Mass transfer across two-fluid interfaces in microfluid systems

Christoffer Plamboeck (s991545)
Haissam El-Safadi (030808)

Supervisors: Martin Manscher and Henrik Bruus

Mikroelektronik Centret (MIC)
Technical University of Denmark
June 2003
Abstract

This report is the final assignment in the course no. 33430 Introduction to Bio/Chemical Microsystems held at the Microelectronics Centre (MIC) at DTU. The purpose of the project is to investigate the phenomena of mass transport across a two-fluid interface in a micro-fluidic system. This project is based on literature studies and simple computer calculations and no practical work has, therefore, been carried out during the 3 weeks.

The project has been divided into two subjects where the first subject is an investigation of the possibilities for extraction of dissolved compounds across an interface between two fluids in a micro-system. This is done by looking at diffusion and a simple diffusion model is set up and compared to more advanced models met in the literature.

The second subject is to investigate the possibilities for controlling immiscible fluids with different pressures in a micro channel. This is done by a introducing a notch across the micro-channel and then comparing different notch geometries in order to determine the possible maximum pressure-difference across the two immiscible fluids.

The basic theory of fluid dynamics, diffusion and surface tension is briefly outlined to explain the mathematics used in the project.
# Table of contents

1 Part I. Diffusion and Fluid Dynamics of a micro-fluidic system ..............4
   1.1 The forces acting on an incompressible fluid .................................................. 4
       1.1.1 Analytical solution to the Navier-Stokes Equation ................................... 4
   1.2 Diffusion in micro-channels........................................................................ 6
       1.2.1 One-dimensional diffusion in liquids ............................................................ 7
   1.3 One-dimensional diffusion model (liquid/liquid systems).............................. 8
       1.3.1 Discussion of the one-dimensional diffusion model .................................... 12
       1.3.2 Discussion of further work on the model .................................................. 13
   1.4 Sub-conclusion .............................................................................................. 13

2 Part II - Notch geometry ............................................................................. 15
   2.1 The Young-equation ..................................................................................... 15
   2.2 The Young-Laplace equation ..................................................................... 16
   2.3 Triangular Notch Geometry ....................................................................... 17
       2.3.1 Sub-conclusion ............................................................................................ 21
   2.4 Half-Circle Notch Geometry ....................................................................... 21
       2.4.1 Sub-conclusion ............................................................................................ 25

3 Final conclusion .................................................................................................. 25

References ............................................................................................................. 26
1 Part I. Diffusion and Fluid Dynamics of a micro-fluidic system

This part of the report introduces the basic equations used in fluid dynamics and explains the diffusion phenomena. A one-dimensional diffusion model is derived and compared to models found in the literature.

1.1 The forces acting on an incompressible fluid

Navier-Stokes Equation for a small fluid volume of constant density $\rho$ and viscosity $\eta$ is given by

$$
\rho \left[ (\mathbf{v} \cdot \nabla) \mathbf{v} + \frac{\partial \mathbf{v}}{\partial t} \right] = -\nabla P + \eta \nabla^2 \mathbf{v} + \rho \mathbf{g} + \rho_d \mathbf{E}
$$

(I-1)

The Navier-Stokes equation is basically Newton’s second law applied on fluids, where the left hand side of the equation corresponds to mass times acceleration. The left hand side accounts for both the inertial forces ($\rho (\mathbf{v} \cdot \nabla) \mathbf{v}$) and the time evolution of the system ($\rho \frac{\partial \mathbf{v}}{\partial t}$). The right hand side of the equation accounts for pressure forces ($-\nabla P$), viscous forces (also known as frictional forces within the fluid, $\eta \nabla^2 \mathbf{v}$), gravitational forces ($\rho \mathbf{g}$) and electrical forces ($\rho_d \mathbf{E}$) acting on the fluid [9].

For an incompressible fluid, the continuum equation tells us that $\nabla \cdot \mathbf{v} = 0$. This means that the total directional velocity change must be zero. If this is not the case, mass would accumulate in the small fluid volume, which is impossible for a fluid of constant density. The Navier-Stokes equation can be further simplified for a micro-fluidic systems considered in this report. Many microfluidic applications, most notably capillary electrophoresis, utilize electroosmotic flows. In many cases, however, it is preferable to use pressure driven flow because relative ease and flexibility of implementation and insensitivity to surface contamination, ion strength, and pH [5]. No electrical forces are, however, applied to the systems considered in this report. In a micro-fluidic system viscous forces will also dominate over gravitational forces, which mean that the two last parts of the right hand side of the Navier-Stokes Equation disappears. For a micro-fluidic system with no velocity change over time the Navier-Stokes Equation then simplifies to

$$
\nabla P = \eta \nabla^2 \mathbf{v}
$$

(I-2)

