Effect of surface roughness: comparison between continuum and kinetic approaches

O Rovenskaya and G Croce
University of Udine, via delle Scienze 208, 33100 Udine, Italy
E-mail: olga.rovenskaya@uniud.it, giulio.croce@uniud.it

Abstract. In the present work a numerical analysis of the flow field in rough microchannels is carried out using two approaches: Navier-Stokes equations provided with first order slip-boundary condition and kinetic S-model equation with Maxwell diffuse reflecting boundary condition. An implicit scheme is used for the solution of S-model equation and an algorithm allowing massive parallelization in both physical and velocity spaces has been developed. The roughness geometry is modelled as a series of triangular obstructions with relative roughness $\varepsilon$ equals to 1.25%, 2.5% and 5%. A wide range of Mach numbers is considered, from nearly incompressible to choked flow conditions and a Reynolds number up to 170. To estimate rarefaction effect the flow at Knudsen number ranging from 0.01 to 0.08 and fixed pressure ratio has been considered. Accuracy and discrepancies between full Navier - Stokes and S-model solutions are discussed, assessing the range of applicability of first order slip condition in rough geometries. The effect of the roughness is discussed via Poiseuille number as a function of local Knudsen and Mach numbers.

1. Introduction
In MEMS fabrication, due to the small scale, it is nearly impossible to create an actual smooth surface. On the other hand, surface roughness may have a significant impact on microchannel performances, both in terms of pressure drop and heat transfer. In the recent past several studies have been devoted to the estimation of roughness effect in these systems. Since roughness may assume different shapes depending on the manufacturing processes, a popular approach is to analyse artificial, ad hoc designed rough textures. This is necessary for numerical analysis, but allows easier parametrization also in experimental work; as an example, an experimental analysis of artificially generated roughness has been carried out as by Kandlikar et al. [1]. In most cases, experimental investigation detected relatively small roughness effect [2, 3], in the sense that its magnitude may be masked by the relatively large uncertainty bar. Nonetheless, even recent experimental works strongly suggest that roughness does affect Poiseuille number in microchannel rarefied flow, although the magnitude of experimental uncertainty does not allow a definitive answer [4]. Thus, the numerical modelling offers an appealing alternative to an experiment, allowing a detailed description of the surface imperfections, where we can easily separate roughness from other microscale effects.

The roughness problem has been first addressed, both via direct numerical analysis and simplified modelling, mainly in the incompressible, no-slip flow regime. The numerical simulation of pressure drop in the presence of three dimensional square box-shaped rough elements was studied in [5], while other authors [6] investigated the effect of several geometries based on 2D squared and saw-tooth obstruction. Both pressure drop and heat transfer in tube and plane channels were considered.
There are few works devoted to the rarefied gas flow through rough channels using direct Monte Carlo simulation [7-9]. Knudsen numbers from 0.02 to 0.12 were considered, in the presence of very rough geometries, from 5% up to 12%. In both papers, the low Mach number level prevented any compressibility effect. In [10] coupling effects of rarefaction and roughness without the effect of compressibility has been considered using the Lattice Boltzmann equation. Numerical results show that the roughness effect increases the friction factor near the wall, while the rarefaction effect decreases it.

Thus, in the literature the interaction with compressibility effect is generally not taken into account. Only recently Ji et al. [11] studied the influence of roughness in slip flow regime with second order slip boundary conditions up to a maximum exit Mach number around 0.5. They simulated the roughness with rectangular elements on two parallel plates and showed that the effect of wall roughness is reduced with increasing Knudsen number. The prediction of roughness effect for gaseous flow, in the presence of compressibility up to chocked flow conditions and/or rarefaction effects, has been analyzed by Croce [12] and Hakak Khadem [13] using Navier-Stokes equations.

While for incompressible flow the numerical tools for roughness analysis are just the usual, well established Navier-Stokes equations, for gaseous flow the rarefaction effect may require different models. The applicability of continuum numerical approach based on the solution of Navier-Stokes equations should be, in fact, limited to flows where the roughness size is larger than the mean free path of the gas. This condition is obviously stricter than the usual condition of hydraulic diameter larger than the mean free path, and may not be fulfilled in actual application of practical interest. Thus, even if the use of appropriate slip boundary conditions allows to partially overcome this limitation, a correct description of the gas-roughness interaction should require an expensive kinetic numerical approach, at least near the roughness surface.

The aim of this paper is, thus, to investigate the effects of rarefaction, compressibility and roughness using two approaches: Navier-Stokes equations provided with first order slip-boundary condition and kinetic S-model equation with Maxwell diffuse reflecting boundary condition. The analysis is limited to first order slip, since second order models are still geometry dependent and not so developed for reliable, arbitrary geometry simulations. Accuracy and discrepancy between full Navier-Stokes and S-model solutions are discussed, assessing the range of applicability of first order slip condition in rough geometries. The effect of the roughness is discussed via Poiseuille number as a function of local Knudsen and Mach numbers.

