Asymptotic Modeling of Flows in Micro-Channel by Using Macroscopic Balance Equations

Renée Gatignol and Cédric Croizet

Université Pierre et Marie Curie (UPMC, Paris 6) & CNRS, Institut Jean le Rond d'Alembert
4 place Jussieu, 75005 Paris, France

Abstract. The introduction of a small parameter related to a micro-channel geometry and the application of the Principle of Least Degeneracy to the dimensionless Navier-Stokes equations produce models for the study of micro-channel flows with small Mach number and small or moderate Knudsen number. The first approximation of the asymptotic solution is calculated for a steady gas flow inside a micro-channel with a temperature gradient along the walls. In addition, Direct Simulation Monte Carlo (DSMC) method is used to analyze the same problem and some comparisons are presented. Analytical asymptotic solutions and DSMC numerical simulations found to be in very good agreement.

Keywords: Microfluidics, Micro-channel, Rarefied Gas, DSMC Simulation.
PACS: 05.10.Ln – 47.10.ad – 47.11.Mn – 47.45.Gx – 47.61.-k

INTRODUCTION

Micrometric apparatii are present in various fields of technology such as process engineering, heat exchangers, etc. For the description of gas flows with heat exchanges in micro-channels which occur in these systems, the Direct Simulation Monte Carlo (DSMC) method is well adapted. However, this method is computationally expensive. Our purpose is to study flows of compressible fluids in micro-channels by using an asymptotic macroscopic approach [1]. The flow equations are the usual Navier-Stokes equations for mass, momentum and energy, with first order jump conditions for the velocity and the temperature written along the walls of the micro-channel.

A large number of theoretical, numerical and experimental work about gas flows in micro-channels through different methods are available. Depending on the Knudsen number, these flows are considered to be in the continuum, slip-flow, transitional, or free molecular regimes [2,3,4,5,6]. The DSMC method is successful in the case of transitional regimes; consequently it is relevant to the study of gas flows in micro-systems [7,8]. Lattice Boltzmann methods are also an interesting approach to compute these flows, particularly for complex geometries, although very few applications have been carried out at the present time [9].

In this paper, an asymptotic modeling is proposed for thermal compressible gas flows in micro-channels with small Mach numbers M and small or moderate Knudsen numbers Kn. Slip boundary conditions of first order for the velocity and the temperature are taken into account [5,6]. It is possible to yield steady analytical asymptotic solutions in order to describe the physical phenomena. In addition, these solutions are compared with DSMC simulations obtained with the code DS2V of Bird [10]. Asymptotic solutions and DSMC simulations are in a very good agreement.

EXAMPLES OF GAS FLOWS IN MICRO-CHANNELS BY DSMC METHOD

Let us consider the steady laminar thermal flow of a gas in a two-dimensional micro-channel of length ℓ and width h, with no volumetric force or heat source. The complete geometry is shown on Fig. 1: It consists of two areas of identical sizes (length $\ell' = 7\ \mu\text{m}$, width $h' = 5\ \mu\text{m}$) filled with a molecular gas, Nitrogen, and connected to each other by a micro-channel of length $\ell = 10\ \mu\text{m}$ and width $h = 1\ \mu\text{m}$. The axis of the micro-channel is a symmetry axis. The gas is flowing from one area to the other one through the channel. We begin with some DSMC simulations. The DS2V code is used in its steady version [10]. The initial values for the pressure and temperature, P_{in} and T_{in}, are given in the area to the left upstream of the channel, whereas P_{out} and T_{out} denote the initial values in the area to the right downstream. The constant pressure boundary conditions defined by Bird [10] are introduced in the left and right ends. The model of diffuse reflection with perfect accommodation is applied to describe the interaction of molecules with the channel walls and the Variable Hard Sphere (VHS) model is chosen for the intermolecular collisions. On the micro-channel walls, the temperature T_w depends on the longitudinal variable with a constant gradient and it varies from T_{in} to T_{out}. The computation is performed with the following numerical values: $P_{out} = 100$ kPa, $T_{out} = 300$ K, $110 \text{ kPa} \le P_{in} \le 200 \text{ kPa}$, $300 \text{ K} \le T_{in} \le 400 \text{ K}$ (simulations n°1 to n°9 on Table 1). The number of test molecules is about 7.2×10^5, and the number of samples about 7.5×10^4. The noise levels for pressure and temperature are deduced from Hadjiconstantinou *et al.* formulas [11] and are of order 0.25% and 0.15% respectively.