1.1.1 Analytical solution to the Navier-Stokes Equation

Let us consider a fluid flowing in a channel of the height $h$ and the length $l$ with the pressures $p_1$ and $p_2$ maintained at the two ends as shown in figure 1.1.1a
The width of the channel is assumed to be infinite and the velocity along the $x$- and $y$-direction is zero. The pressure-gradient will only exist in the $z$-direction which means that the Navier-Stokes Equation on the forces acting on the fluid in the $z$-direction would be reduced to:

\[
\left( \frac{\partial p_z}{\partial z} \right) = \eta \left( \frac{\partial^2 v_z(y)}{\partial y^2} \right) \tag{I-3}
\]

Assuming that the pressure gradient along the $z$-direction of the channel is constant, the pressure force expression simplifies to:

\[
\left( \frac{\partial p}{\partial z} \right) = \left( \frac{dp}{dz} \right) = \frac{p_2 - p_1}{l} = G
\]

-which by insertion into equation I-3 yields:

\[
G = \eta \left( \frac{\partial^2 v_z(y)}{\partial y^2} \right) \tag{I-4}
\]

With the boundary conditions of zero velocity along the channel edges (no-slip condition) equation I-4 integrates to give:

\[
\begin{align*}
y = 0 & \quad \text{for } v = 0 \\
y = h & \\
v_z(y) = \frac{G}{2\eta} \left( \frac{h}{2} \right)^2 - y^2
\end{align*} \tag{I-5}
\]

It has then been shown, that the velocity-profile in the $z$-direction has a parabolic dependency of $y$, if we consider flow in a channel. This velocity-profile will also make a rather good assumption for flow velocities in rectangular shaped channels of high aspect ratios (width/height). For a rectangular channel with an aspect ratio of $\sim 4$, the velocity profile will be parabolic across the $y$-direction (height) and largely uniform across the $x$-direction (width). For channels with an aspect ratio greater than 20, the velocity profile across the $x$-dimension is unchanging for at least 90% its length [4 and 5]. In this project it can, therefore, be assumed that the velocity-profile in a rectangular channel can be
expressed by equation I-5. The velocity profile for a rectangular channel with an aspect ratio of 10 is illustrated in figure 1.1.1b.

![Figure 1.1.1b](image)

The velocity profile of a rectangular tube with an aspect ratio of 10 (A) and the velocity profile of a rectangular channel with no “no-slip” condition along the sides of the channel (B). The figure is plotted in Mathematica 4.1

The solution to the Navier Stokes Equation for a rectangular shaped channel cannot be solved analytically and has to be done numerically. It is, therefore, convenient to utilize equation I-5, in order to ease the calculations.

1.2 Diffusion in micro-channels

Liquid micro space has several characteristic features different from bulk scale, for example short diffusion distances, high interface to volume ratio and low heat capacity. These characteristics in the micro-systems are the important parameters in controlling chemical unit operations such as mixing, reaction, extraction and separation. Especially, to control molecular transport in the micro-systems, the molecular transportation time is given by $t \propto L^2 / D$, where $t$ is the time, $L$ is the diffusion distance and $D$ is the diffusion coefficient [8]. As expressed, the transportation time is proportional to the square of the distance covered. Therefore the diffusion time takes several hours to a day when the diffusion distance is 1 cm since the typical molecular diffusion coefficient is in the order of $10^{-5} \text{cm}^2/\text{s}$. In contrast with that case, it takes only several tenths of seconds when the diffusion distance is $100 \mu \text{m}$. Diffusion is, therefore, becoming a very important method of mass-transfer in micro-fluidic systems, where the dimensions of a flow-channel usually are in the $\mu \text{m}$ scale with respect to width and height.

One device in which diffusion plays a crucial role is in the T-sensor [5] and a schematic representation of flow in a T-sensor with two input fluids is represented in figure 1.2a.
Two fluids enter through channels at the bottom. In the case shown here, the fluid in the right channel contains a diffusible analyte (dark) that spread across the x-direction as flow proceeds along the channel length [5].

Because of the very low Reynolds number of the system (typically less than 1) the flow is strictly laminar and transport between input streams occurs only via diffusion.