2. Numerical method for kinetic approach
In the most general case the gas flow is modelled by the Boltzmann transport equation (BTE), describing the evolution of a particle distribution function $f = f(t, \mathbf{x}, \mathbf{\xi})$ in a six-dimensional phase space:

$$\frac{\partial f}{\partial t} + \mathbf{\xi} \cdot \nabla f = J(f, f)$$

(1)

where $t$ is the time, $\mathbf{x} = (x, y, z)$ is the position vector, $\mathbf{\xi} = (\xi_x, \xi_y, \xi_z)$ is the particle velocity vector, while the operator $J(f, f)$ takes into account the binary collisions between particles. For the sake of simplicity and computational efficiency, the collision integral $J(f, f)$ is replaced by the S-model [14], which can be written as:

$$J_s(f, f) = \frac{P}{\mu} (S - f)$$

(2)

$$S = M \left[ 1 + \frac{2m \mathbf{q} \mathbf{e}}{15 n(kT)^2} \left( \frac{m c^2}{2kT} - \frac{5}{2} \right) \right]$$

(3)
\[ M(n, V, T) = n\left(\frac{m}{2\pi kT}\right)^{3/2} \exp\left[-\frac{mc^2}{2kT}\right] \]  

where \( M \) is the local Maxwellian distribution function, \( c = \xi - V \) is the relative speed of a single particle against a background gas, \( q \) is the heat flux vector, \( p \) is the local pressure and \( \mu \) and \( \lambda \) are the gas viscosity and conductivity at local temperature \( T \), \( Pr = 2/3 \) is the Prandtl number, \( k \) is the Boltzmann constant.

The inlet and outlet boundary conditions for the kinetic equation (1) impose a Maxwellian distribution function for the incoming molecules:

\[ f(\xi)|_{\text{in}} = M (p_i/T_i, 0, T_i) \quad \text{if} \quad \xi \cdot \vartheta(x) > 0 \]  

\[ f(\xi)|_{\text{exit}} = M (p_i/T_i, 0, T_i) \quad \text{if} \quad \xi \cdot \vartheta(x) > 0 \]  

where \( \vartheta(x) \) is the unit vector normal to the boundary directed toward the gas. Note that such boundary condition, assuming Maxwellian distributions, requires equilibrium conditions, and thus the boundaries must be pushed far away from solid boundaries and viscous regions.

Maxwell diffuse reflecting boundary conditions with the full accommodation are applied on solid walls:

\[ f\big|_{\omega}(x) = \omega(x) M (1, V_w, T_w) \quad \xi \cdot \vartheta(x) > 0 \]  

\[ \omega(x) = -\sum_{\xi \cdot \vartheta(x) > 0} \xi \cdot \vartheta(x) f(t, x, \xi) d\xi \]  

\[ \omega(x) = \sum_{\xi \cdot \vartheta(x) < 0} \xi \cdot \vartheta(x) M (1, V_w, T_w) d\xi \]  

The parameter \( \omega(x) \) is determined so as to avoid a mass flux across the wall. All the particles coming off the surface are emitted with the Maxwell distribution functions corresponding the zero mean flow velocity, the temperature is equal to the wall temperature \( T_w \), and the density is calculated from the condition of equality of the fluxes of particles coming on and off the wall. At the symmetry line the specular boundary condition is imposed.

The problem is recast in terms of dimensionless variables introducing the following reference values: the number density \( n_\infty \), is the temperature \( T_\infty \), the most probable velocity \( v_\infty = \sqrt{2RT_\infty} \). The height of the channel \( H \) is taken as thereference length scale. For the hard-sphere molecular model the dimensionless viscosity coefficient is \( \mu/\mu_0 = (T/T_0)^{1/3} \). Thus, non-dimensional variables are \( \xi/v_\infty \), \( x/H, f(n, v, n, T) \), \( \mu/\mu_\infty \), \( n/n_\infty \), \( T/T_\infty \) and \( p/p_\infty \). For sake of simplicity, in the following the dimensionless quantities keep the same designations as the dimensional ones. In the non-dimensional form the S - model equation is thus written as follows:

\[ \frac{\partial f}{\partial t} + \xi \cdot \frac{\partial f}{\partial x} = \frac{8\sqrt{T}}{5Kn\sqrt{\pi}}(S - f) = v(S - f) \]  

where \( v \) is the collision frequency, \( Kn \) is the reference Knudsen number based on the height between plate \( H \) and the mean free path \( \lambda_n \) at reference (isentropic) state which is defined as:

\[ \lambda_n = \frac{16\mu_\infty}{5mn_\infty\sqrt{2RT_\infty}} \]  

