The GASMEMS Network: rationale, programme and initial results

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Abstract GASMEMS is an Initial Training Network supported by the European Commission, which aims at training young researchers in the field of rarefied gas flows in MEMS, and at structuring research in Europe in the field of gas microflows in order to improve global fundamental knowledge and enable technological applications to an industrial and commercial level. The partners and the global objectives of this 4 year programme are detailed, and some initial results are presented. First experimental data about the flow of binary gas mixtures through rectangular microchannels are successfully compared with continuum and kinetic models, in the slip flow and early transition regimes. The behaviour of these mixtures has also been simulated in triangular microchannels, for the whole range of the Knudsen number, using a kinetic approach and the McCormack model. Heat transfer in plane microchannels has been numerically investigated, pointing out compressibility and rarefaction effects. The effect of thermal creep has been studied comparing BGK, S-model and ellipsoidal model with the solution from the full Boltzmann equation. A semi-analytical model of the Knudsen layer has been developed and used to simulate the problem of thermal transpiration in a microchannel. Gaseous flows through rough microchannels have been simulated using kinetic theory and DSMC method, the wall roughness being simulated as a highly porous medium of variable thickness.

Keywords: Gas Microflow, Rarefaction, Heat Transfer, Gas-Wall Interactions, European Network

1. Introduction

GASMEMS is a Marie Curie Initial Training Network (ITN) supported by the European Commission in the framework of the People Programme of the FP7. This network aims at training young researchers in the field of rarefied gas flows in Micro Electro Mechanical Systems (MEMS). This 4-year project has started in October 2008. Details are available on the website http://www.gasmems.eu.

The network is composed of 13 main and 4 associated partners:

- Institut National des Sciences Appliquées, Toulouse, France,
- Università di Bologna, Italy,
- Forschungszentrum Karlsruhe, Germany,
- University of Limerick, Ireland,
- University of Thessaly, Volos, Greece,
- Science and Technology Facilities Council, Warrington, UK,
- Institut of Mechanics, Bulgarian Academy of Sciences, Sofia, Bulgaria,
- Université de Provence, Marseille, France,
- Università degli Studi di Udine, Italy,
- Technische Universiteit Eindhoven, Netherlands,
- AOES Group BV, Leiden, Netherlands,
- University of Strathclyde, Glasgow, UK,
- Technische Universität Dresden, Germany,
- INFICON, Balzers, Liechtenstein,
- Laboratoire d'Analyse et d'Architecture des Systèmes, Toulouse, France,
- Institute for Health and Consumer Protection, JRC, Ispra, EC,
- ENEA Centro Ricerche Casaccia, Roma, Italy.

Gas flows in microsystems are of great interest for various applications that touch almost every industrial field. This diversity is typified through the following examples: fluidic microactuators for active control of aerodynamic flows, vacuum generators for extracting biological samples, mass flow and temperature micro-sensors, pressure gauges, micro heat-exchangers for electronic compo-

nents cooling or for chemical applications, micropumps and microsystems for mixing or separation for local gas analysis, mass spectrometers, vacuum and dosing valves.

Although research in Europe is active in the field of gas microflows, there was no global coordination of these research efforts at the European level. Thus, the two primary objectives of this ITN are:

- to structure research in Europe in the field of gas microflows in order to improve global fundamental knowledge and enable technological applications to an industrial and commercial level;
- to train 15 Early Stage Researchers (ESR), typically PhD Researchers, and 5 Experienced Researchers (ER) or Post-doctoral Researchers at a pan-European level, with the aim to providing them both a global overview on problems linked to gas flow and heat transfer in microsystems, and advanced skills in specific domains of this research field.

