Chapter 4 Health Area

NUMERICAL SIMULATION OF A PDMS MICROFLUIDIC CHANNEL COMPATIBLE WITH BIOSENSORS

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Abstract

Microfluidics has promoted the development of sensors, whose designs, materials, and sizes have been adapted for application in areas such as biology, chemistry, and health. For this, the design of the microfluidic system studies the effect of those parameters on its operation, in addition, the microfluidic design must be compatible with the transducer characteristics. Numerical simulations are powerful tools that allow us to analyze whether microfluidic designs are appropriate, and thereby advance to the microfabrication phase. Nevertheless, performing a numerical simulation of a microfluidics system is not an easy task. In this work, the design of a microfluidic channel is described using COMSOL Multiphysics 5.5. The material is polydimethylsiloxane (PDMS), and its dimensions are chosen to work with a laminar flow. Fluid flow patterns, pressure distribution, and velocity field of water were observed by using the simulation software. The results showed that the velocity and pressure of the water increased, from 0.0012 m/s to 0.06 m/s and from 0.06 Pa to 174.37 Pa, when increasing the flow ratios from 10 μL/h to 500 μL/h. The 3D and 2D graphs showed that the distribution of the water velocity decreased in the walls, due to the interaction between the PDMS and water. Finally, this study provides information to analyze the design of the microchannel and to organize the experimental measurements, establishing suitable geometries, materials, and injection flow ratios.

Keywords: microfluidics, numerical simulation, PDMS, microchannel, pressure, velocity.

1. Introduction

Microfluidics is a field focused on the engineered manipulation of fluids and molecules at the microscale [1]. It studies fluids confined in microchannels typically smaller than 500 μm. It is a growing field of research which is having a significant effect on point-of-care diagnostics and clinical studies[2, 3]. Additionally, microfluidics is very well established in academia [4, 5] and it is rapidly gaining positions in the industry mainly for the development of new methodologies and new products for life sciences [6].

The potential of microfluidics lies in size reduction, scaling down fluidic processes to the microscale, offering significant advantages, for instance; Miniaturized components and processes employing smaller volumes of fluid (pL-μL), thus leading to reduced reagent consumption, as a result, this decreases costs and permits optimized small quantities of expensive samples, thereby the quantities of waste products are reduced [7]. In the microfluidic devices, diffusive mixing is easy and fast, often increasing the velocity and accuracy of reactions. A microfluidic chip allows to reduce measurement times, improve sensitivity, higher selectivity, and greater repeatability [9].

A microfluidic chip is a pattern of microchannels, molded by techniques of microfabrication [4, 5, 9, 10]. Those microfluidic chips can be integrated with transducers (e.g., optical, mechanical, electrical, magnetic, etc.) to form as we know it as a lab on a chip sensor [5, 11, 12]. The microfluidic chip design is essential to obtain an optimized system. It requires analyzing on the effect of the geometry, material, fluids, and temperature etc. Numerical simulations are useful tools to perform preliminary physical tests and investigations on microfluidic chips, also to verify the quality of the microchannel fabrication [13]. A numerical simulation is a calculation to study the behavior of systems whose mathematical models are complex to provide analytical solutions. However, performing a numerical simulation is a very complex task. It requires knowledge about of the software and the physical concepts of microfluidics, to configure the simulation properly and thereby obtain correct results.

In this work, we use the COMSOL Multiphysics program [14] to describe the microfluidic chip design of a polydimethylsiloxane (PDMS) microchannel, with a radius of reservoir of 250 μm, with a length 1000 μm and with a width and height of 70 μm. Its geometry could be compatible with optic (e.g., gold)

[15] and mechanical [11] (e.g., lithium niobate) transducers to create lab on a chip sensors. This study is aimed to describe, step by step, the design of a single microfluidic channel in COMSOL Multiphysics. Additionally, we calculate and analyze the pressure and velocity of water using different flow ratios, commonly used in bio applications.