The macroscopic (bulk) distributions of number density, velocity vector, temperature and heat flux respectively are defined as:

\[ n = \int f d\xi, \quad n(u, v) = \int (\xi_x, \xi_y, \xi_z) f d\xi, \quad nT = \int c^2 f d\xi, \quad (q_x, q_y, q_z) = \int (c_x, c_y, c_z) f d\xi \]
Taking advantage of the two-dimensionality of the flow, the $z$ component of the molecular velocity may be eliminated by the projection procedure. This is performed by introducing the functions:

$$
\begin{align*}
g &= \int f d\xi_z, \\
h &= \int \xi_z^2 f d\xi_z.
\end{align*}
$$

(12)

For the sake of simplicity all schemes will be written for general $S$-model equation (9).

To discretize the $S$-model equation we construct a two-dimensional grid $\{\xi_{\alpha}, \xi_{\beta}\} = (\alpha, \beta = 1, \ldots, N_{\xi})$, bounded by $v_{\text{max}}$, where $\Gamma = (\alpha, \beta)$ defines velocity grid points indices. Velocity space nodes are located at Gaussian abscissas, and Gaussian integration is performed via proper Gaussian weight function. In the discrete form the $S$-model equation (9) is the following:

$$
\frac{\partial f}{\partial t} + \frac{\partial f}{\partial x} \frac{\partial f}{\partial \xi} + \frac{\partial f}{\partial y} \frac{\partial f}{\partial \eta} = \nu \left( S_f - f \right)
$$

(13)

In the physical space a 2D, non uniform grid is defined by nodes $(x_i, y_j)$, for $i = 1, i_{\text{max}}$, and $j = 1, j_{\text{max}}$ and $N_c = i_{\text{max}} j_{\text{max}}$ cells centred around each node. Denoting $f_{\Gamma,i,j}^n$ as the approximations of $f(f^n, \xi, x, y)$ the numerical scheme for the equation (13) can be written as:

$$
f_{\Gamma,i+1/2,j}^{n+1} = f_{\Gamma,i,j}^n - \frac{\Delta t}{\Delta x} \left( f_{\Gamma,i+1/2,j}^n - f_{\Gamma,i-1/2,j}^n \right) - \frac{\Delta t}{\Delta y} \left( f_{\Gamma,i,j+1/2}^n - f_{\Gamma,i,j-1/2}^n \right) + \Delta t \nu_{i,j} \left( S_{\Gamma,i,j}^n - f_{\Gamma,i,j}^n \right)
$$

(14)

where the transport term is approximated by a standard finite volume scheme, while the nonlinear relaxation term is discretized via a standard centred approximation. In particular, the numerical fluxes are defined as:

$$
F_{\Gamma,i+1/2,j}^n = \frac{1}{2} \left( \xi_{\alpha} \left( f_{\Gamma,i+1/2,j}^n + f_{\Gamma,i-1/2,j}^n \right) - \xi_{\alpha} \left( \Delta f_{\Gamma,i+1/2,j}^n - \Phi_{\Gamma,i+1/2,j}^n \right) \right)
$$

(15)

$$
F_{\Gamma,i,j+1/2}^n = \frac{1}{2} \left( \xi_{\beta} \left( f_{\Gamma,i,j+1/2}^n + f_{\Gamma,i,j-1/2}^n \right) - \xi_{\beta} \left( \Delta f_{\Gamma,i,j+1/2}^n - \Phi_{\Gamma,i,j+1/2}^n \right) \right)
$$

(16)

$$
\Delta f_{\Gamma,i,j}^{n+1} = f_{\Gamma,i+1/2,j}^n - f_{\Gamma,i,j}^n
$$

where $\Phi_{\Gamma,i+1/2,j}^n = \min \left( \Delta f_{\Gamma,i+1/2,j}^n, \Delta f_{\Gamma,i,j+1/2}^n, \Delta f_{\Gamma,i,j}^{n+1} \right)$ is the flux limiter function, allowing for a second order of the scheme. Since the scheme is explicit the time step should be limited by the condition:

$$
\Delta t = \frac{CFL}{\max_{i,j} \left( v + v_{\text{max}} / \Delta x + v_{\text{max}} / \Delta y \right)}
$$

(17)

The equation (13) is solved on a curvilinear, structured mesh. If $\zeta(x, y)$ and $\eta(x, y)$ denote curvilinear coordinates, equation (13) may be recast in terms of the new coordinates as in the following:

$$
\frac{1}{J} \frac{\partial}{\partial \zeta} f_{\Gamma} + \frac{\partial}{\partial \eta} \left( \frac{\nabla \zeta}{J} f_{\Gamma} \right) + \frac{\partial}{\partial \eta} \left( \frac{\nabla \eta}{J} f_{\Gamma} \right) = \nu \left( S_{\Gamma} - f_{\Gamma} \right)
$$