Three main scientific domains have been identified from the current state-of-the-art. For each one, the following objectives will be addressed in this ITN:

- **Dynamic aspects**: i) improvement of the existing analytical and numerical models; ii) theoretical and experimental studies on the behaviour of mixture of gas microflows; iii) development of new experimental techniques to measure velocity inside microdevices.
- **Thermal aspects**: i) improvement and validation of heat transfer models for gas microflows; ii) improvement of the experimental data base on the convective heat transfer for gas microflows; iii) development of new experimental techniques to measure the gas temperature.
- **Gas-walls interactions**: i) determination of accommodation coefficients; ii) analysis of the links between fabrication processes of microdevices and thermal and dynamic behaviour of gases; iii) experimental analysis and modelling of microflows with reactive gases.

Annual summer schools and workshops, as well as a final conference will be organised and open to researchers from outside the network. A handbook on gas microflows will be published at the end of the project.

2. Binary mixtures of gas microflows: preliminary results

The hydrodynamic properties of gas microflows are better known than their thermal ones (see next section). The different regimes (continuum, slip flow, transition, and free molecular) are well identified; powerful models and tools are available to accurately describe the flow behaviour in these regimes [1]. However, there is still an important need of research, notably in order to **identify the best boundary conditions** in the slip flow regime, to make a rigorous **link between continuum and kinetic approaches**, to accurately model **unsteady and undeveloped flows** and flows in complex geometries with **curvature effects** as well as **flows of gas mixtures** or on the experimental point a view, to be able to make **local pressure and velocity measurements**. In the GASMEMS network, 5 ESR and 2 ER projects are devoted to these various aspects. We present below some preliminary results about the hydrodynamics of isothermal flows of binary mixtures.

2.1 First experimental data on binary mixtures of gases flowing through rectangular microchannels

Although rarefied gas hydrodynamics through microchannels has been intensively studied during the past decades due to a wide variety of applications, most of the experimental investigations published in the literature concern pure gases, and only a few of them deal with gas mixtures. For example, Bentz et al. [2] made some experimental measurements for binary gas mixtures using a spinning rotor gauge in the slip flow regime. Considering that the accommodation coefficient of each component of the mixture was independent of the composition of this mixture, the authors found a good agreement with theory for He-Ne mixtures, but the agreement was less than satisfactory in the case of He-Ar and He-N_2 mixtures.

In a preliminary work to the ESR4 project, using a novel experimental setup [3], first experimental data of flow rates of He-Ar mixtures through rectangular microchannels

were obtained, in the slip flow and early transitional regimes. They were compared to a continuum model with two kinds of 2nd order boundary conditions (Deissler BC [4] and modified BC [3]) and to a kinetic McCormack model [5]. In the slip flow regime, a good agreement is found assuming that the accommodation coefficients α for both components are close to unity, the value $\alpha = 1$ having been found previously as the best one for each of the pure He and Ar gases.

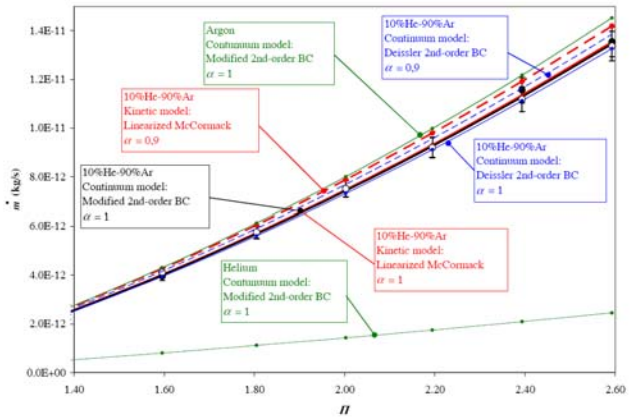

Figure 1: Mass flow rate vs pressure ratio for a mixture of 10% He - 90% Ar through a rectangular microchannel. Comparison between inlet (●) and outlet (○) data with kinetic and continuum models. $T = 298{,}15\,K$, $P_B \approx 5\times10^4\,Pa$, $0.024 < Kn_0 < 0.036$, (from [6])

Figure 1 shows an example of mass flow rate $\dot{m}$ as a function of the inlet over outlet pressure ratio Π. The same behaviour is observed for different compositions of the Ar-He mixture, up to an average Knudsen number Kn_0 in the order of 0.1. However, as rarefaction increases, due to a decrease of pressure or an increase of helium fraction, the best fit is found for a lower value of the accommodation coefficient, around 0.95. This could be caused by the differences of the molecular velocities of each component in the mixture, which could lead to a modification of the concentration inside the microchannel. Further investigations with higher Knudsen numbers and with other mixtures will be done in the ESR4 project for obtaining more definitive conclusions.