1.2.1 One-dimensional diffusion in liquids

For the time dependent diffusion process, the following equation can be derived [2 and 7]:

\[
\frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2}
\]

Equation I-6 is known as Fick’s second law which is derived for the special case of diffusion in one dimension. D is known as the diffusion coefficient and in liquids and solutions, which are said to be isotropic (i.e. uniform in all directions), D has the same value in all directions if the system is in thermal equilibrium. Fick’s second law states, that the change of concentration in time is fast where the concentration difference across distance is large. One solution to Fick’s second law is found by keeping a concentration constant (e.g. at \(x = 0\)) at all times. The following boundary conditions can be defined:

\[
c(0,0) = c_0
\]
\[
c(x > 0,0) = 0
\]
\[
c(x \geq 0,\infty) = c_0
\]

Fick’s law can then be solved to yield [7]:

\[
c = c_0 \left( \text{Erfc} \left[ \frac{x}{2\sqrt{Dt}} \right] \right)
\]

\text{Erfc} is the error function complement which is defined as:
erfc \left( \frac{x}{2\sqrt{Dt}} \right) = 1 - \left( \frac{2}{\sqrt{\pi \sigma^2}} \int_0^\infty e^{-\xi^2} d\xi \right)

-where \( \xi \) is a unitless variable. 1 This type of diffusion is also known as constant-source diffusion which is characterized by the previously presented boundary conditions with a constant concentration at \( x = 0 \). By utilizing this solution to Fick’s second law it is possible to model how diffusion would occur in two liquids flowing next to each other in a rectangular tube.

1.3 One-dimensional diffusion model (liquid/liquid systems)

The diffusion model is based on diffusion of an analyte between two liquids where the analyte is represented in different concentrations. The diffusion coefficient is assumed to be the same in both fluids and it is also assumed that the fluids won’t mix. By looking at a no-flow condition at first, it is possible to determine the start conditions for Fick’s second law. E.g. two similar, but initially separated, fluids with a concentration \( c_0 \) of the analyte in one fluid and zero concentration of the analyte in the other fluid are suddenly brought in contact. In time \( (t \to \infty) \), steady state will be reached and the concentration of the analyte will be similar in the two liquids. By defining origo of the coordinate system in the centerline between the two liquids (as indicated in figure 1.3a), the problem can be argued to follow a constant source diffusion around \( x = 0 \) even though the overall problem is characterized by limited diffusion (There is only a limited amount of analytes present, and the integral below the graph presented in figure 1.3a should be the same at all values of \( r \)).

Since the error function complement is symmetrical around \( x = 0 \) it is possible (by defining a constant concentration at \( x = 0 \)) to utilize the constant-source diffusion solution to Fick’s second law when solving this problem.

---

1 That this is a solution can be verified by using the equation:

\[
\frac{d\text{Erfe}(z)}{dz} = \frac{d}{dz} \left( 1 - \frac{2}{\sqrt{\pi \sigma^2}} \int_0^z e^{-\xi^2} d\xi \right) = -\frac{2}{\sqrt{\pi \sigma^2}} e^{-z^2}
\]

It can then be argued, that:

\[
\frac{\partial c}{\partial t} = \frac{Dc_0 e^{-\xi^2}}{2\sqrt{\pi \sigma^2 Dt}} \quad \text{and} \quad \frac{\partial c}{\partial x} = \frac{c_0 e^{-\xi^2}}{\sqrt{\pi \sigma^2}} \quad \Rightarrow \quad \frac{\partial^2 c}{\partial x^2} = \frac{c_0 e^{-\xi^2}}{2\sqrt{\pi \sigma^2 Dt}}
\]

- whence \( \frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2} \).
By defining the boundary conditions as

\[ \begin{align*}
  c &= c_0 \quad \text{for } x < 0 \\
  c &= 0 \quad \text{for } x > 0
\end{align*} \]

for \( t = 0 \)

-the solution to Fick’s second law can be written as [2]

\[ c = \frac{c_0}{2} \left( \text{erfc} \left( \frac{x}{2 \sqrt{Dt}} \right) \right) \]  \hspace{1cm} (I-8)

The time \( t \) (when the two fluids are exposed to each other in the channel) is variable and dependent on position in the micro-channel. It can be assumed, that the fluid-velocity follows a parabolic velocity profile (which is described in section 1.1.1) across the total width of the channel. Dissolved particles, which are located in the middle of the channel, will, therefore, move faster through the channel than dissolved particles, which are located at the boundaries of the channel. In other words, particles traveling at the channel-boundaries in one fluid will have a larger exposure-time to the other fluid than particles traveling in the middle of the channel. It can therefore be argued, that we will experience a larger diffusion of particles from one fluid to the other at the boundaries of the channel. The exposure time \( t \) is therefore dependent on the location in the channel and can be described as:

\[ t = \frac{L}{v(y)} \]  \hspace{1cm} (I-9)

-which by insertion of equation I-5 yields
\[ t = \frac{2\eta L}{G \left( \frac{h}{2} \right)^2 - y^2} \]  