(18)

Where $\nabla \zeta = (\partial \zeta, \partial \zeta, \partial \zeta)$, $\nabla \eta = (\partial \eta, \partial \eta, \partial \eta)$ and $J = \partial \zeta \partial \eta - \partial \zeta \partial \eta$. If we define a uniform grid $\zeta_i = i \Delta \zeta, \eta_j = j \Delta \eta$ a scheme very similar (14) may be used.
In the implicit scheme the gain term $S_{\Gamma}$ is positive and, thus, can be treated explicitly. Then the implicit first order scheme can be written as:

$$f_{\Gamma,i,j}^{n+1} = f_{\Gamma,i,j}^n - \frac{\Delta t}{\Delta x} \left( F_{\Gamma,i+1/2,j}^n - F_{\Gamma,i-1/2,j}^n \right) - \frac{\Delta t}{\Delta y} \left( F_{\Gamma,i,j+1/2}^n - F_{\Gamma,i,j-1/2}^n \right) + \Delta t \nu_{i,j} \left( S_{\Gamma,i,j}^n - f_{\Gamma,i,j}^{n+1} \right)$$  \hspace{1cm} (19)

or

$$\left( I + T + \nu \right) \delta f = RHS^n$$  \hspace{1cm} (20)

$$(Tf^n)_{\Gamma,i,j} = \frac{1}{\Delta x} \left( F_{\Gamma,i+1/2,j}^n - F_{\Gamma,i-1/2,j}^n \right) + \frac{1}{\Delta y} \left( F_{\Gamma,i,j+1/2}^n - F_{\Gamma,i,j-1/2}^n \right)$$  \hspace{1cm} (21)

where $\delta f = f^{n+1} - f^n$, $I$ is the identity matrix, $(T^n)_{\Gamma,i,j}$ is a matrix with the only first order fluxes, and the right-hand side:

$$RHS^n_{\Gamma,i,j} = -\frac{1}{\Delta x} \left( F_{\Gamma,i+1/2,j}^n - F_{\Gamma,i-1/2,j}^n \right) - \frac{1}{\Delta y} \left( F_{\Gamma,i,j+1/2}^n - F_{\Gamma,i,j-1/2}^n \right) + \nu_{i,j} \left( S_{\Gamma,i,j}^n - f_{\Gamma,i,j}^n \right)$$  \hspace{1cm} (22)

which contains the limiters for the second order scheme. In particularly, If quantities $f_{\Gamma,i,j}$ are stored as $f_{\Gamma} = (f_{\Gamma,i,j})$, it can be seen that $T$ is a $(N_c \times N_c) \times (N_c \times N_c)$ block diagonal matrix with $N_c \times N_c$ pentadiagonal blocks $T_{\Gamma}$:

$$T_{\Gamma,i-1,j} = \frac{1}{\Delta x} \xi_{\alpha}^+, T_{\Gamma,i+1,j} = \frac{1}{\Delta x} \xi_{\beta}^+, T_{\Gamma,i,j} = \frac{1}{\Delta x} \left| \xi_{\alpha} \right| + \frac{1}{\Delta y} \left| \xi_{\beta} \right|$$

$$T_{\Gamma,i,j+1} = \frac{1}{\Delta y} \xi_{\gamma}^-, T_{\Gamma,i,j-1} = \frac{1}{\Delta x} \xi_{\delta}^-$$

The boundary conditions are treated explicitly and the right-hand side contains the boundary terms and the coefficients of $T$ corresponding to the boundary conditions are set to 0.

Thus, equation (20) can be symbolically expressed as for each $\Gamma$:

$$\left[ D + L + U \right] \delta f = RHS$$  \hspace{1cm} (23)

where $D$, $L$, $U$ are the matrices of size $N_c \times N_c$, $\delta f$ and $RHS$ are vectors of size $N_c$ and $D$ consists of only diagonal terms, $L$ only the terms in the lower triangular matrix, and $U$ the upper triangular matrix. The left-hand side of equation (23) can be approximately factored into the product of two operators:

$$(D + L)D^{-1}(D + U) \delta f = RHS$$  \hspace{1cm} (24)

This scheme can be implemented in the following sequence:

$$(D + L)\delta f^* = RHS$$  \hspace{1cm} (25)

$$(D + U)\delta f = D\delta f^*$$  \hspace{1cm} (26)

The distribution function at the next time step is:

$$f^{n+1} = f^n + \delta f$$
The solution of linear systems (23) is local in $\Gamma$, and therefore completely parallelizable. The computation of macroparameters for gain term $S$ and collision frequency $\nu$ is local in $i, j$, thus it is parallelized in physical space. The software code was written in C++ with the use of MPI (Message Passing Interface). The kinetic code ran on double processors, quad core systems, using 8 parallel processes. Running in parallel on 8 cores, on the grid $720 \times 50$ in the physical space the CPU time per time step is $36 \times 8 = 288$ sec. The maximum speed up achieved by 8 processors was 94%.

