A Novel Modeling Method of Surface Roughness in a Microfluidic Channel

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***Abstract*—A novel modeling method of a surface roughness is presented. A straight channel having a random, normally distributed roughness is studied by measuring the change of a hydraulic resistance. A significant amount of attention is focused on a realistic modeling of the surface roughness. Navier-Stokes equations are solved numerically with a finite element method (FEM). Both two and three dimensional cases with roughness varying from 1 to 30 % are studied. The results and developed modeling method create a base for further experimental research on the effect of surface roughness on microchannel flows.**

I. INTRODUCTION

MICROFLUIDICS is used for the transport and handling of small volumes of liquids in an increasing number of applications such as biomedical diagnostics, micro fuel cells and cooling of microelectronics. The most important basic component in microfluidics is a microchannel carrying the liquid.

When the scale is decreased, many macro scale phenomena such as gravitation become negligible. In the microscale, surface phenomena such as hydrophobicity, hydrophilicity and surface roughness become significant. A large surface roughness causes inconvenience in the microchannel by decreasing the flow rate and bounding air bubbles from the liquid to the surface of the channel. Beside these negative effects the surface roughness can be exploited for example in passive valves in microfluidic channels.

The effect of the surface roughness on the pressure driven flow through a microchannel has been studied previously in the Toronto University research [1]. The case in that research was to model the surface roughness with a specific size blocks. The influence of the size and displacement (symmetric and asymmetric) of the blocks was studied using a pressure drop per unit length as a measure.

The approach of the research at the Toronto University has some benefits e.g. simple and lighter analytical solution compared to time consuming numerical simulations in this research. The greatest weakness in Toronto research is the lack of realism. Surface roughness can be considered as random phenomena and this cannot be perfectly modeled with blocks.

This paper studies the effect of the surface roughness on microchannel flow using a finite element method. Section II will present parameters and a basic theory for model construction. Section III focuses on modeling issues like mesh extruding and simplification. Section IV presents and compares the final results.

II. PROBLEM SETTING

An effect of the surface roughness to a liquid flow in a microchannel is studied with numerical simulations. A model construction is made carefully and a lot of attention is focused on a realistic modeling of the surface roughness. The surface roughness is defined here as a percent value from the channel's diameter. Different roughness values varying from 1 to 30 % are studied. Assumptions concerning the distribution of the surface roughness are minimized using normal distribution in roughness definition.

A. *Surface Roughness - Definition*

The surface roughness is understood as an irregularity from a smooth surface caused during a fabrication process. These irregularities appear as microscopic holes and bulges from the expected (smooth) surface.

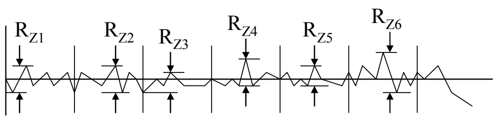

Fig. 1. Surface Roughness can be defined as an average vertical deviation between the highest bulges and lowest holes.

Manuscript received June 30, 2005.

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The surface roughness can be defined as a vertical deviation between the highest bulge and deepest hole within a certain area (Fig. 1). An average surface roughness (for now on just surface roughness) can be specified with Eq.1. [2]

$$R_z = \frac{1}{n}\left(R_{z1} + R_{z2} + R_{z3} + \ldots + R_{zn}\right) \quad (1)$$

In a microfluidic channel, the surface roughness is mostly caused by an inaccurate mask and its imprecise alignment in the fabrication process. These are common problems and expensive to avoid.

B. Hydraulic Resistance

A liquid is moved trough a straight channel with a pressure difference between the channel ends. This causes a specific flow rate to the liquid. If the pressure is kept constant, flow rate depends on the geometry of the channel and the properties of the liquid media. The ratio between the pressure and flow rate defines how the channel geometry limits the flow rate. This is known as hydraulic resistance. Eq. 2 presents the relation between the pressure difference Δp, flow rate Q and hydraulic resistance R_H. It is analogous to Ohm's law and is also known as Hagen-Poisseuille law. [3]

$$\Delta p = R_H Q \quad (2)$$

A smooth, optimal microfluidic channel has the specific hydraulic resistance related to the geometry. The surface roughness on the wall of the channel increases this by decreasing the flow rate. The change of hydraulic resistance is proportional to the change of the surface roughness. For this reason, the hydraulic resistance was selected to measure the effect of the surface roughness on the flow in the microchannel. The results are presented as a percentual change of the hydraulic resistance.