The following notations are introduced: P_i and T_i denote the pressure and temperature values at the centre of the entrance section of the micro-channel ($x = 0$ μm), P_o and T_o at the centre of the exit section ($x = 10$ μm). The DSMC simulations give, among other output quantities, the values P_i, T_i, P_o, T_o, and the Mach number and the Knudsen number at the centre of the micro-channel ($x = 5$ μm, $y = 0$ μm). The Knudsen number Kn varies from 0.035 to 0.066 and Mach number M from 0.0014 to 0.22 (Table 1). In addition, in Table 1, we have given three results from literature. The first one, reference [6], corresponds to a numerical result for a micro-channel with $\ell = 4.52$ μm and $h = 0.226$ μm. The second [7] is a simulation result in a channel with $\ell = 10$ μm and $h = 1$ μm. Finally, the third one is an experimental result [12] where the dimensions of the channel are $\ell = 5000$ μm and $h = 4.48$ μm. In these last results, the Mach number is small but the Knudsen number is not so small. In short, Mach number may be considered as small and Knudsen number as small or moderate.

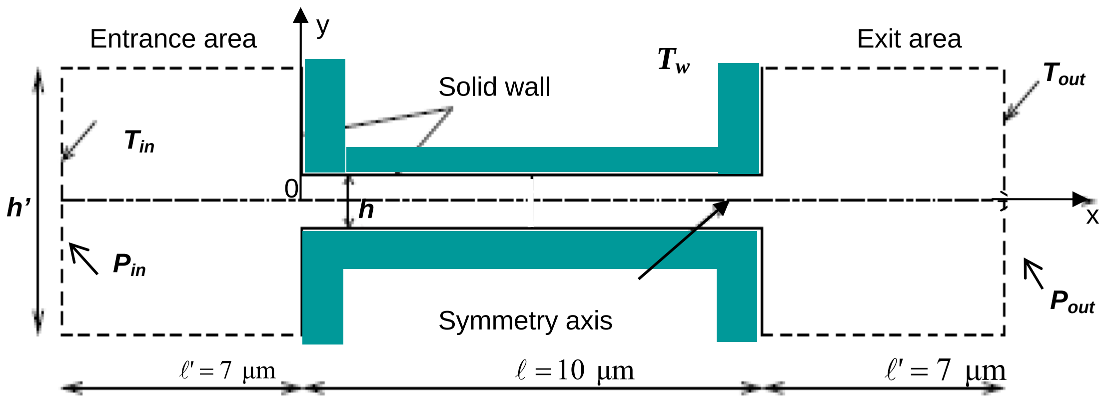

FIGURE 1. Micro-channel geometry for the DSMC simulations.

TABLE 1. Numerical values on the left and right ends and at the centre of the micro-channel.

	P_{in} kPa	T_{in} K	P_{out} kPa	T_{out} K	P_i kPa	T_i K	P_o kPa	T_o K	Kn	M
Simulation n°1	130	300	100	300	131	299	99	301	0.047	0.075
Simulation n°2	140	300	100	300	141	299	98.8	301	0.045	0.097
Simulation n°3	160	300	100	300	162	298	97.5	302	0.041	0.14
Simulation n°4	180	300	100	300	182	298	96.5	302	0.038	0.18
Simulation n°5	200	300	100	300	202.5	298	96	302	0.035	0.22
Simulation n°6	130	400	100	300	118	392	101	303	0.061	0.04
Simulation n°7	120	400	100	300	109	391	101	302	0.064	0.02
Simulation n°8	111	400	100	300	101	392	101	302	0.066	0.0014
Simulation n°9	110	400	100	300	100	392	101	302	0.066	0.0033
Karniadakis *et al.* [6]	360	300	100	300					0.3	0.007
Aktas *et al.* [7]	133	300	100	300					1.1	0.04
Colin *et al.* [12]	252		102.6						0.1	

ASYMPTOTIC MODELING OF GAS FLOWS IN MICRO-CHANNELS

A frame of reference $(O; x, y)$ is attached to the micro-channel with length ℓ and width h (Fig. 1). The walls located at $y = \pm h/2$ are at rest with the same temperature distribution $T_w(x)$. The upstream ($x = 0$) and downstream ($x = \ell$) boundary conditions for the pressure and the temperature will be specified further. The Navier-Stokes equations (1) to (4) are written for an ideal gas with shear viscosity μ and thermal conductivity k. The pressure, volumetric mass, temperature, longitudinal and transversal velocities are denoted p, ρ, T, u and v respectively. The ideal gas law is $p = r\rho T$ with $r = c_p - c_v$ where c_p and c_v are the heat capacities at constant pressure and constant volume. The physical coefficients μ, k, c_p and c_v are assumed to be constant. The indexes x and y denote the partial derivatives in the x and y directions.

