filling of non-trivially shaped microfluidic channels.

DEMCON MULTIPHYSICS

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Goal

In microfluidic channels, the behavior of fluids is the result of a competition between the capillary pressure and viscous resistance. The result of this competition can be analytically predicted for a simple case, such as a cylinder with a constant radius. A different approach is required for non-trivial channel cross sections, such as a rectangle or a trapezoid (see figure 1). Computational Fluid Dynamics (CFD) can be used to simulate the filling behavior of these channels and determine the filling time.

Using CFD we can accurately simulate the filling time of microfluidic channels, a crucial parameter in the design process. This information helps to make informed decisions to optimize the design. Here, we compare the filling time of a microfluidic channel with a trapezoidal and a rectangular cross-section.
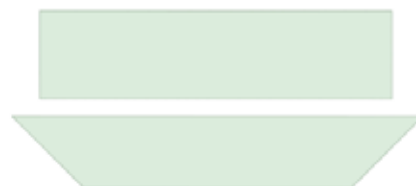

Figure 1. Cross section of microfluidics channel. On top, the rectangular shape. On bottom, the trapezoidal shape.

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Approach

A multiphase CFD simulation is set up using the Volume of Fluid (VoF) method. Two phases were defined: a liquid phase (water) and a gas phase (air) at room temperature, with a surface tension between the phases. The flow is capillary-driven, which means that no driving pressure or velocity is defined at the boundaries. Instead, a wetting contact angle between the liquid and the wall is required to enable the liquid to slowly creep along the wall. This contact angle at the bottom and side walls is set to 60 degrees, while the top wall contact angle is set to 90 degrees. At the start of the simulation the microfluidic channel is filled with air and the adhesion force causes the channel to slowly fill up, as seen in figure 2.

Figure 3. Position of the meniscus over time. The position on the y-axis is normalized with the total distance of the microfluidic channel.

Figure 2a. Snapshot at time t_0

Figure 2b. Snapshot at time t_1

Figure. 2 Snapshots of the filling of the microfluidic channel from the left to right. (Blue=liquid, gray=gas & $t_0 < t_1$)

The meniscus is the curved interface between the liquid and gas phases that arises due to the contact angle at the wall. By recording the average position of the meniscus over time for two designs and plotting the results, a comparison can be made between the filling times of the two designs.

Results

The meniscus is tracked over time to compare the filling time of the two designs. Figure 3 shows a plot with the normalized position of the meniscus as a function of time. It can be observed that the rectangular cross-section fills up to the end of the channel (Ltot) faster than the trapezoidal channel.
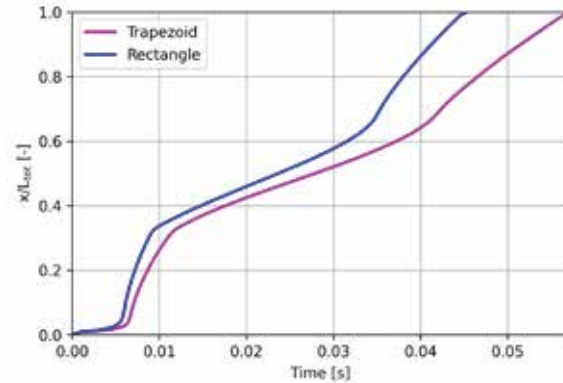
To better understand the faster filling time of the rectangular shaped microfluidic channel, the competition between the capillary pressure and hydraulic resistance is more closely examined.

The capillary pressure in a microchannel is described by the Young-LaPlace equation, see equation 1. The radius of the curvature of the meniscus is straightforward for circular channels, but for rectangular or trapezoidal it is not trivial. A practical approximation for the curvature radius would be the hydraulic diameter. This length scale is commonly used for non-circular tubes and channels. The formula for this diameter is stated in equation 2. The hydraulic diameter and the curvature of the meniscus are closely related as one can imagine. A smaller hydraulic diameter results in a smaller meniscus radius and thus a larger capillary pressure; and vice versa.

$\Delta P = \gamma \cdot 1/R´$ where ΔP pressure drop [Pa], γ surface tension [Pa.m] and R radius of meniscus curvature [m] (eq.1)

$D_h = 4A/P´$ where D_h hydraulic diameter [m], A cross sectional area [m^2] and P perimeter [m] (eq. 2)

During the simulation, the area and perimeter of the liquid-gas interface was recorded to calculate the hydraulic diameter. The hydraulic diameter changes over time due to change in shape of the channel, but only the minimum and maximum values are listed in the table below. The values in the table clearly indicate that the hydraulic diameter of the trapezoidal shaped channel is smaller at every moment in time during filling. Consequently, the capillary pressure is the highest and a faster filling can be expected. It is important to note that this represents only one aspect of the interplay between capillary pressure and hydraulic resistance.

	Minimum D_h [mm]	Maximum D_h [mm]
Rectangle	0.053	0.066
Trapezoid	0.044	0.051

Table 1. Minimum and maximum hydraulic diameter during filling of the microfluidic channel.

Hydraulic resistance is the other parameter at play as mentioned in the paragraph above. The hydraulic resistance of the total channel can be estimated by performing a single phase CFD simulation and recording the flow rate and pressure over the channel. Equation 3 shows the relation between the pressure drop and flow rate. A higher resistance results in a lower flow rate and thus a higher filling time.

$\Delta P = R_H \cdot Q$, where ΔP pressure drop [Pa], R_H the hydraulic resistance [Pa.s/m^3] and Q the flow rate [m^3/s] (eq.3)

The respective hydraulic resistances for the rectangle and trapezoid are stated in the following table. It can be concluded from these values that the hydraulic resistance is the lowest for the rectangular shaped channel. Hence in this competition the rectangular design is the winner.

	R_h [$Pa.s/m^3$]
Rectangle	6.24e+12
Trapezoid	9.77e+12

Table 2. Hydraulic resistances of microfluidic channels.

Conclusion

In conclusion, CFD simulations can be used to determine the filling time of non-trivially shaped microfluidic channels and networks. It is challenging to predict the filling time of a microfluidic channel due to the competition between the capillary pressure and hydraulic resistance. In our comparative study the rectangular cross-section design fills the fastest. Although this design may have a lower capillary pressure, this is offset by its lower hydraulic resistance, resulting in an overall faster filling process.