Analytic solutions for simulated geometries are presented below. Eq. 3 represents solution for a (unreal) smooth 2D channel [kg / m^3 s]. Eq. 4 represents solution for a square cross-section channel [kg / m^4 s]. [3]

$$R_H = 12\eta L \frac{1}{h^3} \quad (3)$$

$$R_H = \frac{12\eta L}{1 - 0.58} \frac{1}{h^4}, \quad (4)$$

where h is height, L is length and η is a fluid dynamic viscosity.

C. Studied Geometry

The modeling is focused on a basic microfluidic channel. The channel can be made e.g. on silicon with photolithography methods. The bottom and top of the channel can be considered to be smooth. That is because an etching is assumed to be perfect on the bottom surface and the top surface has not been affected by the etching process. The walls of the channel suffer by the surface roughness (Fig. 2) caused by the fabrication methods (inaccurate mask, alignment error). If the channel is made on plastics, the quality of the mold has an influence on the quality of the channel walls.

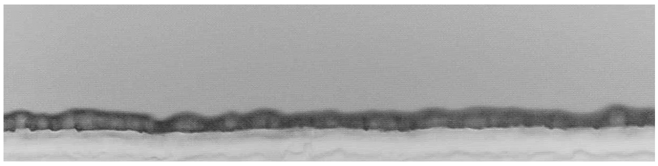

Fig. 2. Top view from the wall of the microchannel [4].

A computer model in Fig. 3 presents the studied channel. All the parameters are listed in Table 1. The liquid media inside the channel is water. The surface roughness in Fig. 3 is about 20 %.

Table. 1. Model parameters.

Parameter	**Value**
Geometry	
Width	100 µm
Height and depth	100 µm
Length	1 mm
Liquid Media	
Density	1000 kg / m^3
Dynamic viscosity	0.001 Pa·s
Pressure	1000 Pa

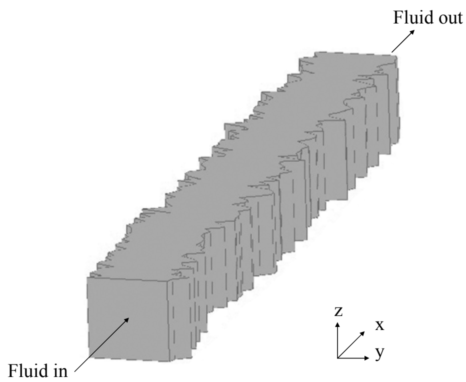

Fig. 3. Studied microchannel with 20 % surface roughness.

Selected dimensions were a compromise between the accuracy and modeling time. The effect of the channel length on the simulation results was studied.

The selected length was found to be adequate for accurate solutions with used surface roughness values (1 to 30 %). With a shorter channel (50 %) the results would be inaccurate.

D. Model Construction

The model was constructed with line elements. The elements were defined to form a continuous edge for the simulated microchannel. The surface roughness on the edge was defined as a normally distributed deviation. This was used because the true distribution of the surface roughness was not known. Normal distribution minimizes the needs to make assumptions.

An expectation value μ was set along the geometry of the channel and a standard deviation σ (factor defining the surface roughness) was given as n % of the width of the channel. The number of roughness peaks (spacing between roughness elements) was fixed by relating it to the standard deviation and channels length. Fig. 4 presents different surface roughness values compared to a smooth channel (0 % roughness)

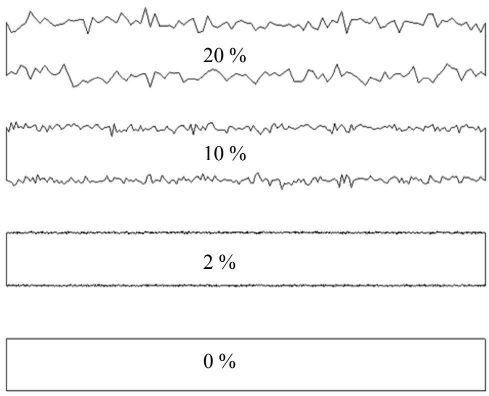

Fig. 4. 2D channel with different surface roughness.

