DSMC SIMULATION OF PRESSURE-DRIVEN FLOWS AND HEAT TRANSFER IN MICROFILTERS

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Abstract. The gas flow in a microchannel is a problem which one encounters in a large number of practical applications such as microfilters or micro cooling systems. These flows are rarefied and are characterized by Knudsen number in the range of transition flows. In this paper a direct simulation of Monte Carlo has been used to calculate the flow in a microchannel. A parametric study on different geometries of microfilters has been done.

Keywords: Rarefied gas, DSMC, microchannel flows, slip flow
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INTRODUCTION

Significant research efforts are devoted to Micro Electro Mechanical Systems (MEMS), in order to develop these systems for industrial applications. Microtechnologies can be found in several domains: Instrumentation, advanced energy systems, etc. More precisely, this paper deals with microfilters. They have several applications. For example, diesel particulate filters are used in the exhaust system automotive engine. However, these systems are not very efficient when the size of the particles is very small (around the nanometer) and, consequently, their optimization is a subject of interest for the scientific community [1, 2]. Our objective is to understand the flow behavior in different conditions in a microfilter composed of thin perforated membranes [3]. Our attention is focused on the gas flow without particles. Due to the size of the system, non continuum effects must be taken into account in MEMS. Consequently, the gas flow cannot be modeled in the frame of continuum hypothesis because the microscopic and wall effects are very important. The rarefaction is characterized with the Knudsen number: $Kn = \lambda/d$ where λ is the mean free path and d the characteristic width of the microchannel. In these applications, the order of the Knudsen number is one and the flow is weakly rarefied. The gas flow is studied using Direct Simulation Monte Carlo and the DS2V code of G. Bird [1].

The execution of DSMC follows the fundamental principles described in [4]. This statistical and particle-based method is inspired by a deterministic approach. A small number of particles are assumed to be representative of all the real particles of the gas and are simulated and followed in time. The flow field is subdivided in very small cells compared to the characteristic size of the flow so that the macrocospic quantities of the flow can be assumed as constant in each cell. The simulation method is based on a splitting of the two main phenomena that determine the motion of a molecule: Displacement and collision. The time step is chosen to be smaller than the mean flight time [5, 6, 7]. During each time step, a particle undergoes a free flight without collision with other other particles. If during its free flight the particle hits a solide surface, its velocity is modified according to a model of interaction with the wall. In this study a diffuse reflexion with perfect accommodation is used, that is that the accommodation coefficient is equal to one. At the end of the time step, the simulated particles undergo collision according to a statistical model and, consequently, the past of the simulated molecules is forgotten. The collision partners are selected in the same cell by the NTC method which allows to respect the real collision frequency of the gas [4, 8]. The collisions represent the most important simulation step. The VHS (Variable Hard Sphere) collision model is used: The molecules are assumed to be rigid spheres and their diameter is assumed to be variable with the velocity of their collision partners. This model allows to reproduce for the viscosity a realistic power law in the temperature T (as with the IPL model) and to keep

[1] http://www.gab.com.au/

easy calculations for the collisions (as in the case of the HS model).

The aim is to describe the gas flow through the microfilter and to build reliable correlations with their validity domain, in order to predict the pressure drop and the effects of heat transfer. Initially, we study the pressure and velocity variations of an isothermal flow through various microfilters. The aim is to predict the best geometry while keeping the same physical problem. After the choice of the microfilter according to the first results obtained, we look at the variation of some parameters as the Mach number and the slip velocity. The velocity profile as well as the flow rate through a given section will be compared with an exact solution of Poiseuille-Hagen flow with first order slip. Finally a problem with a variation of temperature between the entry and the exit of the chosen microfilter is introduced. In that case, the same pressure boundary conditions as in the case with constant temperature are kept.

In the present work, the flow is assumed to be normal to the membrane, the microsized holes are identical and their distribution is periodic. Consequently, periodic boundary conditions allow to reduce the simulation domain to one hole (Fig. 1). The flow field is assumed to be coplanar (Fig. 1). The temperature and the pressure of the inlet (P_{in}) and the outlet (P_{out}) are specified: $P_{in} = 1.3 \times 10^5$ Pa and $P_{out} = 10^5$ Pa. A diffuse reflection condition is assumed at the walls and their temperature T_w is uniform. The first simulations are applied to an isothermal flow of Nitrogen at a temperature equal to 300 K. At the boundary sections AB, EF and x_1x_2, symmetric conditions are adopted. A second set of simulations is actually in progress: The boundary conditions are the same as in the first calculations but the temperature at the inlet is raised to 450 K.