$$(\rho u)_x + (\rho v)_y = 0 \tag{1}$$

$$\rho\left(u u_x + v u_y\right) + p_x - \mu\left(\frac{4}{3}u_{xx} + u_{yy} + \frac{1}{3}v_{xy}\right) = 0 \tag{2}$$

$$\rho\left(u v_x + v v_y\right) + p_y - \mu\left(\frac{4}{3}v_{yy} + v_{xx} + \frac{1}{3}u_{xy}\right) = 0 \tag{3}$$

$$\rho c_v\left(u T_x + v T_y\right) + p\left(u_x + v_y\right) - \mu\left(\frac{4}{3}u_x^2 + \frac{4}{3}v_y^2 - \frac{4}{3}u_x v_y + u_y^2 + v_x^2 + 2u_y v_x\right) - k\left(T_{xx} + T_{yy}\right) = 0 \tag{4}$$

The ratio of heat capacities, γ, the Prandtl number, Pr, and the local mean free path, λ, are classically defined by:

$$\gamma = \frac{c_p}{c_v}, \qquad Pr = \frac{\mu c_p}{k}, \qquad \lambda = \frac{\mu}{\rho}\sqrt{\frac{\pi}{2rT}} \tag{5}$$

The first order boundary conditions on the two walls $y = \pm h/2$ [5,6,12] are given as:

$$\{u\}_{y=\pm h/2} = \left\{\mp\lambda\frac{\partial u}{\partial y} + \frac{3}{4}\frac{\mu}{\rho T}\frac{\partial T}{\partial x}\right\}_{y=\pm h/2}, \quad \{v\}_{y=\pm h/2} = 0, \quad \{T\}_{y=\pm h/2} = T_w \mp \left\{\frac{2\gamma}{\gamma+1}\frac{\lambda}{Pr}\frac{\partial T}{\partial y}\right\}_{y=\pm h/2} \tag{6}$$

The characteristic scales for the longitudinal and transversal lengths, the longitudinal and transversal velocities, the pressure, the temperature and the volumetric mass are respectively denoted ℓ and h, U_c and V_c, P_c, T_c and ρ_c (with $P_c = r\rho_c T_c$). Then, we write down the conservation equations (1) to (4) with the dimensionless quantities $\bar{x}$, $\bar{y}$, $\bar{u}$, $\bar{v}$, $\bar{p}$, $\bar{\rho}$ and $\bar{T}$ defined as $x = \ell\,\bar{x}$, $y = h\,\bar{y}$, $u = U_c\,\bar{u}$, $v = V_c\,\bar{v}$, $p = P_c\,\bar{p}$, $\rho = \rho_c\,\bar{\rho}$ and $T = T_c\,\bar{T}$. As usual for gas flows in micro-channels, the small parameter $\varepsilon = h/\ell$ is introduced, as well as the Reynolds number Re, the Knudsen number Kn and the Mach number M:

$$\varepsilon = \frac{h}{\ell}, \quad M = U_c\sqrt{\frac{\rho_c}{\gamma P_c}}, \quad Kn = \frac{1}{h}\frac{\mu}{\rho_c}\sqrt{\frac{\pi}{2rT_c}}, \quad Re = \frac{\rho_c U_c h}{\mu} = \frac{M}{Kn}\sqrt{\frac{\pi\gamma}{2}} \tag{7}$$