Equation I-10 is then inserted into equation I-8 and an expression of the concentration as a function of position in the channel is derived:

\[ c = \frac{c_0}{2} \text{erfc} \left( \frac{x}{\sqrt{2y} \sqrt{D_0 \left( 1 - \left( \frac{2y^2}{h^2} \right)^{1/2} \right)}} \right) \Rightarrow 
\]

\[ c = \frac{c_0}{2} \text{erfc} \left( \frac{x}{D_0 \left( 1 - \left( \frac{2y^2}{h^2} \right)^{1/2} \right)} \right) \]  

where \( D_0 = \sqrt{32\eta LD/h^3G} \). The concentration profile across the micro-channel can then be plotted for different lengths and heights of the micro-channel. It is important to note, that the model is independent of the width of the channel. This can be explained by the assumption that the velocity-profile is uniform across the width of the channel. This is, however, only a reasonable assumption for large aspect ratios. The concentration profile in the channel is also dependent on the pressure gradient down through the channel, the diffusion coefficient of the analyte and the viscosity of the fluid, as can be argued from \( D_0 \). Contour plots for different \( D_0 \) values are presented in figure 1.3b.
The figure shows concentration contour plots for different $D_0$ values ($D_0 = \sqrt{32\eta LD/h^2G}$). The flow is normal to the page, and the white zone corresponds to a high concentration, and the black zone corresponds to zero concentration. Aspect ratio 4 is used. The figure is plotted in Mathematica 4.1.

The diffusion is getting more extensive with higher $D_0$ as can be seen from figure 1.3b. The diffusion will, therefore, increase with increased length of the channel ($L$), increased viscosity of the fluid ($\eta$) and increased diffusion coefficient ($D$) of the analyte. The diffusion will decrease with increased pressure drop down through the channel. A 3D plot is presented in figure 1.3c to illustrate the concentration profile.

Concentration profile across two flows in a rectangular tube. The ratio between width, height and relative concentration is distorted. The figure is plotted in Mathematica 4.1.
1.3.1 Discussion of the one-dimensional diffusion model

It can be seen from figure 1.3b, that more diffusion occurs in the top and the bottom surfaces of the rectangular channel, where the velocity is slow. This causes the inter-diffusion zone to be shaped like a butterfly as observed in figure 1.3b, hence the name “the butterfly effect”[3]. This effect can be explained by the parabolic velocity profile, which generates a substantial distribution in residence time across the $y$-direction (height). The butterfly effect in a T-sensor was only recently directly discovered for the first time (year 2000) by measuring fluorescence generated from binding between calcium ions and an indicator using confocal microscopy [1].

The butterfly effect would, however, be suppressed by considering diffusion in both the $x$- and $y$-direction [5 and 6]. The model presented in this report considers only diffusion in one dimension, which is in the $x$-direction. It can then be argued; that diffusion in the $y$-direction would occur as a concentration gradient builds up across the $y$-direction. Diffusion in the $y$-direction would also exceed diffusion in the $x$-direction when the concentration gradient in the $y$-direction exceeds the concentration gradient in the $x$-direction. This can be illustrated in figure 1.3.1a

![Figure 1.3.1a](image)

Diffusion is symbolized by arrows. Both diffusion in the $x$- and $y$-direction would occur in praxis, and the butterfly effect would eventually be “outwashed”.$D_0=0,5$ The figure is plotted in Matematica 4.1

As an indication of the models credibility, a plot of $\frac{\partial c}{\partial y} / \frac{\partial c}{\partial x}$ is generated. The higher the concentration gradient in the $x$-direction is compared to the concentration gradient in the $y$-direction, the better the model gets. Figure 1.3.1b shows a number of curves, representing iso-curves of a fixed value of $\frac{\partial c}{\partial y} / \frac{\partial c}{\partial x}$. The inner iso-curve is represented for $\frac{\partial c}{\partial y} / \frac{\partial c}{\partial x}=0,1$ and the outer iso-curve is represented for $\frac{\partial c}{\partial y} / \frac{\partial c}{\partial x}=1,0.$
It can be seen from figure 1.3.1b, that the credibility of the model is best in the center regions of the rectangular channel. At the surface of the channel the diffusion in the y-direction becomes too extensive and the model fails to predict an accurate concentration in these regions.

1.3.2 Discussion of further work on the model

The model considered in this report is based on the assumption of a constant diffusion coefficient over time and position. The next natural step would, therefore, be to examine Fick’s second law for variable diffusion coefficients. The diffusion coefficient would vary as a function of position, if diffusion between two different liquids were considered. The analyte would then have two different diffusion coefficients depending on which liquid it was traveling in.