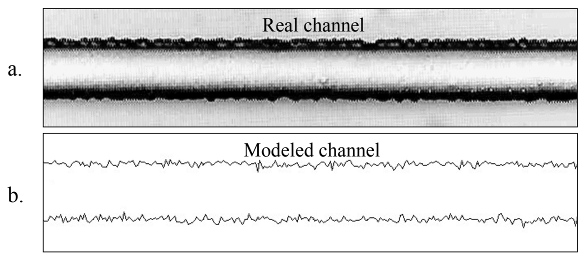

Fig. 5. Real surface roughness [4] and randomly generated model with the same surface roughness.

Assumptions concerning the surface roughness model quite accurate the real case. Fig. 5 represents a true micromachined microchannel (Fig. 5.a) and randomly generated channel geometry (Fig. 5.b). The percentual roughness for the modeled case is 8 % and for the real case about 7-9 %.

III. Modeling Surface Roughness

A numeric estimate for the hydraulic resistance with the different surface roughness values is studied. Partial differential equations are solved with a finite element method using Matlab and Femlab.

A. Modeled Cases

The modeling of the surface roughness was first focused on a 2D case (Fig. 6). A modeling method was developed and tested to be reliable. Fig. 6 shows the velocity field for the simulated surface roughness values.

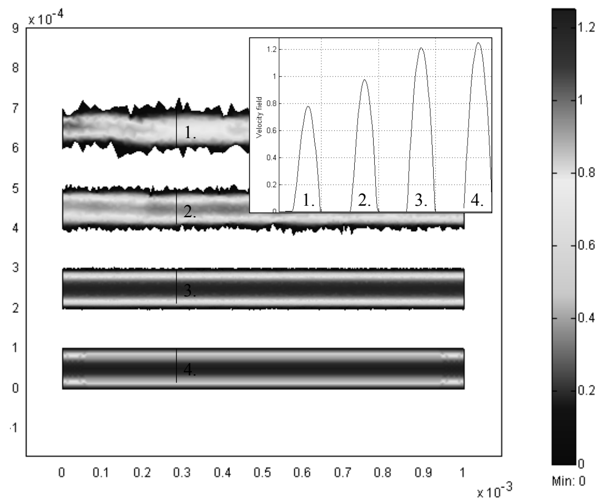

Fig. 6. Velocity field of the 2D microhannel with surface roughness of 0,2,10 and 20 %. Velocity profiles and amplitudes can be compared in the additional graph.

The 2D solution describes the problem imperfectly. It assumes that the channel has an infinite depth. In the real case, the aspect ratio (ratio between the deepest and widest structure) of the microfluidic channel is usually about 1.

A full 3D structure was based on the code used in the 2D model. The 2D geometry was extruded up to 3D and equations were changed to describe a three dimensional modeling space. The 3D model caused memory problems which were solved using symmetry and mesh extruding.

Studied structures were the full 2D channel, a half 2D channel with a symmetry and quarter of the 3D channel with symmetries. The 3D case was also studied with different numbers of mesh layers to optimize accuracy.

B. Simplification of the 3D Model

The 3D model (Fig. 3) was simplified using symmetry. Fig. 7 shows the planes used for simplification. The channel was cut in half with the vertical XZ-plane (Fig. 7). Both sides of the channel were assumed to be equal with some certainty. The left side of the channel was selected and re-cut with the XY-plane. The entire channel was now modeled with one quarter of the channel. At this point, it was clear that a result would suffer a bit because of a reflected pattern. With large percentual roughnesses this was noted to cause deviation and inaccuracy.

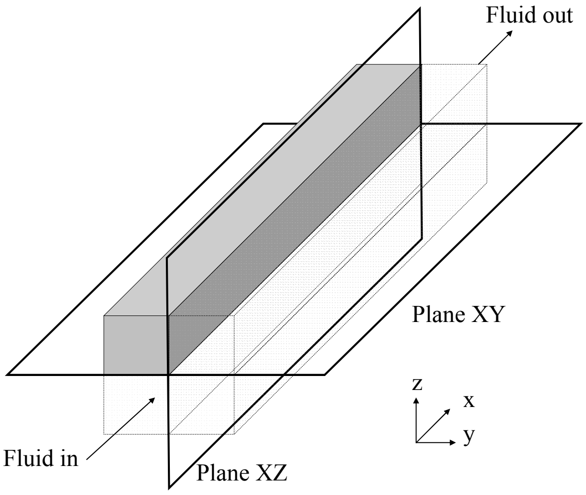

Fig.7. Simplifying 3D channel to quarter of channel.