Due to the Principe of Least Degeneracy [1], we must keep the two terms in the dimensionless mass law; we then obtain $V_c = \varepsilon U_c$. In order to look for the degenerate systems, we set: $Kn = \varepsilon^\alpha$, $M = \varepsilon^\beta$. A comparison of the order of magnitude for the different terms in the dimensionless balance equations for momentum and energy, gives one degeneracy solution with $\alpha = 0$ and $\beta = 1$, among others [8]. This particular one corresponds to small Mach numbers and to Knudsen numbers of order unity. From this point on, we substitute $M = \varepsilon M_0$ and $Kn = Kn_0$ where both M_0 and Kn_0 are of order unity. For the sake of simplicity, we omit the use of bars to denote the dimensionless variables and we obtain:

$$(\rho u)_x + (\rho v)_y = 0 \tag{8}$$

$$\gamma M_0^2\,\varepsilon^2\left(\rho u u_x+\rho v u_y\right)+p_x-\sqrt{\frac{2\gamma}{\pi}}\,M_0 Kn_0\left(u_{yy}+\varepsilon^2\,\frac{4u_{xx}+v_{xy}}{3}\right)=0 \tag{9}$$

$$\gamma M_0^2\,\varepsilon^4\left(\rho u v_x+\rho v v_y\right)+p_y-\sqrt{\frac{2\gamma}{\pi}}M_0 Kn_0\,\varepsilon^2\left(\frac{4v_{yy}+u_{xy}}{3}+\varepsilon^2\,v_{xx}\right)=0 \tag{10}$$

$$\begin{aligned}&\rho\left(uT_x+vT_y\right)+(\gamma-1)\left(u_x+v_y\right)p-\sqrt{\frac{2\gamma}{\pi}}(\gamma-1)M_0 Kn_0\,\frac{4}{3}\varepsilon^2\left(u_x^2+v_y^2-u_x v_y\right)\\&-\sqrt{\frac{2\gamma}{\pi}}(\gamma-1)M_0 Kn_0\left(u_y^2+\varepsilon^4 v_x^2+2\varepsilon^2 u_y v_x\right)-\sqrt{\frac{2\gamma}{\pi}}\,\frac{1}{Pr}\,\frac{Kn_0}{M_0}\left(T_{xx}+\frac{1}{\varepsilon^2}T_{yy}\right)=0\end{aligned} \tag{11}$$

In addition, the dimensionless ideal gas law takes the simple form $p=\rho T$. The boundary conditions (6) are now written with dimensionless variables. We have, for $y=\pm 1/2$:

$$u=\mp\,Kn_0\,\frac{1}{\rho\sqrt{T}}\frac{\partial u}{\partial y}+\frac{3}{4}\sqrt{\frac{2}{\pi\gamma}}\frac{Kn_0}{M_0}\frac{1}{\rho T}\frac{\partial T}{\partial x}\quad,\quad v=0\quad,\quad T=T_w\mp\frac{2\gamma}{\gamma+1}\frac{Kn_0}{Pr}\frac{1}{\rho\sqrt{T}}\frac{\partial T}{\partial y} \tag{12}$$

It is important to note that the small parameter ε does not appear in (12). If the boundary conditions (6) had been written with second order terms [5,6], then all these additional terms would appear in Eq. (12).

THE ASYMPTOTIC SOLUTION IN THE FIRST APPROXIMATION

In order to find the first approximation of the problem (8) to (12), we substitute: $u=\tilde{u}+O(\varepsilon^2)$, $v=\tilde{v}+O(\varepsilon^2)$, $\rho=\tilde{\rho}+O(\varepsilon^2)$, $p=\tilde{p}+O(\varepsilon^2)$, $T=\tilde{T}+O(\varepsilon^2)$. The terms $O(\varepsilon^2)$ are neglected and we obtain:

$$\left(\tilde{\rho}\,\tilde{u}\right)_x+\left(\tilde{\rho}\,\tilde{v}\right)_y=0\quad,\quad \tilde{p}_x-\sqrt{2\gamma/\pi}\,M_0 Kn_0\,\tilde{u}_{yy}=0\quad,\quad \tilde{p}_y=0\quad,\quad \tilde{T}_{yy}=0 \tag{13}$$

$$\tilde{u}=\mp Kn_0\,\frac{1}{\tilde{\rho}\sqrt{\tilde{T}}}\frac{\partial\tilde{u}}{\partial y}+\frac{3}{4}\sqrt{\frac{2}{\pi\gamma}}\frac{Kn_0}{M_0}\frac{1}{\tilde{\rho}\tilde{T}}\frac{\partial\tilde{T}}{\partial x}\quad,\quad \tilde{v}=0\quad,\quad \tilde{T}=T_w\mp\frac{2\gamma}{\gamma+1}\frac{Kn_0}{Pr}\frac{1}{\tilde{\rho}\sqrt{\tilde{T}}}\frac{\partial\tilde{T}}{\partial y} \tag{14}$$