The temperature of the system would also contribute to the size of the diffusion. In the liquid phase molecules vibrate and interact with each other but there can still be said to exist a state of near-order. The analyte would therefore have to climb an energy-barrier in order to break free from the near-order arrangement of the fluid molecules. The diffusion coefficient in a liquid is defined as $D = d^2 fe^{-\Delta E / kT}$, where $d$ is the distance between liquid molecules in near-order, $f$ is the frequency of the fluctuations made by the analyte and the exponential factor describes the statistical possibility for the analyte to receive the energy $-\Delta E$ required to climb the energy-barrier and break free from the surrounding liquid molecules [7]. The diffusion coefficient is, therefore, very temperature dependent in a liquid and this dependency should be considered when diffusion between to liquids of different temperature is modeled.

A liquid/gas interface could also be considered. The diffusion coefficient in a gas is defined as $D = l \sqrt{\frac{2kT}{m}}$, where $T$ is the temperature, $k$ is the Boltzmann’s constant, $m$ is the mass of the molecule of interest and $l$ is the mean free path [7]. The diffusion would in every case be dependent on temperature, and it could therefore be interesting to model diffusion of an analyte between in two different fluids in a rectangular channel with a temperature gradient along either the x- or the y-direction.

1.4 Sub-conclusion

It has been shown, that diffusion in a T-sensor where two fluids meet in a rectangular channel can be modeled by assuming simple one-dimensional diffusion. The model is, to some extend, in agreement with the phenomena observed and reported in the literature.
The boundary for the models credibility is investigated and it has been shown, that the models prediction of diffusion is most accurate in the middle of the rectangular channel.
Part II - Notch geometry

This section of the report investigates the possibilities for controlling interfaces of immiscible fluids with different pressures by re-shaping the micro-fluidic channel. Re-shaping is suggested to be done by adding a small notch to the wall of the micro-fluidic channel.

A micro fluidic channel with two immiscible fluids could form bobbles along the channel under different pressures. In order to avoid such bobbles a small notch to the wall is integrated in the micro fluidic channel.

The suggested notch geometries taken into consideration were triangular, circular, rectangular and a notch with concentric rings. A theoretical analysis study of these notches will be done in order to discuss which notch geometry would be the most appropriate to keep a stable interface along the micro-fluidic channel. Due to the limited time available for this project, it was not possible to investigate the last two geometries, rectangular and a notch with concentric rings.

The theoretical analysis of the notch geometry is based on Young-equation and the Young-Laplace equation. Therefore, a brief introduction to the mentioned equations is considered at first.

2.1 The Young-equation

Consider a situation with three surface interfaces involved, a solid-gas interface, a liquid-gas interface and a solid-liquid interface as outlined in figure 2.1a.

For a liquid to spread out over a part of the solid surface, two conditions must be met. First, the surface energy of the solid-gas interface must be greater that the combined surface energies of the liquid-gas and solid-liquid interfaces. Second, the surface energy of the solid-gas interface must exceed the surface energy of the solid-liquid interface. The relation between the three surface energies can be summarised in the so called Young-equation [10].

\[ \sigma_{lg} \cos \theta = \sigma_{sg} - \sigma_{sl} \]  

(II-1)
-where $\sigma_{lg} \cos \theta$ is the force component of the liquid-gas surface tension, $\sigma_{sg}$ is the solid-gas surface tension and $\sigma_{sl}$ is the solid-liquid surface tension. The angle $\theta$ is the contact angle that is formed by the solid-liquid interface.

2.2 The Young-Laplace equation

The intermolecular bonds or cohesive forces between the molecules of a liquid cause surface tension. The molecules at the surface of a liquid have a higher energy than molecules within the liquid. The liquid will therefore minimize its energy by configuring itself with as small a surface area-to-volume ratio as possible. Surface tension can, therefore, be defined as a measure of the energy required to form a unit surface area. This can be illustrated by considering figure 2.2a, which shows a small change in surface area of a liquid surrounded by a gas.

The following relations can be derived:

$A_i = A_0 + \partial A$

$A_i = (R_1 + \partial r)\partial \theta_1 (R_2 + \partial r)\partial \theta_2$

$A_0 = (R_1 \partial \theta_1)(R_2 \partial \theta_2)$

$A_i$ can then be reduced to

$A_i = A_0 + \left(\frac{\partial r}{R_1} + \frac{\partial r}{R_2}\right)A_0 \Rightarrow$

$\partial A = \left(\frac{1}{R_1} + \frac{1}{R_2}\right)\partial r A_0$

The system has two types of energies, the surface energy ($\partial E_{surf}$) and the pressure energy ($\partial E_{press}$) which is defined as:
\[
\begin{align*}
\partial E_{\text{surf}} &= \sigma \partial A = \sigma \left( \frac{1}{R_1} + \frac{1}{R_2} \right) \partial r A_0 \\
\partial E_{\text{press}} &= -(P_1 - P_2) \partial V = -(P_1 - P_2)(A_0 + \partial A) \partial r
\end{align*}
\]

The total energy change of the system is zero since the system is in thermal equilibrium, which means, that

\[
0 = \partial E_{\text{surf}} + \partial E_{\text{press}} \Rightarrow -\partial E_{\text{press}} = \partial E_{\text{surf}} = \sigma \left( \frac{1}{R_1} + \frac{1}{R_2} \right) \partial r A_0 = (P_1 - P_2)(A_0 + \partial A) \partial r
\]

\[
\sigma \left( \frac{1}{R_1} + \frac{1}{R_2} \right) = (P_1 - P_2) = \Delta P \tag{II-2}
\]

-which is defined as the Young-Laplace equation\(^2\).