2.2 Numerical simulation of the isothermal flow of binary mixtures of gases through triangular microchannels

These first data concern isothermal flows of mixture through rectangular microchannels, but another section of interest is the triangular section, easily obtained by wet etching in silicon wafers. In the beginning of ESR4 project, the flow of a binary gas mixture through a channel of triangular cross section is investigated. The flow is due to a pressure gradient and considered as fully developed. The analysis is based on the McCormack kinetic model subject to Maxwell diffuse boundary conditions. The kinetic equations are solved on a triangular lattice coupling accordingly the discretization in the physical and molecular velocity spaces. Preliminary results for the flow rates and the velocity profiles are provided for an equilateral triangle cross section and a binary mixture of He-Ar for various concentrations. One main interest of using the kinetic theory is that results are valid in the whole range of the Knudsen number.

For the discretization of the problem, 500500 grid points are used for a rarefaction parameter $\delta \le 2$ and 980700 for $\delta \ge 5$. In the molecular velocity space, the velocities are discretized in 16 magnitude values and in 280 polar angles for $\delta < 0.5$ and 72 for $\delta > 1$.

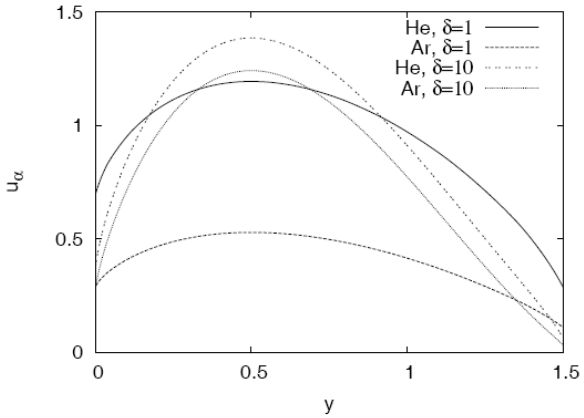

Figure 2: Velocity profiles for a He/Ar mixture with C = 0.25, (from [7]).

Typical velocity profiles of the mixtures in the channel are shown in Figure 2. The velocities are plotted along a bisectrix of the equilateral triangle, for different values of the rarefaction parameter. The velocity exhibits a maximum at the channel centre. It is also observed that the lighter molecules haves always a larger velocity than the heavier ones. This velocity difference between the two

species increases with the flow rarefaction.

Concerning the flowrate, the classical Knudsen minimum phenomenon is observed, in the transition regime, for a value of the rarefaction parameter close to unity. This work will be continued in the short future in order to obtain complete data for binary gas flows through isosceles triangular and trapezoidal channels, and the obtained data will be compared to experimental measurements.

3. Heat transfer in gas microflows: preliminary results.

The analysis of the convective heat transfer in rarefied gas flows is an interesting topic from both technical and scientific point of view because: 1) the **temperature jump conditions** at the wall, used in the slip flow regime together with the classical energy equation in order to determine the temperature distribution, have not been extensively studied for complex geometries and for various roughness (i.e. inhomogeneous) conditions of the walls. 2) There are problems in treating **complex cases** of industrial interest that involve **different flow regimes** and **heat transfer**, since, up to now, the various models use specific mathematical and numerical tools for specific regimes. 3) There are **few available experimental local data** (temperature, heat fluxes) allowing the validation of the complex mathematical models proposed for the analysis of rarefied gases in slip, transitional and free molecular regimes.