In equation (14), the dimensionless temperature T_w on the two walls depends only on the longitudinal variable x. As a consequence of (13), $\tilde{p}$ depends only on the coordinate x, and $\tilde{T}$ is a linear function of the variable y with its coefficients depending on x. By using the third condition in (14), due to the symmetry of the problem, one sees that $\tilde{T}=T_w$. The second equation in (13), the ideal gas law $\tilde{p}=\tilde{\rho}\tilde{T}$ and the first boundary condition in (14) are used to write the expression of the longitudinal velocity:

$$\tilde{u}=\frac{\tilde{p}_x}{\sqrt{2\gamma/\pi}\,M_0 Kn_0}\left(\frac{y^2}{2}-\frac{1}{8}-\frac{Kn_0\sqrt{T_w}}{2\,\tilde{p}}\right)+\frac{3\sqrt{2/\pi\gamma}\,Kn_0}{4\tilde{p}\,M_0}\frac{dT_w}{dx} \tag{15}$$

Now we consider to the first equation in (13), the ideal gad law $\tilde{p}=\tilde{\rho}\,T_w$ and the boundary condition for $\tilde{v}$ in (14). The equation is integrated between $y=-1/2$ and $y=1/2$ and at the upstream and downstream ends of the micro-channel, we set the pressures to be: $\tilde{p}=\tilde{p}_i$ for $x=0$ and $\tilde{p}=\tilde{p}_o$ for $x=1$. The pressure $\tilde{p}=\tilde{p}(x)$ is obtained by solving a second order differential equation with boundary conditions,

$$\frac{d}{dx}\left\{\frac{\tilde{p}\,\tilde{p}_x}{6\,Kn_0 T_w}+\frac{\tilde{p}_x}{\sqrt{T_w}}-\frac{3\,Kn_0}{\pi\,T_w}\frac{dT_w}{dx}\right\}=0\quad,\quad \{\tilde{p}\}_{x=0}=\tilde{p}_i\quad,\quad \{\tilde{p}\}_{x=1}=\tilde{p}_o \tag{16}$$

In the particular case where T_w is constant, the pressure and the longitudinal velocity have known explicit expressions [5,6]. With a temperature gradient along the walls, Eq. (15) shows that the flow velocity and the slip velocity along the wall will depend on this gradient, i.e. the dynamic and thermal effects are coupled. In order to obtain $\tilde{p}$, it is necessary to perform a numerical integration of Eq. (16). Then, the velocity $\tilde{u}$ is deduced from (15). Three cases for the dimensionless temperature $T_w(x)$ along the channel walls are chosen: a) $T_w = 1+(1-2x)/7$, b) $T_w = 1+(1-4x)7$ for $0 \le x \le 0.5$ and $T_w = 6/7$ for $0.5 \le x \le 1$, c) $T_w = (2/7)(-2x^2+x+1)+6/7$. In each case $Kn_0 = 1/6$, $p_i = 2.998$ and $p_o = 2.306$. In Fig. 2, the three pressure solutions of equation (16) are given, and we observe that these pressure profiles are different. In Fig. 3, the associated velocity profiles in the micro-channel section x = 0.4 are shown. The effect due to the temperature gradient is obvious.