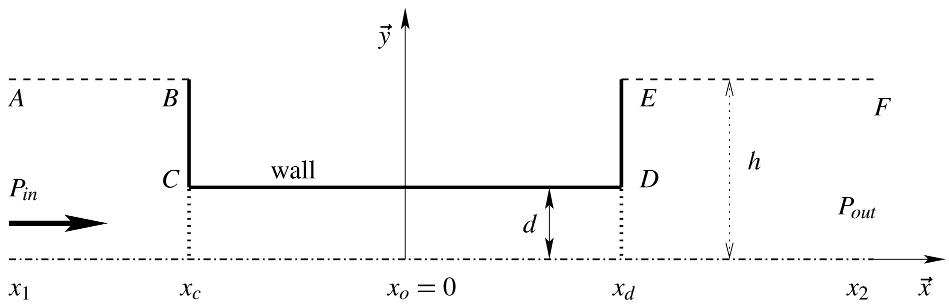


FIGURE 1. Filter geometry

RESULTS AND DISCUSSION

The main disadvantage of the DSMC method is its very high cost in computation time. In order to find an optimal compromise between the simulation time and the quality of the results, a parametric study of the length of entry (AB) compared to that of exit (EF) is made. Dependence of the characteristics of the flow on the length of entry is studied by using several geometries given in table 1. For all the calculations the channel length is fixed at $CD = 10\mu$m, the exit length is $EF = 7\mu$m ; the diameter of the microchannel and the height of the area of entry are respectively fixed equal to $d = 0.5\mu$m and to $h = 2.5\mu$m.

The number of molecules simulated during each calculation is about 6×10^5 molecules. The temperature of reference of the gas is $273.15K$, the diameter of the Nitrogen molecules is 4.17×10^{-10}m and the mass of each molecule is 4.65×10^{-26} kg. The real computation time for each microfilter is about a few hundred hours. The characteristics of the computer are the following : CPU 2 × 3.00 GHZ and 2 GB RAM. In this statistical method the noise level, is inversely proportional to the square root of the number of samples [7]. Consequently the number of required samples depends on the level of desired accuracy. In this study, the number of samples is about 7×10^5.

TABLE 1. Dimensions of different filters and simulation results

	Filter I	Filter II	Filter III	Filter IV	Filter V	Filter VI
AB (μm)	3	4	5	6	7	8
Pressure at x_1 (Pa) x10^5	1.3346	1.3298	1.3259	1.3260	1.3236	1.3225
Pressure at x_2 (Pa) x10^5	0.9950	0.9969	1.0001	0.9982	0.9980	0.9992
P_{x_1}/P_{x_2}	0.745	0.749	0.754	0.752	0.754	0.755
Flow rate from DSMC (kg/s) x10^{-5}	1.40	1.38	1.36	1.36	1.35	1.35

Pressure

A first set of simulations for several lengths of the inlet zone (AB) (see Table 1), allows to optimize the domain dimensions in order to reach a good compromise between the required accuracy and the computation time. In all the cases, an overpressure is observed at the microchannel upstream. When the length of the inlet area decreases, the difference between the upstream pressure P_{in} and the pressure P_{x_1} calculated by the DSMC method increases. The table 1 shows this difference in absolute value. We note that the pressure difference is weaker in the microfilters (III) to (VI) in comparison with the microfilters (I) and (II). Moreover, the difference between P_{out} and P_{x_2} is less important for all the geometries. Overpressure at the upstream was noticed in [3], this could be explained with the reinjection condition in the calculation field of the molecules which leave it. The microfilter (VI) needs 480 hours of computation and the microfilter (V) needs 380 hours. Consequently, we can conclude that the geometry of the microfilter (V) presents the best compromise between the optimization of the computing times and the error on the pressure at the entry and the exit.