3. Numerical solution of the Navier–Stokes equation

The viscous, compressible Navier-Stokes equations for 2D laminar flow can be written in terms of conservative variables:

$$\frac{\partial U}{\partial t} + \frac{\partial F(U)}{\partial x} = 0$$  \hspace{1cm} (27)

$$U = (\rho, \rho V, e_{tot})$$  \hspace{1cm} (28)

where the flux vector $F(U)$ may be decomposed into the convective (inviscid) and diffusive (viscous) components:

$$F = F^{inv} - F^v$$  \hspace{1cm} (29)

$$F^{inv} = (\rho V, \rho VV + pI, V(e_{tot} + p))^T$$  \hspace{1cm} (30)

$$F^v = (0, \tau, \tau \cdot V + q)^T$$  \hspace{1cm} (31)

where $I$ is the identity matrix and $q$ is the heat flux vector. Pressure $p$ and total energy per unit volume $e_{tot}$ are linked by the equation of state for ideal gas:

$$p = (\gamma - 1) \left( e_{tot} - \frac{\rho V^2}{2} \right)$$  \hspace{1cm} (32)

Navier-Stokes solver is based on a hybrid finite difference-finite volume method. The in-house FORTRAN code was developed by Croce, has formal second order accuracy in space and time, has already been applied and validated for the microflow simulations of (Croce et al. [12]) and, thus, is here only briefly outlined. Adopting a curvilinear, structured mesh we may define a computational cell of volume $\Lambda_{ij}$ with faces $A_k$, $k = 1, 4$ around each node. At each of these computational cells the flux balance offers:

$$\Lambda_{ij} \frac{\partial U_{ij}}{\partial t} = \sum_{k=1}^{4} F(U) \cdot A_k \eta(x)_k$$  \hspace{1cm} (33)

Fluxes are defined via neighbouring value averaging, and an artificial dissipation term $d$ is added to prevent checker boarding and numerical instabilities. Thus, considering a face located at $i+1/2$ we get:

$$F^{inv}(U)_{i+1/2} = \frac{F^{inv}(U)_i + F^{inv}(U)_{i+1}}{2} + d_{i+1/2}$$  \hspace{1cm} (34)

Artificial dissipation term $d$ are given by a blend of second and fourth order differences, scaled by the maximum eigenvalue of jacobian matrix of vectors $F^{inv}$, as suggested in (Pulliam [15]). Second order terms are switched on near discontinuities, as in Pulliam [15]. Viscous flux vectors are evaluated with second order finite differences at $i+1/2$. The solution is advanced in time via Crank Nicolson
integration scheme. The use of the spatially factored ADI scheme originally proposed by Beam and Warming (Hirsh [16]) leads, at each time step, to the resolution of two series of block tridiagonal algebraic systems, rather than the original pentadiagonal block system arising from flux discretization.

So far, no general consensus has yet been reached on the expression of second order slip conditions for arbitrary geometries and most of the proposed models are related to a specific reference case and geometry, and are, thus, not easily extended to arbitrary geometry. For these reasons, the Maxwell first order slip boundary condition is here used. Thus, at solid walls we have:

$$u_{\text{gas}} - u_w = s_p Kn \left( \frac{\partial u_{\phi(x)}}{\partial \hat{\theta}(x)} + \frac{\partial u_{\psi(x)}}{\partial t(x)} \right)$$  \hspace{1cm} (35)$$

$$s_p = \frac{\sqrt{2}}{2 - \sigma_s} \left( 1 + 0.1366 \sigma_s \right)$$  \hspace{1cm} (36)$$

where $\hat{\theta}(x)$ and $t(x)$ are the unit vectors respectively normal and tangential to the solid wall. $\sigma_s$ is the tangential momentum accommodation coefficient, which is not only a function of the material property of gas–solid interface, but depends also on Knudsen number. In the computations $s_p$ is close to one (since the portion of incident particles scattered diffusely $\sigma_s$ is equal to one). The additional derivative along the tangential direction is essential in capturing even the qualitative behaviour of slip flow along curved walls.

A Dirichlet temperature boundary condition is imposed at the wall. The wall temperature is fixed at the inlet total temperature value to minimize the effect of viscous dissipation. In the energy equation, the Smoluchowski temperature jump is used:

$$T_{\text{gas}} - T_w = s_T Kn \frac{\partial T}{\partial \hat{\theta}(x)}$$  \hspace{1cm} (37)$$

$$s_T = \frac{2 - \sigma_T}{\sigma_T} \left( \frac{2}{\gamma + 1} \frac{1}{Pr} \right)$$  \hspace{1cm} (38)$$

where $s_T$ is the temperature jump coefficient. Since the isothermal flow is considered we assume the temperature accommodation coefficient $\sigma_T$ equals to one.