C. Mesh Extruding with Mesh Layers

A 3D model can be constructed in many ways. After several experiments it was discovered that they all use too much memory. Due to the laminar flow in a microchannel it is possible to use a coarser mesh without loosing accuracy. This was the first step to lighter the model. The second step was to use an extruded mesh, simplifications and mesh layers to model the 3D case.

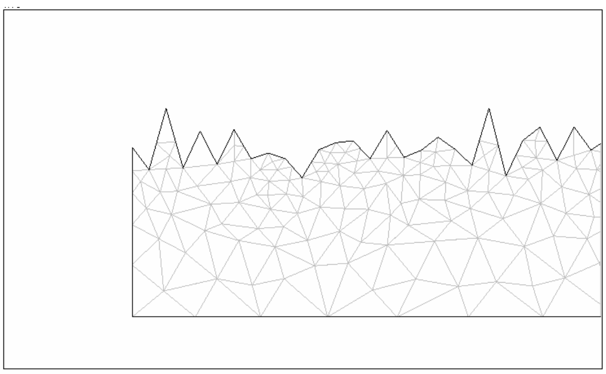

Fig. 8. Half channel 2D model meshed with coarse mesh.

The half channel 2D geometry (Fig. 8) was first meshed with a specified mesh. After this the mesh was extruded up to the 3D model. The number of mesh elements in Z-direction was studied with additional simulations. It was discovered that with five mesh layers the results are accurate enough (Fig. 9).

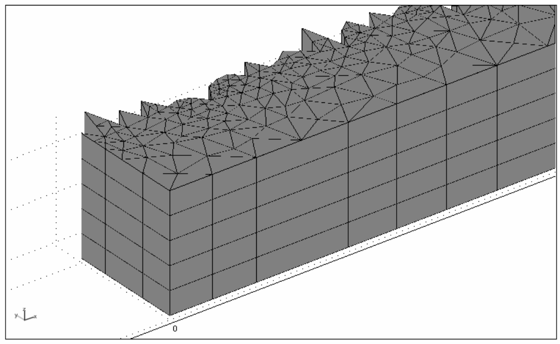

Fig. 9. 3D quarter channel with five mesh layers.

D. Finite Element Method

The modeling problem is solved using incompressible Navier-Stokes equations for laminar flow. These nonlinear partial differential equations can be presented as follows:

$$\rho\frac{\partial u}{\partial t} - \eta\nabla^2 u + \rho(u\cdot\nabla)u + \nabla p = F \tag{5}$$

$$\nabla\cdot u = 0, \tag{6}$$

where η is the dynamic viscosity, ρ is the density, u is the velocity field depending on the modeling space, p is the pressure and F is a volume force containing e.g. gravity. Solving of these PDEs is made numerically with Femlab.

IV. Results

Simulations were repeated to increase repeatability and reliability of the results. The average and the standard deviation of 100 simulations for each surface roughness value are presented. The surface roughness values from 0 % to 30 % are studied.

A. Reference Models

An ideal smooth channel is used as a reference. The simulated channels are compared to the smooth channel. Both numerical and analytical solutions are presented for the reference channel. The analytical solution is presented to connect numerical simulation to the real world. Table 2 presents these reference results. Analytical values are in italics.

Table. 2. Reference values for the hydraulic resistance.

	2D	3D
Q	83.560 ml /s·m *83.333 ml /s·m*	3.514 µl / s *3.539 µl / s*
$\mathbf{R_{hd}}$	$1.1968 \cdot 10^7$ kg / m^3 s *$1.2000 \cdot 10^7$ kg / m^3 s*	$2.8459 \cdot 10^{11}$ kg / m^4 s *$2.8258 \cdot 10^{11}$ kg / m^4 s*

B. Reliability

The reliability of one simulation should be taken with a caution. A simulation may be disturbed for many reasons. The simulated channel can be e.g. blocked with some probability (tails of the normal distribution). The probability increases with higher surface roughness values and when only a half of the channel is modeled. Amount of statistical errors was minimized repeating each simulation 100 times. The results could now be presented with the average and deviation.

C. 2D Channel vs. 2D Half Channel

The results in Fig. 10 present the change of hydraulic resistance as a function of surface roughness. Both 2D model and 2D half channel model are plotted with the average line (bolded lines) and with deviation lines (1σ).