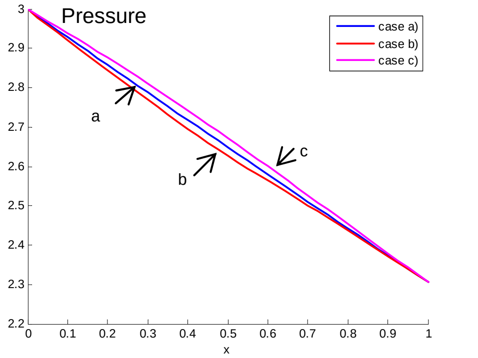

FIGURE 2. Pressure profiles along the micro-channel

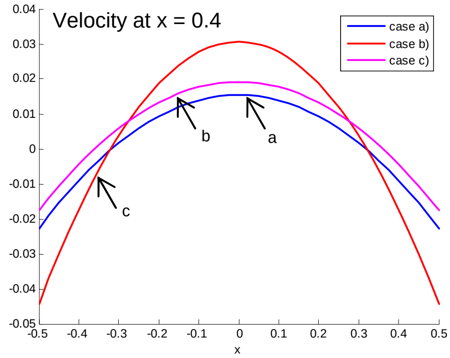

FIGURE 3. Velocity profiles in the section x= 0.4

ASYMPTOTIC SOLUTION AND DSMC SIMULATION COMPARISON

The aim of this section is to compare, for a number of flows inside a micro-channel, the results given by DSMC simulations and by the asymptotic method. For each simulation (n°1 to n°9), the pressures P_{in} and P_{out} and the temperatures T_{in} and T_{out} take different values, as shown in Table 1. The DS2V code is used in its steady version [10]. At its last stage, the code yields the steady solution for the flow inside the channel. The values P_i, T_i, P_o, T_o are taken from the simulation results (see Table 1). The following characteristic scales are introduced: $T_c = (T_i + T_o)/2$, $P_c = (3\mu/h)\sqrt{2\pi r T_c}$, $U_c = (3h/\ell)\sqrt{2\pi r T_c}$. Then $\tilde{p}_i = P_i/P_c$ and $\tilde{p}_o = P_o/P_c$. By using these values as data for the solution of (15) and (16), one obtains the solution through the asymptotic method.

Two sets of result are now shown. First, the particular case where T_w is a constant is considered (simulations n°1 to n°5). In Fig. 4, the dimensionless pressure profiles along the micro-channel axis are presented with the solid lines corresponding to the asymptotic solutions and the dots to the DSMC simulations. The two results are in very good agreement. In Fig. 5, the difference between the two results, *i.e.* $100(1-P_{AS}/P_{DSMC})$, is shown. The fluctuations between the two solutions are smaller than 0.5%. For the longitudinal velocity, similar comparisons have been made, and give fluctuations between asymptotic and DSMC results less than 2.5% for the simulations n°1, n°2 and n°3. As in many studies [5,6,8,12], we note the nonlinear evolution of the pressure (solid lines compared to the dashed lines on Fig. 4).

The second result set corresponds to the four simulations n°6 to n°9 where the temperature decreases linearly from 400 to 300 K along the micro-channel walls, and where the entrance pressure P_{in} varies from 130 to 110 kPa. In Fig. 6 the pressure and the longitudinal velocity profiles along the channel axis are presented (here, all the quantities are dimensional and $X = x - 5\,\mu\text{m}$). The dots correspond to the DSMC simulation values. For the pressure, we present the asymptotic solution of Eq. (16) shown by a solid line. As before, the asymptotic and DSMC results, are in good agreement. Depending on the simulation conditions, the pressure gradient inside the channel may be negative (n°6, n°7), near zero (n°8), or positive (n°9). The associated velocity is positive (n°6, n°7), near zero (n°8) or negative (n°9). This conclusion is in agreement with Eq. (15) where a negative pressure gradient increases the velocity and a negative temperature gradient decreases the velocity. This thermal effect is well known in the scope of rarefied gas dynamics [14].

CONCLUSION

The asymptotic analysis of the flow in a micro-channel leads to solutions in good agreement with DSMC numerical simulations, in the flow configurations considered here. The analytical expressions deduced from the asymptotic process underline the influence of a temperature gradient along the walls. In particular, it is clear from the expression for the longitudinal velocity that a negative temperature gradient can induce a change in the flow direction.

The DSMC simulations n°1 to n°9 were done on a personal computer requiring a computational time to obtain each steady result of about 170 hours. It is important to emphasise that to obtain the asymptotic solution is, in contrast, very fast.

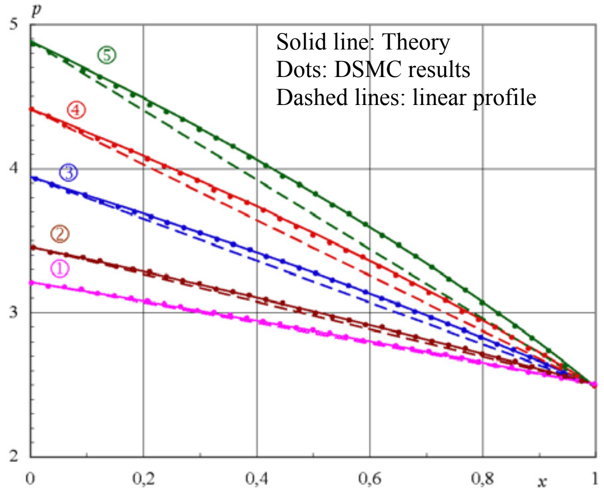

FIGURE 4. Dimensionless pressure profiles along the micro-channel axis for the simulations n°1 to n°5.