4. Results and discussion

The two-dimensional problem geometry is illustrated in figures 1 and 2. A plane channel of length $L$ and height $H$ connects two large reservoirs of size $L_x \times L_y = 30H \times 10H$. The reservoir size was chosen as to be sufficiently large, so that their further increase by 50% did not change the mass flow rate beyond 0.5%. The flow is driven by the pressure difference between the two reservoirs and is examined using both kinetic and continuum approaches. Due to the symmetry of the flow only one half of the domain was modelled. The inlet and outlet reservoirs are included in the computational domain. This allows a realistic description of inlet and outlet losses and is required, as noted above, for the kinetic solution. In order to save computational resources, we considered a channel with an inlet smooth section of length $L_s = 9H$ followed by a rough one of length $L_r = 3.15H$ (see figure 1). The roughness geometry is modelled as a series of triangular obstructions with sharp angle of 45°, as shown in figure 2. The details of the roughness element shape, as well as their pitch, have certainly an impact on the quantitative evaluation of the channel performances, as shown in [17]. However, the characterization of the actual surface texture (which is a function of the manufacturing process and parameters) with the level of detail required for the CFD discretization is a demanding task and beyond the scope of the present paper. As such, any choice of range of pitch, height or random distribution of peaks would be somewhat arbitrary. Thus, we focus on the qualitative interaction...
between compressibility, rarefaction and representative length scales, rather than on the detailed geometrical effect. Due to this choice, the computations are limited to a single geometry, properly scaled in order to get different relative roughness.

The height of a single peak is \( h = \varepsilon H \) and the peaks spacing is \( s = 5h \). We consider relative roughness \( \varepsilon \) of 1.25\%, 2.5\% and 5\%. Thus, the rough section \( L_r \) includes 12 roughness ridges at \( \varepsilon = 5\% \), 24 ridges at \( \varepsilon = 2.5\% \) and 48 ridges at \( \varepsilon = 1.25\% \).

The results have been obtained on non uniform, structured meshes in physical space; in particular, we used 672 \( \times \) 50 nodes for \( \varepsilon = 5\% \), 720 \( \times \) 50 nodes for \( \varepsilon = 2.5\% \) and 1.25\%, and 440 \( \times \) 50 nodes for the smooth channel. For all of these grids the minimum grid spacing close to the wall is of the order of 0.001 \( H \), with around 21 nodes within the rough layer. The velocity space \(-v_{\text{max}} \leq \xi_x, \xi_y \leq v_{\text{max}}\) (\( v_{\text{max}} = 4.68 \)), is discretized on a non uniform 16\( \times \)16 mesh; the node spacing is based on the proper Gaussian abscissas, allowing for accurate integration. Grid independence analysis was carried out for both space and velocity domain discretization: doubling velocity mesh points gives a 1\% variations in mass flow rate.

The gas in the reservoirs is assumed in equilibrium at constant inlet pressures \( p_{0i} \) or outlet pressure \( p_e \), with \( p_{0i} > p_e \), and temperature \( T_{0i} \). The compressibility effect is monitored via the local value of \( Ma \) and the isentropic exit Mach number \( Ma_{0i} \) (i.e., the \( Ma \) that would arise from an isentropic flow with the same pressure ratio as the real one):

\[
\frac{p_{0i}}{p_e} = \left(1 + \frac{\gamma - 1}{2} Ma_{0i}^2 \right)^{\gamma/(\gamma-1)}
\]

The temperature of the walls is equal to the temperature in reservoirs \( T_{0i} \). We define also the isentropic Reynolds number as following:
Thus, the corresponding Knudsen number based on the isentropic values is:

\[ Kn_{is} = \frac{16}{5} \sqrt{\frac{\gamma Ma_{is}}{2\pi \text{Re}_{is}}} \]  

The following computations have been carried out for pressure ratios \( \frac{p_0}{p_e} = 1.1, 2 \) and 3, allowing for a \( Kn_{is} \) range from 0.01 to 0.08. Maximum local Knudsen number \( Kn_e \) is reached after the rough region and ranges from 0.01 to 0.055.

Global and local channel performances are defined in terms of the Poiseuille number \( Po \), where the friction factor \( f \) is computed as an average value either over a portion of rough section of the channel or over a single geometrically periodic roughness element of length \( s \). In both cases, \( f \) is defined as:

\[ f = 2 \frac{\Delta p}{\Delta L \langle u \rangle} \frac{D_h}{\mu} \]  

where \( D_h = 2H \) is the hydraulic diameter, the variations \( \Delta L \) and \( \Delta p \) are computed between the inlet and outlet section, either of the whole rough portion of the channel or of the single roughness element, \( \langle \cdot \rangle \) means average over cross section.