2. Methodology

2.1. *Setting*

The simulation of the microfluidic channel is carried out in the engineering modeling software COMSOL Multiphysics version 5.5. The settings are mentioned in Table 1.

Table 1. COMSOL configuration for the microfluidic channel

Settings	Details
Space Dimension	3D
Physic	Fluid Flow, Single-Phase Flow, Laminar Flow
Study Type	General Studies, Stationary
Module	Microfluidic

2.2. *Geometry of the PDMS microfluidic channel*

The Figure 1a shows the geometry of the microchannel, where L represents the length, it is parallel to the Y axis that connects two reservoirs, Ri for the inlet and Ro for the outlet, the radius is 250 µm. For a correct union between the

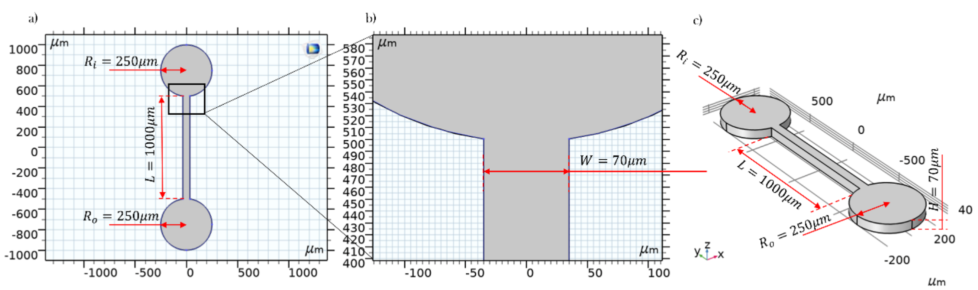


Figure 1. Geometry of the PDMS microfluidic channel. a) Top view of the reservoirs, inlet and outlet, with 250 µm of radius, b) Reservoir connecting to the rectangular part of the microchannel with a width (W) of 70 µm, and c) Microchannel dimensions.

rectangular part of the channel and the reservoir, it is necessary to extend the length of the channel as shown in the Figure 1b. An extrusion of 70 μm is set for the height (H) as shown in Figure 1c.

2.3. *Materials of the microfluidic channel*

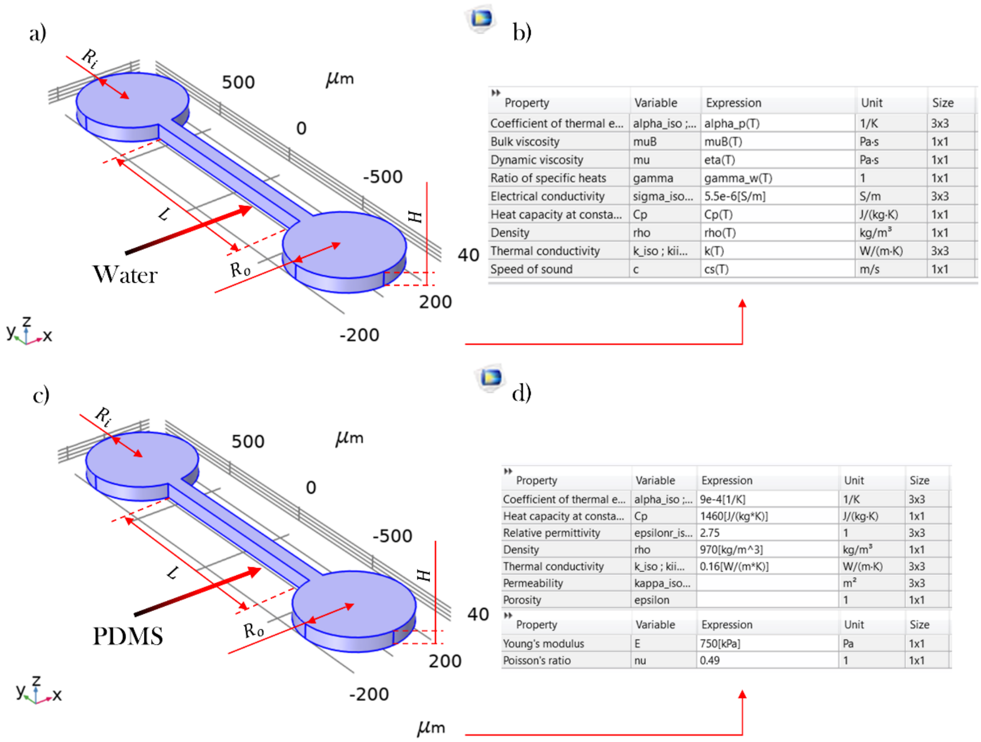
Polydimethylsiloxane (PDMS) is chosen as the material for the walls due to its excellent properties that allow molding at microscale a channel. This polymer is transparent, and a biocompatible polymer widely used in microfluidics due to its compatibility with biosensors. [5, 16] as for example cellular adhesion. Cellular adhesion is a multipart process with crucial implications in physiology (i.e. immune response, tissue nature, architecture maintenance, or behaviour and expansion of tumor cells We can set its Young's modulus, so we have the option to modify the design or make the study more efficient.