### 2.3 Triangular Notch Geometry

Consider a micro fluidic channel with three surface interfaces liquid-gas-solid in thermal equilibrium conditions in the system. The region of the three-phase system - where the three immiscible co-existing phases - is characterized in figure 2.3a.

![Figure 2.3a](image)

*Front view slice of the triangular notch geometry integrated in the rectangular micro fluidic channel*

\(^2\) Derived by Associate Professor Henrik Bruus
The micro fluidic channel is divided into two halves that are completely symmetrical. Therefore, the theoretical analysis of the triangle notch geometry will be done on one half of the channel. \( \frac{h}{2} \) is the height of the one-half of the micro fluidic channel. \( \varphi \) is the angle between the curved radius interface \( R \) and the symmetry line. \( P_L \) is the pressure for the liquid, and \( P_g \) is the pressure for the gas. \( P_L \) has a larger value than \( P_g \), which is assumed to be constant, \( \Delta P = P_L - P_g \). \( \theta_n \) is the notch’s angle and \( h_n \) is the height of the notch. \( L \) is the length of the notch’s side, and \( x \) is the position of the interface from the bottom of the notch. \( \theta \) is the contact angle between the solid-liquid interface.

The theoretical analysis will focus on the following:
1. Determination of the interface’s location in relation to the notch geometry (The length of \( x \) as a function of the interface’s radius \( R \)).
2. Determination the maximum and the minimum value of \( \Delta P \) by using the Young-Laplace equation.

First, a value for \( \frac{h}{2} \) is found

From the above model consideration, the triangle notch geometry has an angle \( \theta_n \)

\[
\sin \theta_n = \frac{h_n}{x} \Rightarrow h_n = x \sin \theta
\]  

(II-3)

The triangle with the interface radius \( R \) has an angle \( \varphi \)

\[
\sin \varphi = \frac{d}{R} \Rightarrow d = R \sin \varphi
\]  

(II-4)

Then the value for \( \frac{h}{2} \) can be defined as

\[
\frac{h}{2} = R \sin \varphi + x \sin \theta_n
\]  

(II-5)

Now a value for the angle \( \varphi \) is found. We know that the sum of the angles in a triangle is \( \pi \).

\[
\pi - \theta_n + \frac{\pi}{2} - \theta + \varphi = \pi \Rightarrow \\
\varphi = \theta_n + \theta - \frac{\pi}{2}
\]  

(II-6)

By insertion of the value for \( \varphi \) in the Eq. (II-5)

\[
\frac{h}{2} = R \sin \left( \theta_n + \theta - \frac{\pi}{2} \right) + x \sin \theta_n
\]  

(II-7)

\( x \) can be written as a function of \( R \)

\[
x = \frac{\frac{h}{2} - R \sin \left( \theta_n + \theta - \frac{\pi}{2} \right)}{\sin \theta_n}
\]  

(II-8)
where \( 0 \leq x \leq L \)

The second task is to find the maximum and the minimum values for the pressure (\( \Delta P_{\text{max}} \) and \( \Delta P_{\text{min}} \)). In order to determine the maximum and the minimum value of \( \Delta P \), a theoretical analysis of the curved radius interface must be done in relation to the Young-Laplace equation. Therefore, having a side view slice of the triangular notch geometry, that shows how the curved radius interface behave along the channel, will help in shaping the Young-Laplace equation for this case. This is shown in figure 2.3b.

![Figure 2.3b](image)

*Figure 2.3b*

*Side view slice of the triangle notch geometry, that shows the curved radius \( R_1 \) of the interface, where \( R_2 \rightarrow \infty \).*

For \( R_2 \rightarrow \infty \) the Young-Laplace equation can be released to

\[
\Delta P = \sigma \left( \frac{1}{R_1} + \frac{1}{\infty} \right) \\
\Rightarrow \\
\Delta P = \frac{\sigma}{R} 
\]

(II-9)

Figure 2.3c shows the relation between \( \Delta P \) and the radius \( R \). The radius \( R \) has a minimum value at the top of the triangle notch. The value for \( R \) increases along the bottom of the notch. In terms of the Young-Laplace equation, \( \Delta P \) has a larger value for \( R = R_1 \), than for \( R = R_2 \).
As a conclusion we can write

$$\Delta P_{\text{max}} = \frac{\sigma}{R_1} > \Delta P_{\text{min}} = \frac{\sigma}{R_2}$$