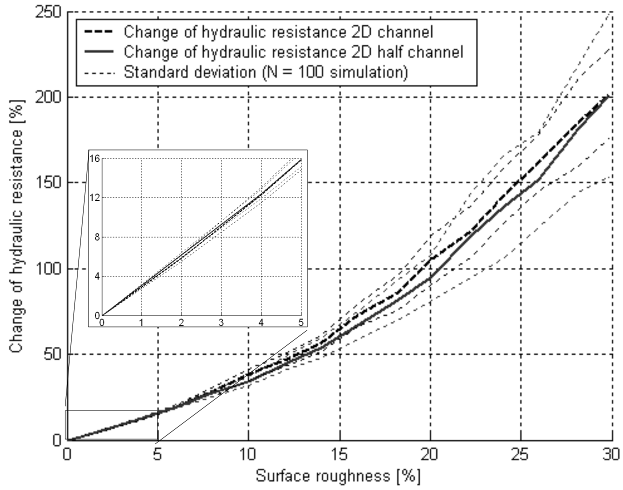

Fig. 10. The change of hydraulic resistance as a function of percentual surface roughness in 2D channels.

The lack of randomness in the 2D half channel increases the deviation as can be seen in the figure. The results are still comparable and the half channel two dimensional geometry can be used as a base for the three dimensional model.

D. 2D Channel vs. 3D Quarter Channel

The results in Fig. 11 are plotted as in section IV- C. The 2D model is compared to the 3D quarter model. It can be seen that the effect of the surface roughness is slightly smaller for the 3D case than for the 2D case. That is because the bottom and roof of the 3D channel were considered as smooth. The 2D model was notified to have almost linear relationship with the 3D model. This will be studied more in further research.

Despite the fact that the more realistic 3D case is less sensitive to the surface roughness than the 2D case, it must be notified that e.g. with 10 % surface roughness 30 % more pressure is needed to achieve the same flow rate.

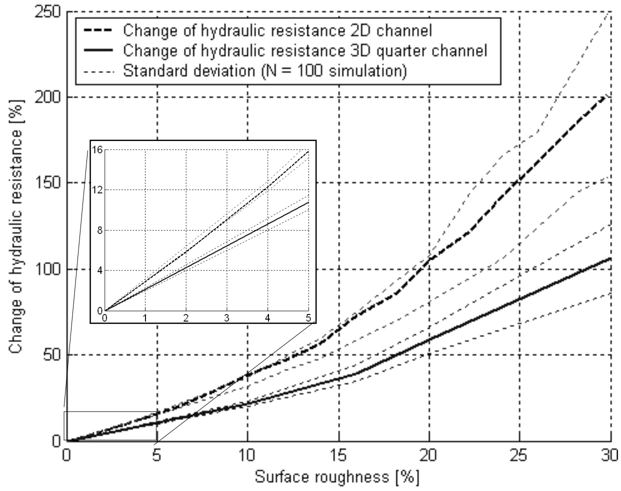

Fig. 11. The change of hydraulic resistance as a function of percentual surface roughness. 3D quarter channel model is plotted with solid line and 2D half channel model is plotted with dashed line.

V. CONCLUSION

The effect of the surface roughness in microchannel was studied. Hydraulic resistance was used as a measure for the effect of the surface roughness. The modeling was focused on 2D and 3D models. The 2D model was used to give guidelines and limits for the 3D model. The 3D model gives more realistic results basing on true boundary conditions.

The change of the hydraulic resistance was presented as a function of surface roughness. The reliability of the results was increased by repeating the simulations 100 times. The results were shown with the average and deviation. The results show that e.g. 10 % surface roughness leads to 30 % increase of hydraulic resistance. The relationship between the surface roughness and the change of hydraulic resistance is not linear but exponential.

The research is significant, since the created surface roughness model can now be used in a further experimental research. One interesting case is to study how the varying surface roughness can be utilized as passive valves in microfluidics channels.

The next step is to verify achieved results with an experimental research. This can be connected to the current model with an image based measurement. The shape of the real channel with a surface roughness can be imaged and used as geometry for the numeric model.

VI. ACKNOWLEDGMENT

The authors would like to express their sincere thanks to S. Lukkarinen and J. Pennanen from Comsol Oy, to N. Matintupa from University of Jyväskylä and to Hong Yu from Tampere University of Technology.

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