Water is chosen as fluid because it is the universal dissolvent and its properties are used as a reference to understand the behavior of the fluid through the microchannel, and thereby, we could compare the behavior with other biological fluids.

The PDMS and water do not need to be registered, COMSOL software has their properties in the library. The properties are specified in the following Figure 2. We select the entire microchannel for water, it must be configured as one solid, see Figure 2a-b. We select the walls, one by one, to configure PDMS material as shown in the Figure 2c-d.

2.4. *Inlet and outlet port microfluidic channel*

In this section, the inlet and outlet of the microchannel are configured as well as the water as a laminar flow. The inlet reservoir (Ri) is selected as shown in Figure 3a, where a tubing is connected to inject the water inside the microchannel, then, due to the same pressure, water passes through the microchannel and reaches the outlet reservoir as shown in Figure 3b. The water leaves the microchannel due to the pressure and through another tubing connected at the outlet reservoir as shown in Figure 3c. We test three different flow ratios, 2.778×10^{-12} m^3/s, 9.772×10^{-12} m^3/s, and 1.3889×10^{-10} m^3/s which are equivalent to 10 μL/h, 35 μL/h, and 500 μL/h, respectively. These flow ratios are commonly used in biofunctionalization and droplet generation processes [2]. It's important to verify that at the end of this configuration, when entering the Inlet, Outlet and Wall option, the selection is displayed as shown in Figure 3.



Property	Variable	Expression	Unit	Size
Coefficient of thermal e...	alpha_iso ;...	alpha_p(T)	1/K	3x3
Bulk viscosity	muB	muB(T)	Pa·s	1x1
Dynamic viscosity	mu	eta(T)	Pa·s	1x1
Ratio of specific heats	gamma	gamma_w(T)	1	1x1
Electrical conductivity	sigma_iso...	5.5e-6[S/m]	S/m	3x3
Heat capacity at consta...	Cp	Cp(T)	J/(kg·K)	1x1
Density	rho	rho(T)	kg/m³	1x1
Thermal conductivity	k_iso ; kii...	k(T)	W/(m·K)	3x3
Speed of sound	c	cs(T)	m/s	1x1

Property	Variable	Expression	Unit	Size
Coefficient of thermal e...	alpha_iso ;...	9e-4[1/K]	1/K	3x3
Heat capacity at consta...	Cp	1460[J/(kg*K)]	J/(kg·K)	1x1
Relative permittivity	epsilonr_is...	2.75	1	3x3
Density	rho	970[kg/m^3]	kg/m³	1x1
Thermal conductivity	k_iso ; kii...	0.16[W/(m*K)]	W/(m·K)	3x3
Permeability	kappa_iso...		m²	3x3
Porosity	epsilon		1	1x1

Property	Variable	Expression	Unit	Size
Young's modulus	E	750[kPa]	Pa	1x1
Poisson's ratio	nu	0.49	1	1x1

Figure 2. a) Scheme showing the selected parts of the microchannel where the water will flow, b) Properties of water, c) Selected geometry of the microchannel to configure the PDMS material, and d) Properties of PDMS polymer.