Now it is possible to write $\Delta P_{\text{max}}$ and $\Delta P_{\text{min}}$ as a function of $R$. $\Delta P$ has a maximum value when the curved radius interface $R = R_{x=L}$ (at the top of the triangle notch). 

$$x = L \Rightarrow \quad \frac{h}{2} - R \sin \left( \frac{\theta_n + \theta - \pi}{2} \right) = \sin \theta_n \Rightarrow \quad \frac{h}{2} - R \sin \left( \frac{\theta_n + \theta - \pi}{2} \right) = L \sin \theta_n \Rightarrow$$

$$R = \frac{\frac{h}{2} - L \sin \theta_n}{\sin \left( \frac{\theta_n + \theta - \pi}{2} \right)} \quad (\text{II-10})$$

By insertion of Eq. (II-10) into the Young-Laplace equation we get

$$\Delta P_{\text{max}} = \sigma \frac{\sin \left( \theta_n + \theta - \frac{\pi}{2} \right)}{\frac{h}{2} - L \sin \theta_n} \quad (\text{II-11})$$

$\Delta P$ has a minimum value when the curved radius interface $R = R_{x=0}$ (at the bottom of the triangle notch). 

$$x = 0 \Rightarrow \quad \frac{h}{2} - R \sin \left( \frac{\theta_n + \theta - \pi}{2} \right) = 0 \Rightarrow \quad \frac{h}{2} - R \sin \left( \frac{\theta_n + \theta - \pi}{2} \right) = 0 \Rightarrow$$

$$R = \frac{h}{2 \sin \left( \frac{\theta_n + \theta - \frac{\pi}{2}}{2} \right)} \quad (\text{II-12})$$

By insertion of Eq. (II-12) into the Young-Laplace equation we get:
\[
\Delta P_{\text{min}} = \sigma \frac{2\sin\left(\theta_n + \theta - \frac{\pi}{2}\right)}{h}
\]  

(II-13)

The values for \(\Delta P_{\text{max}}\) and \(\Delta P_{\text{min}}\) are valid for the following conditions:

\[
\begin{align*}
\theta_n + \theta & \geq \frac{\pi}{2} \\
\theta_n & \geq \varphi
\end{align*}
\]

For \(\theta < \frac{\pi}{2}\)

2.3.1 Sub-conclusion

For \(R_{x=L} < R_{x=0}\) \(\Rightarrow\) \(\Delta P_{x=L} > \Delta P_{x=0}\)

In the term of Young-Laplace equation the pressure will have a maximum value at the top of the notch, where the interface is located \((x=L)\). This is due to the curved radius \(R\) that has a minimum value. The pressure will have a minimum value at the bottom of the notch. This due to the fact that the curved radius \(R\) has a maximum value where \(x=0\).

2.4 Half-Circle Notch Geometry

The conditions for the micro fluidic system remain identical to the previous one concerning the triangular notch geometry. The only difference is that a half-circle is integrated instead of the triangle as shown in figure 2.4a.
$\beta$ is the angle between the curved radius interface $R$ and the symmetry line. $\varphi$ and $r$ are the angle and the radius of the notch, respectively. $\theta$ is the contact angle between the solid-liquid interface.

First, a value for $\frac{h}{2}$ is found

From the above model consideration, the half-circle notch geometry has an angle $\varphi$

$$\sin \varphi = \frac{x + r - L}{r} \Rightarrow x = r \sin \varphi - r + L \quad \text{(II-14)}$$

The triangle with the interface radius $R$ has an angle $\beta$

$$\sin \beta = \frac{d}{R} \Rightarrow d = R \sin \beta \quad \text{(II-15)}$$
Then the value for \( \frac{h}{2} \) can be defined as
\[
\frac{h}{2} = R \sin \beta + r \sin \varphi - r + L \tag{II-16}
\]
A value for \( \beta \) is then found. We know that the sum of the angles in a triangle is \( \pi \).
\[
\beta + \left( \frac{\pi}{2} - \theta \right) + \left( \pi - \frac{\pi}{2} - \varphi \right) = \pi
\]
\[
\beta = \theta - \varphi \tag{II-17}
\]
By insertion of the value for \( \beta \) in the Eq. (II-16) we get
\[
\frac{h}{2} = R \sin(\theta - \varphi) + r \sin \varphi - r + L \Rightarrow
\]
\[
R = \frac{h}{2} - r \sin \varphi + r - L \sin(\theta - \varphi) \tag{II-19}
\]
-where \( \text{Arc.sin}\left(\frac{r-L}{r}\right) \leq \varphi < \theta \). It is possible to write \( \Delta P_{\text{max}} \) and \( \Delta P_{\text{min}} \) as a function of \( R \). \( \Delta P \) has a maximum value when \( R \) has a minimum value (at the top of the half-circle notch geometry). In the term of Eq. (II-19)

1. \( R \) has a minimum value when \( \sin(\theta - \varphi) \) has a maximum value.
2. \( \sin(\theta - \varphi) \) has a maximum value when \( \varphi = 0 \).

