the numerical simulation of Aoki et al. [19].

| Case | 1          | 2          | 3          |
|------|------------|------------|------------|
| $D$ (m) | 1          | 1          | 1          |
| $L_s$ (m) | 3.14       | 6.28       | 15.7       |
| $R_c$ (m) | 1          | 2          | 5          |
| Mass flow rate (10$^{-8}$ kg s$^{-1}$ m$^{-1}$) |   |   |   |
| [19] | 79.645     | 8.833      | 0.511      |
| UDF  | 78.867     | 8.734      | 0.513      |
| Deviation (%) | 0.977      | 1.126      | 0.314      |

In figure 7 the distribution of the dimensionless temperature, density and pressure along the centerline of the whole channel are shown, for all cases described in table 2. In this figure the normalization has been done with the cold temperature $T_L$, the average density $\rho_{av}$, and the term $R\rho_{av}T_L$, respectively, and $S$ represents the dimensionless curvilinear abscissa normalized by the length of the straight part $L_s$ with $S = 0$ corresponding to the inlet $A$ of the curved channel. In addition, in table 2 the mass flow rate per unit of depth is included for both methods. In every case the UDF method shows a very good agreement with the numerical analysis and especially for case 3.
Figure 7. Distributions of the dimensionless temperature $T$, density $\rho$ and pressure $P$ along the centerline of the channel for a) case 1, b) case 2 and c) case 3. The thick curves correspond to the results of the present UDF model and the thin ones to the numerical solution of Aoki et al. [19].

5. Application to the design of a multistage Knudsen micropump

The device presented in figure 2b, which actually is a Knudsen pump (compressor) consisting of $N$ stages, and has been proposed by Aoki and co-workers [18, 19] is now simulated. The cascade system consists of two basic units joined alternately: the unit ABC of figure 6a and the mirror image of part ADC of figure 6b. It is considered that the end of the first stage is closed by a wall kept at temperature $T_L$, while the other end of the $N$ stage is open and kept at pressure $P_o$ and temperature $T_H$. The slip and temperature jump conditions are also imposed at the wall of the closed end of the pump. Again, $S$ is the dimensionless curvilinear abscissa across the centerline, with $S = 0$ referring to the closed end and $S = N$ to the open end of the cascade system.

The size of each unit is defined by $D = 100 \, \mu m$, $L_s = 314 \, \mu m$ and $R_c = 100 \, \mu m$. The hot and cold temperatures are $T_H = 900 \, K$ and $T_L = 300 \, K$, respectively, and the pressure at the open end of the device is $P_o = 1500 \, Pa$. The Knudsen number calculated for this conditions is $Kn = 0.04$ (or equal to 0.1 if calculated based on the average density in the whole device). The mesh of one unit (stage) contains $200 \times 100$ cells and the grid is non-uniform in the spanwise direction with higher density near the walls. The simulations are made for $N$ equal to 1, 2, 4, 8 and 25 stages.

In figure 8a the dimensionless pressure $P$ along the centerline of the whole channel for the different cascade systems is shown as a function of the dimensionless distance $S$. As expected, the pressure profiles oscillate with the same frequency as the imposed wall temperature and the cumulative effect of the number of stages is evidenced. Calculating the dimensionless average pressure $P_{\text{average}}$ for every stage (figure 8b) it can be concluded that the dependence on the number of stages is rather close to a linear function which depends on each system. In figure 8c the pressure gain $P_{\text{gain}}$, defined as the ratio of the pressure difference (between the two ends of the cascade system) to the outlet pressure $P_o$, and the density gain $\rho_{\text{gain}}$, defined as the ratio of the density difference between the two ends of the cascade system to the density on the open end, are plotted in percent. Both pressure and density gains are linearly dependent on the number of stages. Additional simulations with a larger number of stages and under different conditions, however, are required in order to confirm this observation. For the present simulated device the pressure and the density gains are almost 45% for the 25 stage device. Extrapolating the line of figure 8c, it is found that 100% of gain could be achieved with around 60 units.

In their work Aoki et al. [19] have simulated a different multistage Knudsen pump ($D = 1 \, m$, $L_s = 6.28 \, m$, $R_c = 2 \, m$, $T_H = 900 \, K$, $T_L = 300 \, K$, $Kn = 0.5$, $N = 2$-16). In their system a gain of 100% is achieved with around 32-36 units. The results of figure 8, however, present the same trend and the observations are almost identical. The difference in the required number of stages for achieving 100% of gain is most likely due to the different Knudsen number which is higher in the case simulated by Aoki et al. It is expected that the operation of the Knudsen pump in this early transition regime is a bit
more efficient. Nevertheless, the similarities between the results from the present simulation and the numerical simulation using the Boltzmann-BGK model support our methodology.

![Figure 8. a) Distributions of the dimensionless pressure $P$ along the centerline of the channel, b) distributions of the dimensionless average pressure $P_{\text{average}}$, and c) pressure and density gain due to the pumping of the device.]

6. Conclusions
It has been proven that thermal transpiration in the slip flow regime can be numerically simulated using commercial CFD codes, if the correct boundary conditions at the walls are used and handled in an appropriate way. The numerical model that has been developed showed a very good agreement with analytical and other numerical approaches when compared for benchmark cases.

The present numerical model proved that Knudsen pumps based on curved channels can be efficient in the slip flow regime. The simulation results are close to the numerical data obtained from a kinetic approach [18, 19].

Motivation of the present project is the development of a simulation tool which would be useful in the design of Knudsen pumps. At the moment, a multistage Knudsen pump with curved segments (see figure 2b) at millimetric scale has been designed, taking into account manufacturing limitations and based on the numerical results, and is being fabricated at the Karlsruhe Institute of Technology (Germany). Its performance will be experimentally analyzed and compared with the numerical results and its structure and operation will be optimized.

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