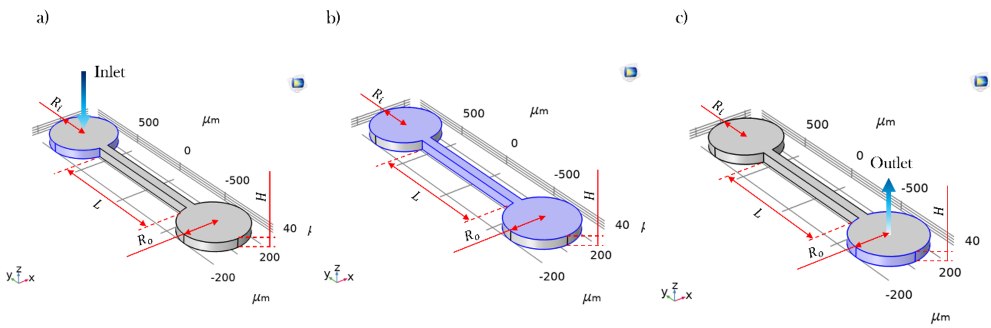


Figure 3. Port settings. a) Inlet port settings, reservoir Ri where the water enters, b) Walls port settings where the water flows and c) Outlet port settings, reservoir Ro where the water comes out.

2.5. *Mesh settings*

In this section, we select a normal mesh for a stationary study, this configuration has a suitable characteristic to perform it, see Figure 4c. Each crossing of lines in the mesh, called nodes, is where the resolution of equations is generated

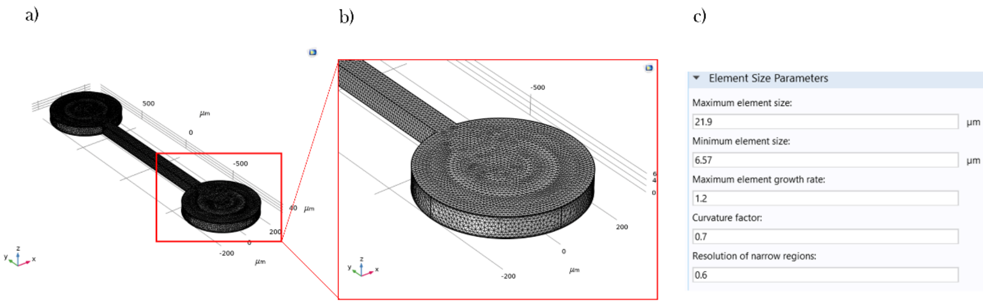


Figure 4. Normal mesh settings. a) Normal mesh along the entire geometry, b) Outlet reservoir with the mesh and c) Default properties of a normal mesh for a stationary study.

by COMSOL to obtain, speed, pressure, among other parameters. Figure 4a-c shows the main parameters for a normal mesh as well as an approach to the mesh produced in the outlet reservoir.

2.6. *Study Settings*

To generate a stationary study, slices of the areas of interest are needed. In this case, three types of slices are generated. The slice 1 is parallel to the microchannel in the yz plane, and it is in middle of the microchannel, as shown in the Figure 5a. The second plane (slice 2) is created parallel to the microchannel in the yx plane, see Figure 5b. Finally, we configure five slices in the zx plane, in the transversal form, as shown in the Figure 5c.

The slices are used to generate the stationary study in which the speed appears in each one to calculate the pressure and velocity of the water at different flow ratios.