In the framework of the GASMEMS project, 6 ESR and 1 ER positions have been devoted to the analysis of thermal aspects in rarefied gas flows. There is a strong cohesion and complementarities between the concerned projects, with the goal to provide accurate models covering a wide rarefaction range, from low *Kn* to high *Kn*, benefiting from the implementation of promising new numerical tools. The striking lack of experimental data about heat transfer in gas microflows has motivated our willpower to accentuate efforts on experimental aspects, including the development of new techniques for local temperature measurements and the creation of accurate experimental databases on convective heat transfer. In the following section, we present a selection of results on heat transfer obtained by the first researchers enrolled in the GASMEMS network.

3.1 Heat transfer combined effects of rarefaction and compressibility on the Nusselt number

The first activities of ESR6 have been devoted to become familiar with the numerical code used by Croce and D'Agaro in previous studies of rarefied gases [8, 9]. A numerical investigation on heat transfer, compressibility and rarefaction effects in the slip flow regime was carried out using Navier-Stokes equations with classical Maxwell first-order slip boundary conditions and Smoluchowski first order temperature jump definitions for a microchannel with parallel plates geometry.

Under fixed flux boundary condition, friction factors and heat transfer performances are evaluated for relatively short microchannels, with a length to hydraulic diameter ratio of 10. Both positive (heating) and negative (cooling) heat flux are considered in the numerical analysis, as well as different pressure ratios and Reynolds numbers. More in detail, the numerical analysis focuses on rarefied gases for relatively small Knudsen numbers ($Kn < 0.05$). In microchannels, due to huge pressure drop and/or significant density variations induced by heat transfer, strong compressibility effects can be experienced. A Mach number increase results in a static temperature decrease. This reduces heat flux in cooled flows and increases it in heated ones. Rarefaction can reduce all the above mentioned effects, since it reduces wall shear stress and pressure drop, as well as the wall heat transfer rate. In Figure 3 the Nusselt numbers, Nu_0, based on the stagnation temperature at each section of the microchannel, for a heated and a cooled case, are plotted versus the local, mass flow averaged Mach number, *Ma*. Various values of the isentropic Mach number Ma_{is}, i.e. of the inlet over outlet pressure ratio, are considered. It is quite clear that the compressibility is by far the dominant effect. The pressure drop tends to increase the Mach

number along the channel; an incoming heat flux (heated flow) also acts in the same direction, while flow cooling increases density, inducing a reduction in both velocity and Mach number. However, at moderate cooling rate, as in Figure 3, the pressure drop effect is prevalent and *Ma* increases along the microchannel. However, the heating flow enhancement is more evident.

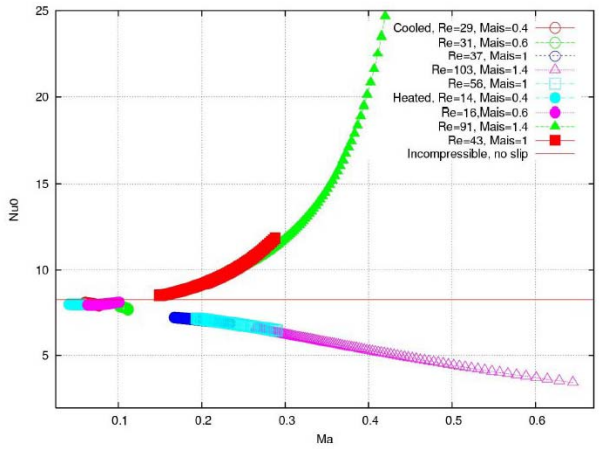

Figure 3: Compressibility effect: Nu_0 vs. local Ma, cooled and heated microchannel (from [10]).

