Proc. Eurosensors XXV, September 4-7, 2011, Athens, Greece

Simulation and Experimental Evaluation of Gas Mass Flow Transfer Rate in Microchannels

G. P. Patsis[a*], K. Ninos[a], D. Mathioulakis[b], and G. Kaltsas[a]

[a]*Department of Electronics, TEI of Athens, Athens, Greece*

[b]*School of Mechanical Engineering, NTUA, Athens, Greece*

Abstract

Continuum hydrodynamics accurately describes the flow of fluids over a wide range of systems. However, continuum models are unable to adequately describe the flow of fluid under extreme confinement. In particular, the no-slip boundary condition invoked in continuum flow calculations is violated for low density gases flowing in microtubes or nanoporous materials. The calculation of gas mass transfer rate in microtubes using experiments and simulation is investigated in the case of small absolute pressures. Specifically, in the present work, Argon gas is considered in a 3D model of two metallic tanks connected through microchannels. The pressure difference between the inlet and the outlet of the structure is monitored as a function of time. Thus the gas transfer rate is evaluated and compared with experimental data, in order to verify the departure from the standard Navier – Stokes equations with the no-slip boundary condition.

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Keywords: Rarefied gas; microchannels; microfluidics; mass transfer rate; simulation; COMSOL.

Nomenclature

ρ	fluid's density (kg/m^3)
$\vec{u}$	velocity vector (m/s)
p	pressure (Pa)
η	dynamic viscosity ($Pa\ s$)
$\tau_{n,t}$	shear stress along the boundary (Pa)
λ	mean free path (m)
$\vec{I}$	unity matrix
R	Gas constant ($J / kg\ K$)
T	absolute temperature (K)
m	gas mass in the metallic tank (kg)
V	metallic tank volume (m^3)
a_v	tangential momentum-accommodation coefficient

*Corresponding author, e-mail: patsisg@teiath.gr

1. Introduction

The mass flow rate of gases in micro channels under small absolute pressures is underestimated when the theory of continuum mechanics is applied. This deviation becomes evident when Knudsen number takes values above *0.1*, namely when the gas is considered as rarefied [1]. Under these conditions the number of atom collisions with the internal wall of the tube have to be taken into consideration. In fact, the failure of the continuum model happens when the shear stress and the heat flux in the continuum equations of mass, momentum and energy conservation can no longer be characterized by the macroscopic magnitudes of lower order (velocity, temperature) i.e., when the expressions of the transport coefficients are no longer valid. This happens when the scale length of the gradients of the macroscopic quantities becomes so small that it is comparable with the molecular mean free path of the gas [1]. The scale length of the gradients of the macroscopic magnitudes is:

$$L = \rho / (d\rho / dx) \qquad (1)$$

To characterize the degree of rarefaction the Knudsen number is introduced and is defined as the ratio of the molecular mean free path λ (the average distance traveled by a molecule between two collisions) and the characteristic length of the flow L:

$$K_n = \lambda / L \qquad (2)$$

Reference [2] divides the rarefied gas flows into three realms according to the degree of rarefaction, i. e., the slip flow regime, the transitional regime and the free molecular regime. According to the range of the properly chosen Knudsen number K_n the three regimes are *0.01 < K_n < 0.1* : slip flow regime, *0.1 < K_n < 10* : transitional regime, and *K_n > 10* : free molecular regime.

In section 2, a 3D model of the experimental apparatus is developed which is used in section 3 for comparison with the experimental mass flow rate measurements.

2. Model Description

The experimental set up of this work consists of two tanks which were connected through eight parallel micro-channels of rectangular cross section (made by PMMA). Fig. 1a shows a 3D view of a structure with the two tanks and their connection through microchannels, along with some geometric details. The simulation was performed in COMSOL [3] using finite elements. The weakly compressible Navier – Stokes equations (WCNSE) are suitable where small density variations arise due to temperature differences. They are not suitable for high velocities or where fluid compression or expansion results in substantial internal work or heat effects. Specifically they are given by:

$$\rho \frac{\partial \vec{u}}{\partial t} + \rho \vec{u} \cdot \nabla \vec{u} = \nabla \cdot \left[-p\mathrm{I} + \eta \left(\nabla \vec{u} + \left(\nabla \vec{u} \right)^T \right) - \frac{2\eta}{3} \left(\nabla \cdot \vec{u} \right) \mathrm{I} \right] \text{ and } \frac{\partial \rho}{\partial t} + \nabla \cdot \left(\rho \vec{u} \right) = 0 \qquad (4)$$