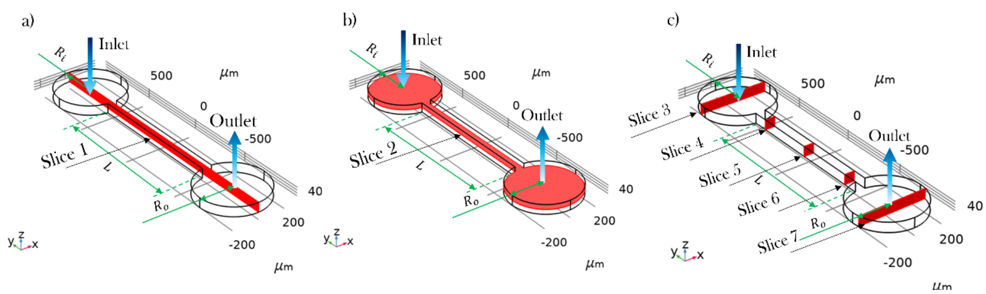


Figure 5. Settings of the slices. a) Slice 1 is parallel to the microchannel in the yz plane. b) Slice 2 is parallel to the microchannel in the yx plane. c) Slice 3 to Slice 7 is transversal to the microchannel in the zx plane.

3. Results and Discussion

3.1. *Velocity of the water through the PDMS microchannel*

To calculate the results, it is necessary to indicate the type of study that COMSOL will perform, if it is not given by default in the options box on the left of interphase, we must create it by selecting a new study in the tool ribbon at the top of interphase. Once this is done, to obtain the velocity, we select a 3D PLOT GROUP in the same tool ribbon and configure it to refer to Slice 1, created in the previous section, see Figure 5a. Once inside the 3D PLOT GROUP configurations, we will find a variable selector indicated with a red and a green triangle, in this section, we will search the variable of interest to analyze (e.g., velocity). Once this is done, we return to the study settings and press the Compute button to generate the study, as shown in Figure 6.

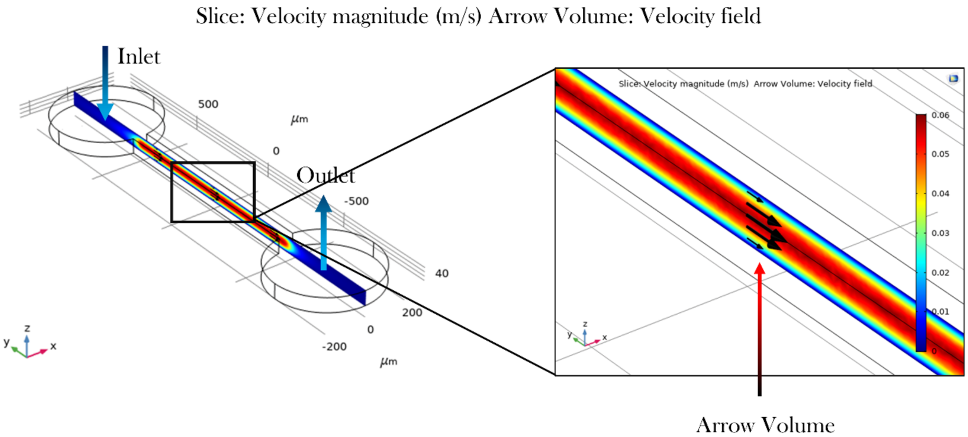


Figure 6. Slide 1 of velocity flowing through the microchannel and flow lines of that velocity indicating the direction from the inlet to outlet.

We can see in Figure 6 that the water velocity is less than 0.02 m/s in the inlet reservoir and in the outlet reservoir, while through the microchannel the velocity can reach 0.06 m/s. We can observe the water direction from the inlet to the outlet. For the second stationary study referenced to Slice 2, see Figure 5b. We repeat the previously mentioned steps but selecting the Slice 2. Then, we can see in Figure 7 that the velocity is transversely along the microchannel.