For the filter (V), the evolution of the pressure along the $\vec{x}$ axis for differents value of y is given in (Fig. 2). In order to analyse the behavior of the flow near the wall of the microchannel, three interesting values for y are chosen: $y = 0$ (channel axis), $y = 0,25 \times 10^{-6}$ m and $y = 0,45 \times 10^{-6}$ m (close to the solid surface). The results are identical for all the values of y: The maximum variation with the reference value (in $y = 0$) is 0.06%. Then, the pressure is quasi-independent of y.

The comparison of our results with those obtained in [3] for the same problem (but with a different simulation code) shows a good agreement. More simulations have been done and some cases are still in progress. In each case, we try to obtain the pressure drop: $\Delta P = P(x_d) - P(x_c)$ and the mass flow through the section x_o.

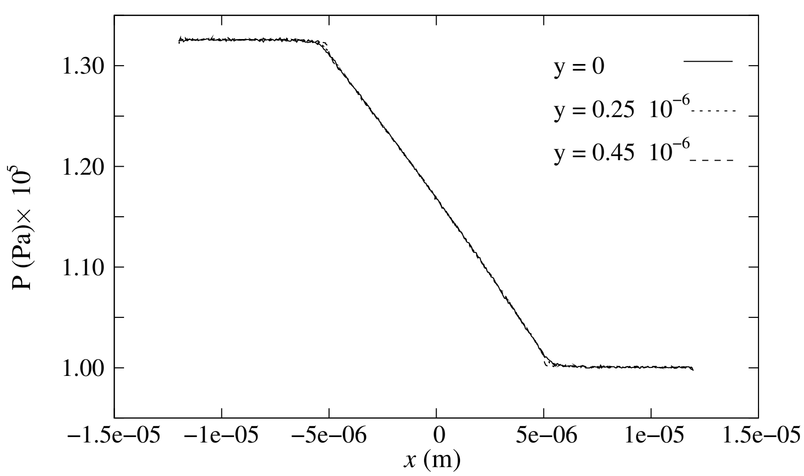


FIGURE 2. Pressure at various value of y

Velocity and slip on the walls

In this paragraph we are interested in the variation of the velocity components (u, v) and of the flow rate. The variation of the component u along axis in the microfilters (I) and (VI) is represented on (Fig. 3). It is noticed that the values of this component are close in the two microchannels. Nevertheless it is slightly higher when the entry length is smaller. The velocity y-component v is about 10^{-2} m/s in all the microfilters and the ratio (u/v) is about 10^{-3} and thus very small compared to one.

Velocity slip is observed for all the filters. The slip velocity on the channel wall is shown in (Fig. 4 (a)) for the microfilter (V). At the entrance and the exit of the channel the flow is undeveloped and, consequently, a rapid change of the slip velocity is observed. Beyond these regions, the flow is fully developed and then the slip velocity on the channel wall increases, as it was expected [3]. The velocity slip on the membrane walls at the entry and at the exit of the channel is shown in (Fig. 4 (b)). We observe that this slip velocity is equal to zero except in a small area around the hole because of high local Kn at the points C and D.