For \( \varphi = 0 \)
\[
R_{\text{min}} = \frac{h}{2} + r - L \sin \theta \tag{II-20}
\]
Insert Eq. (II-20) into the Young-Laplace equation we get:
\[
\Delta P_{\text{max}} = \sigma \frac{\sin \theta}{h - L + r} \tag{II-21}
\]
\( \Delta P \) has a minimum value when \( R \) has a maximum value (at the bottom of the half-circle notch geometry). In the term of Eq. (II-19) we get

1. \( R \) has a maximum value when \( \sin(\theta - \varphi) \) has a minimum value.
2. \( \sin(\theta - \varphi) \) has a minimum value when \( \text{Arc.sin}\left(\frac{r-L}{r}\right) \leq \varphi < \theta \)

For \( \text{Arc.sin}\left(\frac{r-L}{r}\right) \leq \varphi < \theta \)
\[
R_{\text{max}} = \frac{h}{2} - r \sin \varphi + r - L \sin(\theta - \varphi) \tag{II-22}
\]
By insertion of Eq. (II-22) into the Young-Laplace equation we get:
\[ \Delta P_{\text{min}} = \sigma \frac{\sin(\theta - \varphi)}{h - r \sin \varphi - L + r} \]  

(II-23)

In order to determine the most appropriate notch geometry model, either the triangle or the half-circle, the following theoretical analysis is required. One way of comparing the two geometries could be to assume that the notches have the same cross section area as shown in figure (2.4b) and figure (2.4c). Therefore, the area of the two notches is considered:

The area for the triangle is
\[ A_{\Delta} = \frac{1}{2} gh_n \]  

(II-24)

By insertion of the values for \( g \) and \( h_n \) in Eq. (II-24) we get:
\[ A_{\Delta} = \frac{1}{2} 2L \cos(\theta_n) L \sin(\theta_n) \Rightarrow \]
\[ A_{\Delta} = L^2 \cos \theta_n \sin \theta_n \]  

(II-27)

For \( L = 10^{-6} \) m and \( \theta_n = 50^\circ \) the area of the triangle is \( A_{\Delta} = 4.92 \cdot 10^{-13} \) m²

The area for the half-circle is
\[ A_0 = \frac{1}{2} \pi r^2 \]  

(II-28)

\[ A_{\Delta} = A_0 \Rightarrow \]
\[ 4.92 \cdot 10^{-13} = \frac{1}{2} \pi r^2 \Rightarrow \]
\[ r = 3.15 \cdot 10^{-7} \text{ m} \]

In order to determine which is the most appropriate notch geometry that is able to keep the interface along the micro fluidic channel, some values has to be involved.
### For a triangle | For a half-circle
---|---
h = $10^{-5}$ m | h = $10^{-5}$ m
L = $10^{-6}$ m | r = $3.15 \times 10^{-7}$ m (r = L)
$\sigma = 0.075 \text{ J/m}^2$ for water / air | $\sigma = 0.075 \text{ J/m}^2$ for water / air
$\theta = 60^\circ$ | $\theta = 60^\circ$  
$\theta_\phi = 50^\circ$ | $\varphi = 50^\circ$

$\Delta P_{\text{max},A} = 6058.5 Pa$ | $\Delta P_{\text{max},O} = 12990.4 Pa$
$\Delta P_{\text{min},A} = 5130.3 Pa$ | $\Delta P_{\text{min},O} = 2736.85 Pa$

#### 2.4.1 Sub-conclusion
The values for $\Delta P$ maximum and minimum for the two notches are determined in the term of Young-Laplace equation. The half-circle notch geometry is able to keep the interface along the micro fluidic channel better than the triangle at a higher pressure difference.

#### 3 Final conclusion
It has been possible to investigate the literature and test a simple diffusion model with the relative sparse time available in a 3-week course. The simple diffusion model developed in this project resembles (to some extent) the more complex 2-dimensional models derived in the literature.

It has also been possible to derive expressions for the location of an interface between two immiscible fluids on two different notch geometries. The geometries has been compared with respect to the pressure-difference across the fluids, and it has been found that the circular notch geometries would be preferable to a triangular notch geometries based on the assumptions made for similar cross-sectional area.
References