The Poiseuille number \( Po \) is then computed as:

\[ Po = f \times \text{Re} = 2 \frac{\Delta p}{\Delta L} \frac{D_h^2}{\mu \langle u \rangle} \]  

For uncompressible flow through smooth channel with first order slip boundary condition it’s possible to compute an analytical expression for the Poiseuille number:

\[ Po_{\text{smooth}} = \frac{96}{1 + 12 \cdot s_p \cdot Kn} \]  

For either compressible or rough surface flows no analytical solution is available. However, a few correlations have been proposed. In particular, an expression for rough surfaces, based on the results obtained by the Lattice Boltzmann computations, was proposed in [10]:

\[ Po_{\text{rough}} = Po_{\text{smooth}} \times (1 + 0.8 \varepsilon + 24 \varepsilon^2) \]  

while Asako et al. [18] suggested a local Po correlation for a developing compressible flow:

\[ Po_{\text{comp}} = 96 - 4.55 \times Ma + 274.8 \times Ma^2 \]  

Equation (44) allows for a first assessment of numerical results. Figure 3 compares Poiseuille numbers from kinetic and NS computations in a smooth channel with the first order expression equation (44) and numerical results of Varoutis et al. [19] obtained by BGK-model equation. We consider a small pressure ratio \( \frac{p_0}{p_e} = 1.1 \) (small compressibility effect) and an exit Knudsen number \( Kn_e \) range from 0.01 to 0.81. It can be seen that S-model results are close to the BGK-model ones from [19] in the whole range of \( Kn \), thus the numerical scheme for the solution of S-model can accurately predict rarefied flow. We should expect that first order expression is accurate at lower \( Kn \). The NS results well correlate with both analytical expression and kinetic computations. As expected, kinetic results deviation from slip solutions become apparent above \( Kn = 0.05 \).

Figure 4 shows the averaged Poiseuille \( Po \), defined by equation (43), between the inlet and outlet section of a rough sector of length \( L^* = 2.3 \) \( H \) at the end of the channel, i.e. including 9, 18 or 36 rough modules, depending on \( \varepsilon \). The length and the position of \( L^* \) was chosen in order to exclude the
developing flow region at the beginning of the rough sector. The Poiseuille number increases with \( Re \); due to equation (41), this means also an increase in \( Po \) related to a decrease in \( Kn \). The picture for a higher pressure ratio (higher actual \( Ma \)), but roughly comparable width of \( Re \) range, shows a much steeper slope. This clearly suggests that the dominant effect is the compressibility.

Figure 3. The rarefaction effect on the Poiseuille number in a smooth channel: \( p_{oi}/p_e = 1.1 \).

Figure 4. Averaged Poiseuille number vs. averaged Re: (left) \( p_{oi}/p_e = 2 \), (right) \( p_{oi}/p_e = 3 \).

Figure 4 shows significant discrepancies between NS and kinetic results at low level of \( Re \) and high roughness. These conditions correspond to the higher rarefaction levels: as an example, at \( \epsilon = 5\% \), \( p_{oi}/p_e = 3 \) and \( Re = 21 \) we have an exit Knudsen number equals to 0.055. In particular, NS overestimates the rough effect in comparison with S-model results, at higher rarefaction level, up to nearly 30%, while for \( Re = 100 \) the discrepancies are negligible.

In figures 5, the local Poiseuille number for \( \epsilon = 0, 2.5\% \) and 5% and pressure ratios \( p_{oi}/p_e = 3 \) and 2 respectively is plotted as a function of the cross section averaged Mach number. The Reynolds number is nearly constant along the channel, but the Mach number increases due to the acceleration of the gas flow. For rough channels the local \( Po \) is computed between the inlet and outlet sections of each rough module. In figures 5 we can easily identify the transition region between the smooth and rough sectors. The developing flow in this area yields a quick decrease in Poiseuille. As soon as this transition is completed (i.e., at the minimum in the \( Po \) curve), Poiseuille becomes a monotone function of \( Ma \). Figure 5 shows, at the \( p_{oi}/p_e = 2 \) and lower \( Kn_{ei} \), that for the same value of local \( Ma \) both kinetic and NS solutions offer the same value of \( Po \), for both smooth and rough channels. For rough geometries and higher rarefaction, on the other hand, NS over estimates the roughness effect.