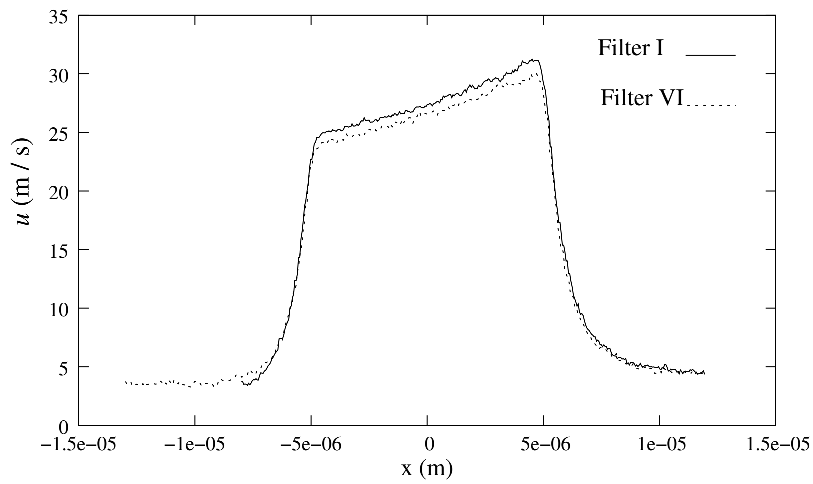
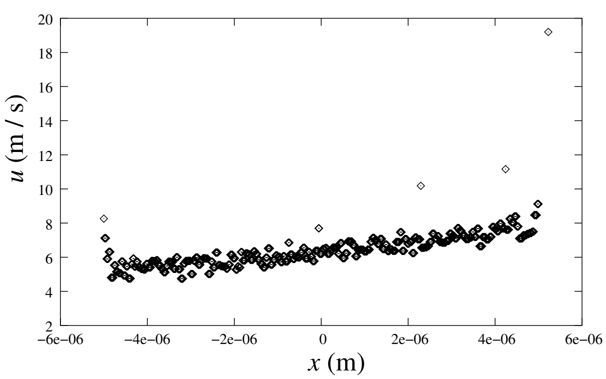
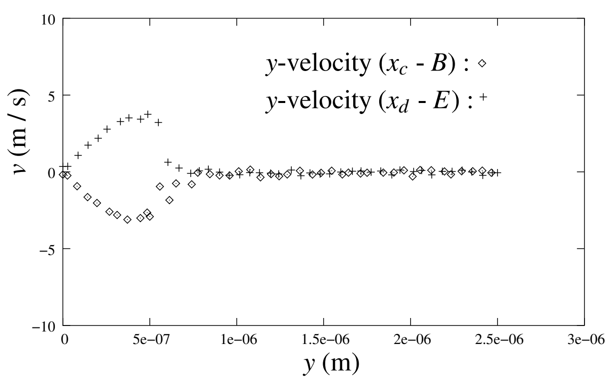


FIGURE 3. Longitudinal velocity along the x-axis of the filters (I) and (VI)



(a) : x-velocity a long the wall CD



(b) : y-velocity along the lines $(x_c - B)$ and $(x_d - E)$

FIGURE 4. Slip velocities in the microfilter (V)

In (Fig. 5), the Mach number levels in the microfilter (V) are plotted. This figure shows that the Mach number increases along the microchannel. Its maximum value is reached at the exit of the channel and it remains relatively small ($M_a < 0.2$). Consequently the effects of compressibility are negligible, and the flow is always in the range of the incompressible flows. In the case of the computationed filters, the Knudsen number vary from 10^{-2} to 10^{-1}. Consequently the incompressible flow inside the microchannel can be caculated by using Navier-Stokes equations with slip boundary conditions. Besides, the previous results show that the gradient of pressure is constant (Fig. 2)

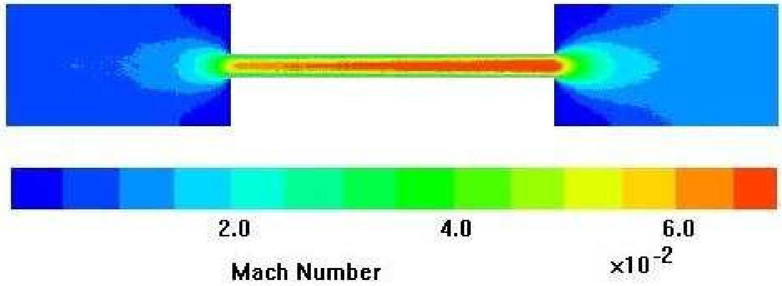


FIGURE 5. Mach number in the filter (V)

and that the pressure does not depend on y. In addition, the velocity transverse component v is small compared to the velocity longitudinal component u. Consequently, the Poiseuille-Hagen flow assumptions are almost satisfied. For all the DSMC calculations that have been carried out, the variation of the local density in section $x_0 = 0$ is about 10^{-3} kg/m^3. The pressure gradient, the density and the shear viscosity are assumed to be constant and their values are respectively: -3×10^9 , 1.44 kg/m^3 and 1.656×10^{-5} Pa×s. The velocity profile u in section $x_0 = 0$ of the