In the microscale, flow at a boundary is seldom strictly no slip or slip. Instead, the boundary condition is something in between and there is a slip velocity at the boundary. The following equation relates the viscosity-induced jump in tangential velocity to the tangential shear stress along the boundary, and they are also implemented in COMSOL:

$$\Delta u = \frac{1}{\beta}\tau_{n.t} \tag{5}$$

For gaseous fluids, the coefficient β equals:

$$\beta = \frac{\eta}{\left(\dfrac{2-a_v}{a_v}\right)\lambda} \tag{6}$$

A simpler expression for β is:

$$\beta = \frac{\eta}{L_s} \tag{7}$$

$$L_s = \left(\frac{2-a_v}{a_v}\right)\lambda \tag{8}$$

where L_s (the slip length) for a straight channel is a measure of the distance the flow profile extrapolates to zero away from the boundary. This equation holds for both liquids and gases. Fig. 1b shows a magnified portion of the microchannel/tank junction and the directions along which velocity and pressure profiles are recorded. Examples of velocity and pressure profile for He, Ar and Air as the flowing medium along x and z direction are shown in Fig.1c and Fig.1d respectively. The mean free path and the slip length is a function of the position x, through the relations shown in the inset of Fig.1c.
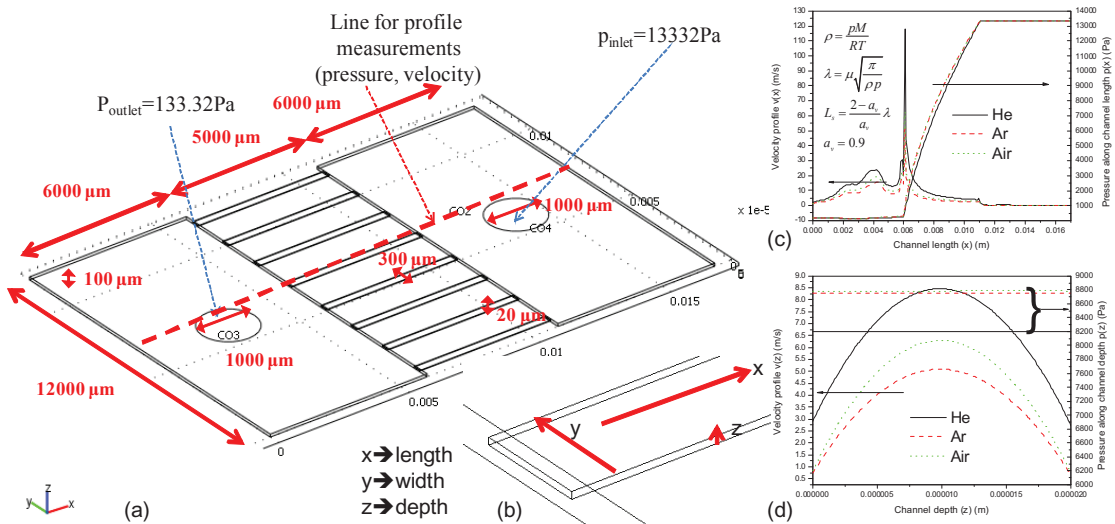

Fig. 1. (a) Simulation geometry. (b). Velocity profile with no slip and velocity slip boundary condition along the center of one micro-channel, for Air and Ar as flowing medium. Average velocities are shown obtained by the average of the corresponding profiles every 2μm within the 20μm deep channel.

3. Results and Discussion

The flow of a gas (Argon in this work) was established by applying a pressure difference between the metallic tanks. The mass flow rate was calculated employing the ideal gas equation for the gas of the higher pressure tank, namely $p = \rho RT$ and since $\rho = m/V$, it is possible to calculate the mass flow rate from:

$$\dot{m} = \frac{V}{RT}\frac{dp}{dt} \tag{9}$$

Therefore, using a manometer, the pressure of the inlet tank is measured as a function of time. In Fig. 2, the continuous line is the experimentally determined mass flow rate for Ar. Velocity and pressure fields and their profiles in various sections of the structure were simulated. Fig. 2 also shows the simulation results (discrete points) in the case of Argon gas. The slip-flow regime in the pressure range is found based on K_n which is shown along with R_n in the right axis of Fig. 2. Numerical predictions, although they agree in order of magnitude, and follow roughly the shape of the experimental curve, they overestimate the experimental measurements. Such deviation is attributed to the limitations of the WCNSE along with the velocity slip boundary condition and to the computational grid which most probably has to be denser. For a more accurate description computational results should be obtained by solving the Boltzmann equation and the BGK model of molecule collisions [4, 5].
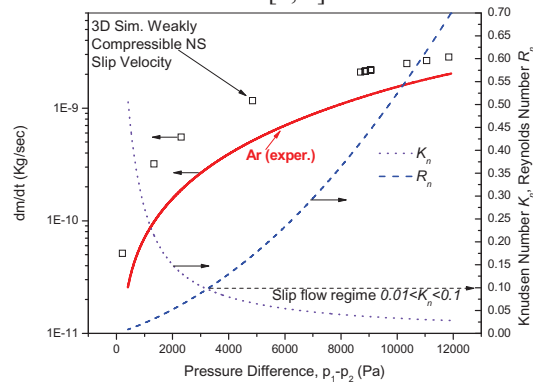
Fig. 2. Comparison of experimental and simulated mass transfer rate. Knudsen and Reynolds numbers obtained using the experimental measurements of pressure differences in the two tanks.

4. Conclusions

The gas mass transfer rate in microtubes using experiments and simulation is investigated in the case of small absolute pressures. Finite element analysis software was used for the design and simulation of the model. It was verified that in the velocity slip regime i.e., for $0.01<K_n<0.1$, the weakly compressible form of the Navier-Stokes equations with the velocity slip boundary condition on the structure walls is not enough to accurately model the gas transfer rate, and one should use more elaborate calculation methods.

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