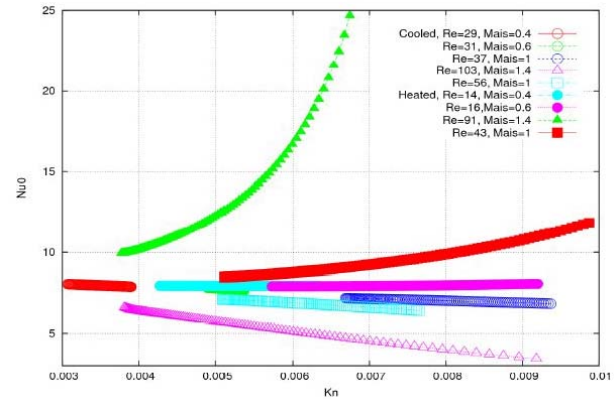

Figure 4: The rarefaction effect on heat transfer, cooled and heated channel (from [10]).

Figure 4 addresses the rarefaction effect: the local Nusselt number is plotted versus the local Knudsen number *Kn*. The results do not appear as clearly aligned along a line as when plotted vs. the local Mach number; the spread is clearly due to the compressibility effect. The presence of slip and temperature jump obviously decreases the Nusselt number: however, this effect seems to be more than compensated by the increase induced by compressibility. In all of the cases in Figure 4, the Knudsen number is monotonically increasing with the streamwise direction. For each line, the lower values of *Kn* represent the end of the entrance region. Thus, rarefaction has smaller impact on either the extension or the performances near the channel inlet.

3.2 Thermal creep effects on heat transfer and mass flow rates

Among the first activities of ESR10, a numerical simulation of a rarefied gas confined between two heated plates with an imposed uniform temperature has been conducted. The steady-state heat transfer problem has been investigated using three non-linear kinetic models of the Boltzmann equation: BGK, S-model and ellipsoidal (ES) model. The aim of this preliminary work is to test the accuracy and the applicability of these kinetic models to describe correctly the heat flux in the transitional flow regime. The same problem has been extensively studied by many authors in the past, but especially using the linearized formulation of the full Boltzmann or kinetic model equations [11].

Table 1: Normalized heat flux q/q_{FM}, comparison between different models, from [12].

δ	BGK	S-Model	ES-model	Full. Boltz. [11]
1.1906	0.6759	0.7393	0.7488	0.7558
3.0150	0.4774	0.5637	0.5684	0.5807
4.6483	0.3811	0.4694	0.4719	0.4843
6.4710	0.3117	0.3966	0.3980	0.4094
13.7189	0.1813	0.2462	0.2466	0.2538

By using the analytical value of the heat flux obtained for a free molecular flow (q_{FM}) for the normalization of the calculated heat flux, the numerical results obtained using respectively BGK, S-model, ES-model and full non-linear Boltzmann equation associated to the hard sphere model [11] are compared in Table 1, for various values of the rarefaction parameter δ. It is possible to note that the difference between the results derived from the full non-linearized Boltzmann equation and the results of the ES kinetic model is less than 3% for $\delta = 13.7189$ and less than 1% for $\delta = 1.19058$. The results of S-model are also close to that of ES model. On the contrary, the BGK model gives smaller values of heat flux and this fact can be explained by considering that in the BGK method the Prandtl number is always settled equal to 1.

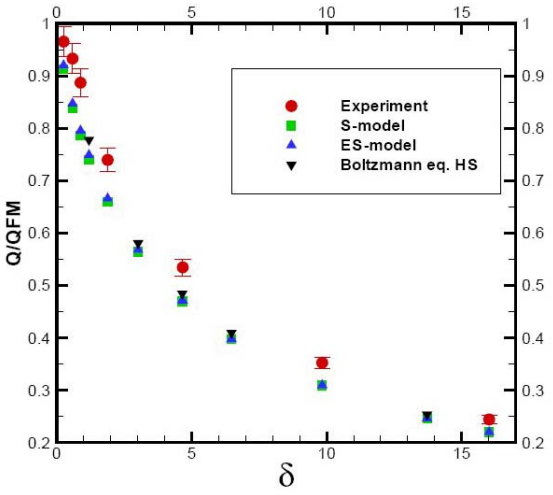

Figure 5: Normalized heat flux for different kinetic models and experimental data (from [12]).