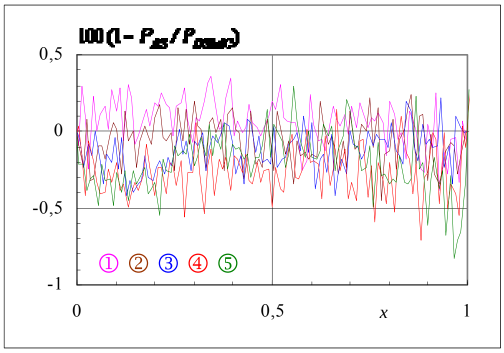

FIGURE 5. The pressure fluctuations for the simulations n°1 to n°5.

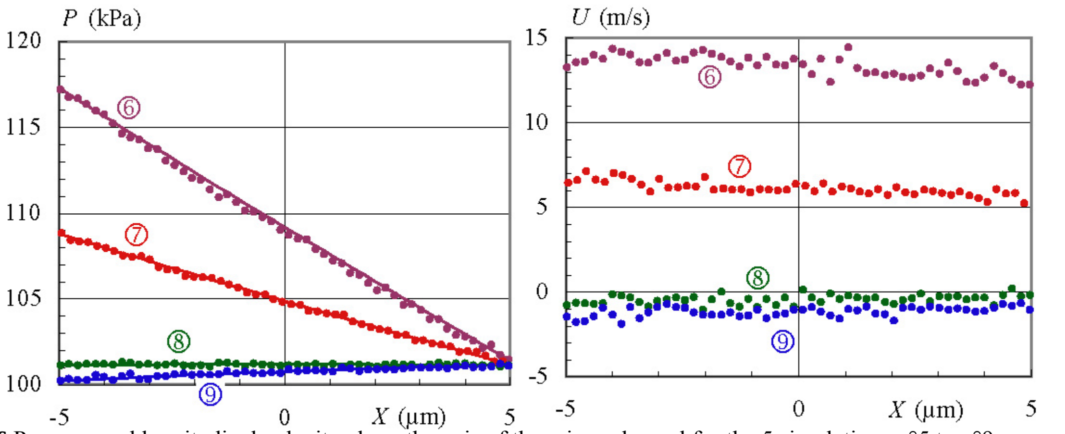

FIGURE 6 Pressure and longitudinal velocity along the axis of the micro-channel for the 5 simulations n°5 to n°9.

REFERENCES

1. M. Van Dyke, *Perturbation methods in fluid mechanics,* New-York, Academic Press, 1964.
2. S. Chapman, T.G. Cowling, *The mathematical theory of non-uniform gases,* Cambridge, University Press Cambridge, 1952.
3. M. Kogan, R*arefied Gas Dynamic",* New-York, Plenum Press, 1969.
4. G.M. Bird, *Molecular gas dynamics and the direct simulation of gas flows*, New-York, Oxford University Press, 1994.
5. S.G. Kandlikar, S. Garimella, D. Li, S. Colin, M.R. King, *Heat transfer and fluid flow in minichannels and microchannels*, Paris, Elsevier, 2005.
6. G. Karniadakis, A. Beskok, *Microflows – Fundamentals and Simulation*, New-York, Springer, 2002.
7. O. Aktas, N.R. Aluru, U. Ravaioli, *Journal of Microelectromechanical Systems*, **10**, 538-549 (2001)
8. D. Ameur, C. Croizet, F. Maroteaux, R. Gatignol, in "*Rarefied Gas Dynamics-2008"*, ed. T. Abe, AIP Conference Proceedings 1084, Kyoto, 2009, 1129-1134
9. J.W. Shim, R. Gatignol, in "*Rarefied Gas Dynamics-2008"*, ed. T. Abe, AIP Conference Proceedings 1084, Kyoto, 2009, 1033-1038.
10. G. M. Bird, DSMC of Graeme Bird, http://gab.com.au
11. N.G. Hadjiconstantinou, A.L. Garcia, M.Z. Bazant, G. He, *Journal of computational physics*, **187**, 274-297 (2003).
12. S. Colin, P. Lalonde, R. Caen, *Heat Mass Engineering*, **25**, 23-30, (2004).
13. R. Gatignol, C. Croizet, Second European Conference on Microfluidics (µFlu10), Toulouse, December 2010.
14. Y. Sone, *Molecular gas dynamics*, Boston, Birkhausen, 2007.