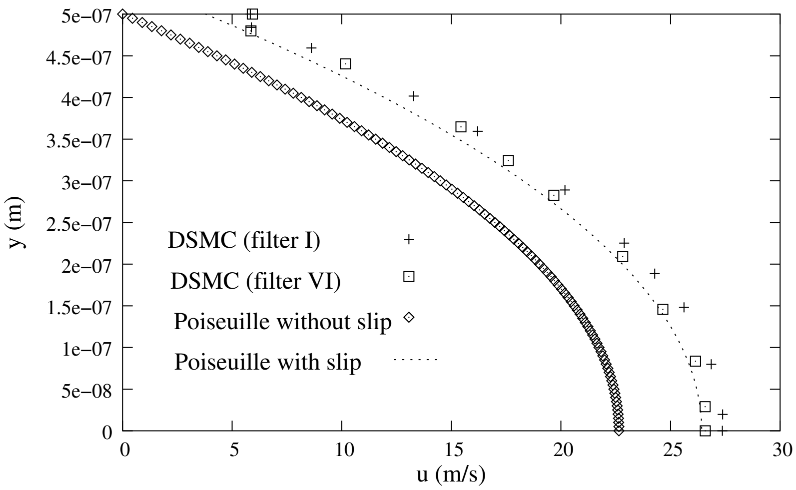


FIGURE 6. X-velocity along the X-axis of the filters (I) and (VI)

microchannel of filters (I) and (VI) was compared with the solution of Poiseuille-Hagen flow with slip condition. A first order Maxwell boundary condition has been used and then, the following velocity jump on the wall is introduced:

$$u \mid_{wall} = \frac{2-\sigma}{\sigma} \lambda \frac{\delta u}{\delta y}\Big|_{wall}$$

where $u \mid_{wall}$ is the mean velocity of the gas at the wall and σ an accomodation coefficient which summarizes the details of interaction of gas molecules with a given solid surface. This coefficient depends on the preparation details of the surface. Here the reflexion on the wall is assumed to be perfectly diffuse ($\sigma = 1$). In (Fig. 6) we plot the Poiseuille-Hagen velocity profile (with and without slip) and the datas coming from the DSMC simulations for the filters (I) and (VI). The results shows a good agreement between the two methods. Nevertheless, the results of the microfilter (VI) are better. The Poiseuille-Hagen model allows to calculate the flow rate. The value 1.36×10^{-5} kg/s is obtained. A comparison with the values obtained from the DSMC shows a good agreement in all the cases; nevertheless the agreement is better with the filters (III) and (IV).

Heat transfer problem

A second set of simulations has been done with different temperatures at the entry and the exit of the microfilter (III) in order to study the effects of the temperature gradient on the flow. They are still in progress. The outpout pressure is kept at 10^5 Pa and the input at 1.3×10^5 Pa. The temperature at the inlet is raised to 450 K and it is kept to 300 K on the wall and at the exit of the microfilter. In (Fig. 7), the temperature levels are plotted. We observe that the temperature in the microchannel does not increase very much. This could be explained by the action of the temperature difference that induce a gas motion which is opposed to the motion induced by the pressure gradient [7]. Further simulations are necessary to investigate these effects.

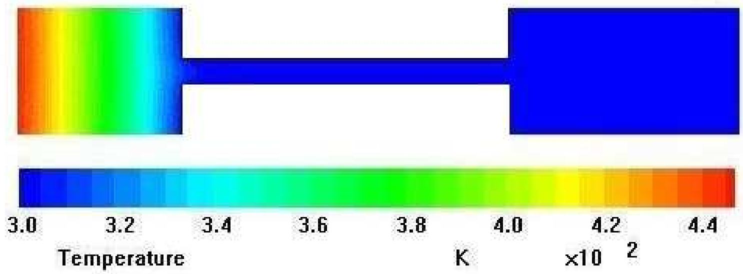


FIGURE 7. Temperature

CONCLUSION

A Nitrogen flow through a microchannel has been studied. The velocity profile as well as the flow rate were compared with a solution of the Poiseuille-Hagen flow. It is noticed that the agreement is better with the microfilters which have a larger entry length. The numerical results show that more the entry length is increased and more the pressure ratio (P_{out}/P_{in}) is increased. The velocity in the microfilters remains very low and the Mach number is about 10^{-2}. A good agreement between the results obtained by the Poiseuille-Hagen model with a Maxwell slip boundary condition and the DSMC is obtained.

This work is still in progress. Our first objective is, of course, to study the problem of heat transfer thoroughly. In the future more complex geometries and the transport of solid particles by the carrying fluid will be investigated.

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