One can note that the agreement between the numerical results obtained during this study (Figure 5) with experimental results [13] obtained for a temperature difference between the plates equal to 0.013K, is not always very good: the discrepancy varies between 4% and 12% and appears greater than the uncertainty of the heat flux measurements (3%). One of the reasons of this discrepancy may be due to the value of the accommodation coefficient used in the calculation which is different from the thermal accommodation coefficient derived from the heat flux measurements in free molecular regime and for a small temperature difference.

4. Gas-walls interactions in microsystems: preliminary results.

In rarefied microflows, the role played by the interaction between the gas and the wall becomes essential but is generally badly known. Numerous models of boundary conditions are currently in confrontation and require an empirical adjustment strongly dependent on the micro manufacturing techniques. On the other hand, the experimental data are fragmentary and difficult to confront. From the current state of the art, the following existing weaknesses and current scientific needs have been identified: 1) not well known **accommodation coefficients** (due the wall surface state) in slip flow and temperature jump models, 2) no clear links between flow behaviour**, materials** and **fabrication processes**, 3) lack of data on **chemical reactions** between gas and walls.

A specific work package of the GASMEMS project focuses on the study of specific effects of gas/material interactions on gas microflows, through 4 ESR and 2 ER projects. The general objective is to better quantify these interactions, focusing on the accurate determination and better use of energy and momentum accommodation coefficients, in particular in complex 3-D micro-geometries. Determining these key parameters remains an open issue which will be tackled in close link with the study of the role of the material and micro fabrication processes. The special case of reactive or selective wall surface, of great industrial interest, will also be studied. The first results obtained within the network on gas-walls interactions are presented below.

4.1 "Knudsen layer" effect on thermal transpiration of rarefied gases

In rarefied gas flows in microsystems, when the Knudsen number increases, the behaviour of the gas near solid surfaces is affected by the gas molecules/wall interactions, which lead to the formation of the so-called Knudsen layer. In this local non-equilibrium region, the constitutive relations for shear stress and heat flux are no longer linear and the thermophysical transport coefficients such as viscosity and thermal conductivity are no longer constant. Thus, even if the Navier Stokes equations, associated to slip boundary conditions, are able to accurately model the moderately rarefied flows outside the Knudsen layer, they cannot predict the flow characteristics inside this layer [14]. It has also been shown [15], that the modified thermo-physical transport in the Knudsen layer influences the global fluid flow characteristics, strongly for high Knudsen numbers but even significantly in the slip flow regime. To avoid using time consuming kinetic methods for the calculation of the non-equilibrium flow in the Knudsen layer, it is proposed to use an effective mean free path semi-analytical model, obtained by calculating the relative intermolecular and boundary collisions [16], [17]. Effective thermo-physical transport coefficients in the Knudsen layer are

derived from this effective mean free path

In the preliminary work of the ESR1 project, this model has been used to solve the thermal transpiration (or "thermal creep") problem: a closed-ended capillary tube with insulated sidewalls is filled with a single-component rarefied gas, and the capillary ends are maintained at different uniform temperatures. In this system, the thermal transpiration (creep), where the fluid starts creeping in the direction from cold toward hot, leads to a pressure difference between the hot and cold ends and a pressure return flow will occur, partially or completely balancing the thermal creep flow. This phenomenon cannot be predicted by Navier-Stokes-Fourier equations associated to no-slip boundary conditions.