Moreover, the impact of compressibility, especially at higher pressure ratio is much more significant than the variation due to roughness: \( Po \) at \( Ma = 0.6 \) is three times higher than at \( Ma = 0.3 \), while the increase between rough and smooth channel at the same \( Ma = 0.6 \) is at most 40%.
Furthermore, in figure 5 the comparison with correlation equation (46) for smooth channel of Asako [19] is presented. For lower $Kn_d$ equals to 0.01 and $p_0/p_e = 2$ there is a small difference between equation (46) and numerical solution. When Knudsen number increases the difference becomes larger and local $Po$ are lower than that obtained from the Asako’s expression. This is due to the rarefaction effect, which is not included in the model of Asako et al. [19]. The rarefaction alleviates the friction effect of the wall on the gas flow. It should be mentioned that for higher pressure ratio $p_0/p_e = 3$ (see figure 5) the deviation from equation (46) is large both for lower $Kn$, due to high $Ma$ numbers exceeding the correlation range of validity, and for higher $Kn$, due to the rarefaction effect.

The increase in Poiseuille number due to the roughness, and the behavior of kinetic and continuum solvers are different at different Mach numbers. Looking at figure 5, for $Kn_d = 0.01$, at $\varepsilon = 5\%$ and local $Ma \approx 0.6$ the Poiseuille number increase, with respect to the smooth channel, is 30$\%$ for kinetic results and 41$\%$ for NS ones. At a lower $Ma$, namely $Ma \approx 0.37$, and the same roughness the increase is smaller, around 30$\%$, and is nearly identical in both kinetic and NS results. Accordingly, for pressure ratio $p_0/p_e = 3$ the difference between NS and kinetic results increases towards to the outlet reservoir (i.e. at higher $Ma$) in the rough channel, while for smooth channel the difference is small. For smaller pressure ratio $p_0/p_e = 2$ there is no difference between kinetic and NS results for smooth and rough channels at lower $Kn$.

![Figure 5. Local Poiseuille number at $p_0/p_e = 2$ (left); $p_0/p_e = 3$ (right).](image)

![Figure 6. $Po/Po_{smooth}$ via $\varepsilon$: (left) $p_0/p_e = 2$, (right) $p_0/p_e = 3$.](image)
In figure 6 we plot the increase of averaged rough Poiseuille number with respect to smooth value, based on the non-entrance region, as a function of roughness height $\epsilon$ for different $Kn_e$ from 0.01 to 0.08. At higher $Kn$ kinetic and continuum solutions show quite different behaviours. For kinetic results the maximum deviation is reached at the lowest $Kn_e$ for both pressure ratios: thus, the surface roughness has a more significant effect on a weaker rarefied gas flow. Similar behavior has also been observed in the DSMC results of Sun [7], whose calculations indicated $Po$ significantly decreased when the Knudsen number increased from 0.02 to 0.08. On the opposite, for NS results maximum deviation of $Po$ reaches at higher rarefaction $Kn_e = 0.04$ ($Kn_e = 0.055$).

![Figure 7](image.png)

**Figure. 7.** The rarefaction effect on the Poiseuille numbers in a rough channel.

In order to concentrate on the coupling effect of rarefaction and roughness the flow for small pressure ratio $p_0/p_e = 1.1$ and $0.01 < Kn_e < 0.08$ has been considered. In figure 7 the Poiseuille numbers for rough surface ($\epsilon = 5\%$) obtained by NS and S-model equations are compared with the correlation equation (45) suggested in [7]. Such picture indicates that kinetic computed $Po$ correlates well enough with expression (45) for high Knudsen number, while at lower ones the correlation fails and NS results offer good agreement with kinetic data. It is worth to notice that, while in a smooth channel continuum and kinetic approaches show good agreement up to $Kn_e = 0.05$, for the rough geometries the discrepancies appear at lower even at $Kn_e = 0.02$. This is due to the fact that the effect is related to geometrical details (peak height) of a much smaller scale than the channel height; thus, the significant length scale is smaller than $H$, and, as a consequence, a representative $Kn$ should actually be higher than the $H$ based one.

5. Conclusion
The numerical analysis of the flow field in rough microchannel with relative roughness ranging from 0% to 5% has been carried out using two approaches: Navier-Stokes equations provided with the first order slip-boundary condition and kinetic S-model equation with Maxwell diffuse reflecting boundary condition. The use of implicit scheme for the solution of S-model equations and the optimization of the algorithm using parallelization in both physical and velocities spaces allow for efficient computations.

It was found that compressibility is the dominant effect increasing the value of Poiseuille number. Such effect often overcomes the Poiseuille number significant decrease due to rarefaction effects. As expected at a fixed pressure ratio and rarefaction level the increase in roughness gives an increase in Poiseuille number which may be significant.

The difference between NS and S-model results is smaller at lower $Kn$ and increase with $Kn$, as expected; however, while for smooth channels the two approaches agrees well up to $Kn = 0.05$, in the rough case the discrepancies arise earlier. This is consistent with the idea that the representative length scale for the flow around the roughness peaks is their height, which is a few percent of $H$. Thus,
locally rarefaction has a greater impact on the flow and first order slip may become inadequate. This interpretation is supported by the fact that NS consistently over-estimates the rough effect in comparison with S-model results.

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