In the case of Slice 3-7 (see Figure 5), we obtain two results. The first one in 3D PLOT GROUP, with the velocity referenced to the transverse planes as

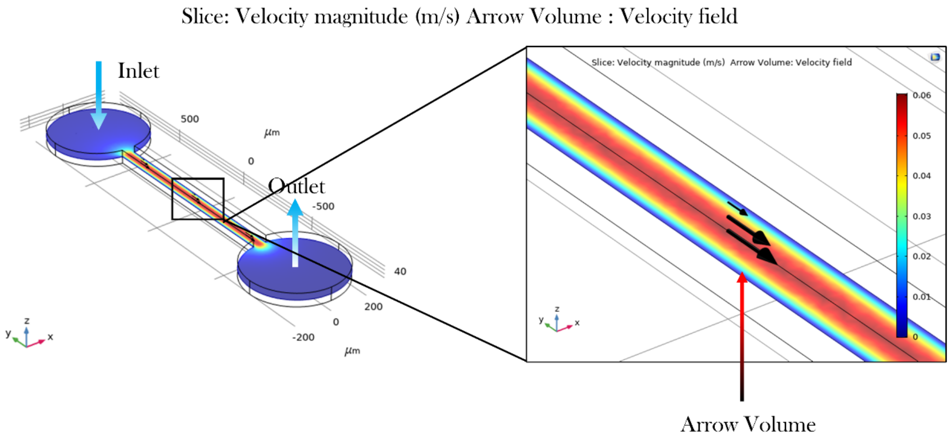


Figure 7. Velocity through the microchannel and flow lines of that velocity in the slice 2.

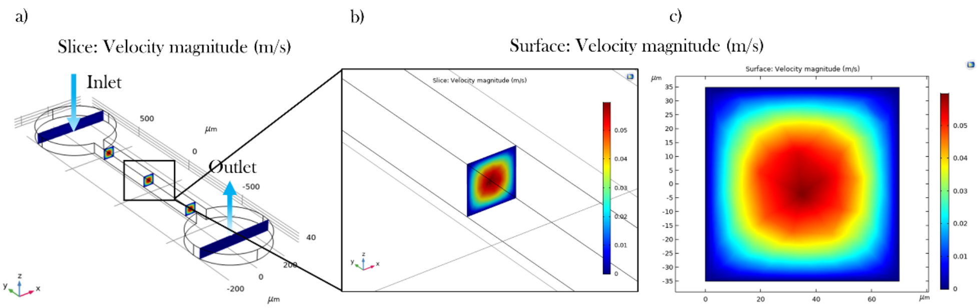


Figure 8. a) Velocity magnitude in the slices 3-7, b) 3D plot of the central slice 5, and c) Surface of the transversal velocity in 2D of the slice 5.

shown in Figures 8a and 8b, following the steps already mentioned. We plot a 2D PLOT GROUP and reference it to Slice 5, which is a central transverse plane, to observe the behavior of the water as shown in Figure 8c.

We can see in the Figure 8 the results of the slides 3-7, the scale is shown that goes from 0.0 m/s to 0.06 m/s, which is the velocity range calculated through the PDMS microchannel. We note that the velocity in the center reaches the largest value (0.06 m/s) while in the base (sensor) and walls (PDMS) the velocity reaches the lowest values (0.01 m/s). We attribute this behavior to the PDMS, due to it is a polymer with a Young´s modulus of 750 kPa that affects the flow of the water. With this simulation, it is possible to calculate the time that the water takes to pass through the entire microfluidic channel at different flow ratios, the results are shown in Table 2.

Table 2. Water injection flow ratios. Calculated pressure and velocity values by numerical simulation, and the travel time of the water through the microchannel.

Water Flow at inlet reservoir		Velocity (m/s)d		Pressure (Pa)e		Maximum Time (s)c
(μL/h)a	(m^3/s)b	min	max	min	max	
10	2.778 e-12	0.0	0.0012	0.06	3.48	0.833
35	9.722 e-12	0.0	0.0040	0.21	12.19	0.250
500	1.389 e-10	0.0	0.0600	2.93	174.37	0.016

a Flow ratio used for microfluidics applications.
b Flow ratio in unit accepted by COMSOL Multiphysics.
c Fill Time of water to pass through the entire microfluidic channel with 1000 μm of length.
d Calculated values of water velocity at Slice 2.
e Calculated values of water pressure at Slice 2.