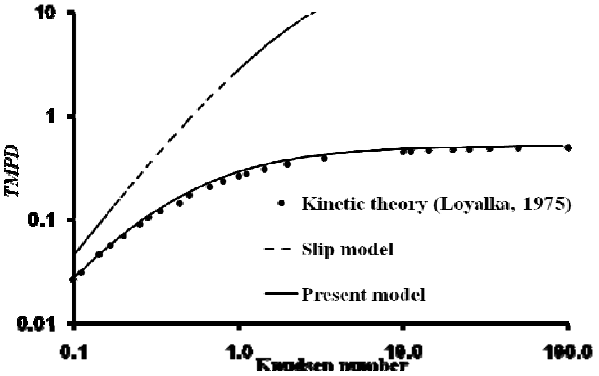

Figure 6: Variation of thermo molecular pressure difference with the Knudsen number for Helium gas (from [19])

However, as shown in Figure 6, the present model predicts very accurately the variation of the thermo molecular pressure difference with the Knudsen number, for Helium gas. The results are indeed very close to the numerical simulations results from Loyalka [18] (kinetic theory with BGK model and diffuse reflection) and much better than classical slip model predictions, whatever the Knudsen number.

Further investigations will concern constitutive scaling models based on the power-law distribution of mean free path and the effect of curvature and surface roughness on the fluid flow characteristics of rarefied gases.

4.2 DSMC simulations of gaseous flows through rough microchannel

In these first studies related to ESR2 and ESR7 projects, the flow of rarefied gas through microchannels with rough walls is investigated. Wall roughness is here simulated as a highly porous medium with randomly distributed body skeleton [20]. The motion of a single gas molecule through the pore skeleton can be described by using the well-known "dusty gas" model, which considers the porous body skeleton as a system of large, compared with the gas molecules, immovable particles randomly distributed within the porous domain. Thus, the velocity distribution function of the molecules moving through the porous body skeleton can be obtained from a linear integral equation describing the scattering of the molecules from the surface of the large immovable particles. In the present model, both processes of intermolecular collisions and molecular scattering from pore boundaries are incorporated into one kinetic equation. The obtained equation is solved by using the widely used, in rarefied gas dynamics, Direct Simulation Monte Carlo (DSMC) method.

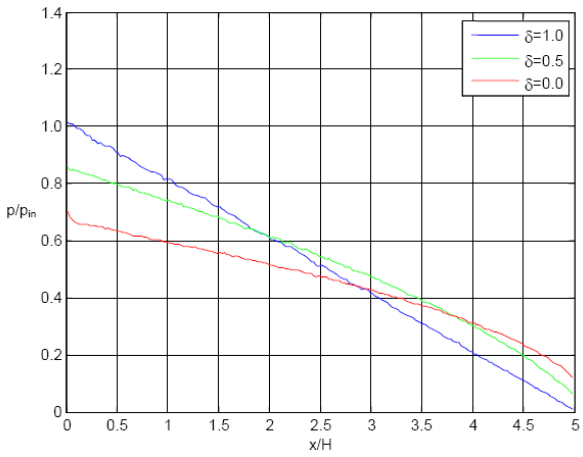

Figure 7: Pressure profiles along the channel centre line for different values of δ (from [21])

First simulations have been done on a classical problem of pressure driven monatomic gas flow in a two-dimensional microchannel with height H and length $L >> H$. The fluid is at the same temperature T_w than the walls. Diffuse reflection is assumed on both channel walls and on the surface of the immovable spheres presenting the porous medium. Numerical simulations have been carried out for a fixed Kn=0.028, and pressures p_{in}=1 and p_{out}=0, where pressure is scaled by $\rho_0 R T_w$. The depth of the porous layer simulating the rough walls is $\delta = H/2 - Y_{por}$.

As shown in Figure 7, the character of the pressure drop along the channel centre line is changed significantly from non-linear for perfectly smooth walls (d=0) to linear for channel filled out with porous medium.

In the near future, these first numerical results will be compared for validation to existing experimental and numerical data.

5. Conclusion - Acknowledgments

The GASMEMS project has been officially launched in October 2008, and the first recruitments of researchers took place in April 2009. A selection of preliminary results obtained a few months later has been presented and replaced in the frame of the global objectives of the GASMEMS network.

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