3.2. *Pressure of the water through PDMS microchannel*

To obtain the water pressure inside the PDMS microfluidic channel, we select a 3D PLOT GROUP, in its settings, in the green and red triangle, we choice the pressure variable. We select the surface of the entire microchannel to obtain pressure values and pressure curves, to appreciate the behavior of the microchannel, as shown in Figure 9 a-d.

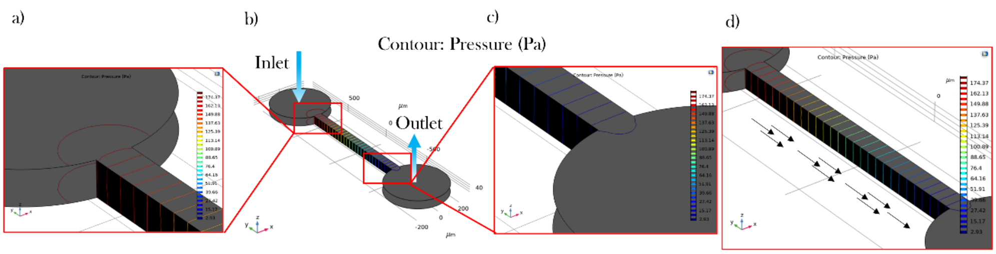


Figure 9. a) Pressure curves in the inlet reservoir, b) Pressure curves along the entire geometry of the PDMS microchannel, c) Pressure curves in the outlet reservoir and d) Pressure curves along the entire PDMS microchannel.

We can see in Figure 9 a-d, that the flow is distributed along the PDMS microchannel causing different pressures from 2.93 Pa to 174.37 Pa for a flow ratio of 500 μL/h. Thus, we can calculate and observe the maximum pressure values that the microchannel supports, without suffering damage or leaks, by varying the flow ratios of the water.

The data of pressure and velocity of water provide information to analyze the design of the microfluidic channel and to organize the experimental measurements, establishing suitable geometries, materials, and injection flow ratios. The pressure values at different flow ratios are shown in Table 2. As we expected, the values increase as the flow ratio increases. On the contrary, the time decreased as the flow ratio increased.

4. Conclusions

In this work, we presented a numerical simulation of a PDMS microfluidic channel whose geometry could be compatible with optic and mechanical sensors. We configured the microchannel geometry to analyze a laminar behavior, and to calculate the pressure and velocity using water.

PDMS material was selected for its well-known biocompatibility, thereby the PDMS microchannel can be applied in biology and chemistry. Water is used as a fluid and as a reference in these simulations.

The design is the basic microfluidic channel with an inlet and outlet. The radius of reservoirs is 250 μm with a length of 1000 μm, a width of 70 μm and a height of 70 μm. The PDMS microchannel can be fabricated with 3D printer or photolithography techniques.

In this work, we described the configuration of ports to analyze the behavior of pressure and velocity of water since this is the universal solvent and the most used in bio applications.

The results showed that the velocity goes from 0.0 m/s to 0.06 m/s decreasing in the walls, due to the interaction between the PDMS and water. The minimum filling time was 0.016 seconds using a flow ratio of 500 μL/h. The pressure goes from 2.93 Pa to 174.37 Pa. In the case of 35 μL/h, the velocity goes from 0 m/s to 0.0040 m/s, with a pressure that goes from 0.21 Pa to 12.19 Pa, with a filling time of 0.250 s.

For the flow ratio of 10 μL/h, the velocity goes from 0.0 m/s to 0.0012 m/s, with a pressure that goes from 0.06 Pa to 3.48 Pa, with a filling time of 0.833 s.

These calculations required at computational cost of 1.61 GB with an execution time of 1 minute and 20 seconds. With this work, we demonstrate the potential of numerical simulations for the suitable design and microfabrication of microfluidic systems compatible with sensors, also by numerical simulation is possible to vary the water for other biochemical substances, modifying its properties according to the study.

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