Modelling of Acoustically Induced Rapid Mixing Processes in Microchannels Using Acoustic Streaming

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Abstract

Technical advancements in miniaturization in the last decades have, among others, brought forth the technology of so called "Lab-on-a-Chip" (LOC) systems. These systems provide the possibility to automate and accelerate certain laboratory processes, e.g., biomedical diagnostics, on the microscale. LOC systems usually consist of a network of sub-millimeter wide channels for processing fluids. Frequently, these fluids need to be mixed, e.g., for diagnostical purposes. Due to the laminar nature of flow in those microchannels the mixing mechanism is governed by slow diffusion processes which would require unsuitably long channels to achieve homogeneous mixing. Actively introducing convection processes into the flow greatly enhances the mixing efficiency.

Various publications in recent years have discussed the possibility of employing ultrasound in combination with sharp edged structures in microchannel walls to achieve rapid mixing. When actuating the channel with ultrasound the sharp edges vibrate and generate local acoustic streaming phenomena which in turn lead to substantially enhanced mixing of the fluids. Using acoustic frequencies in the low kHz-range, the wavelength is much larger than the channel width and thus unified actuation of the channel segment including the sharp edges can be assumed. Building upon this previous work, we employ the new Acoustic Streaming interface in the Acoustics Module of Comsol Multiphysics to simulate the mixing of two identical fluids with different species concentrations in a 2D or 3D segment of a straight microchannel containing sharp, evenly spaced, triangular edges. Our modelling pipeline combines the Acoustic Streaming interface for Pressure and Thermoviscous Acoustics with an additional Laminar Flow interface for the background flow and the Transport of Diluted Species interface to simulate two different species concentrations. The computational grid needs to be highly refined around the sharp edges to resolve the viscous boundary layer. The model is solved using four study steps, first solving the acoustics in the frequency domain, and subsequently calculating the stationary solution of the acoustic streaming flow, the laminar background flow as well as the concentration field.

The obtained simulation results show a remarkable improvement of the mixing efficiency when introducing acoustically actuated sharp edges into the LOC-system. We used this setup to conduct parameter studies for determining optimal geometrical properties of the mentioned sharp edges, e.g., height, tip-angle and spacing, and other process parameters like actuation frequency and inlet velocity. The parameter study identified the sharp edges height and spacing as critical parameters of the geometrical setup. Furthermore, the inlet velocity could be determined as a critical parameter, with improving mixing quality at lower inlet velocities due to the longer residence time. Our results are comparable with previously published findings based on simulations employing the Weak Form interface of the PDE module in Comsol.

Keywords: Acoustic Streaming, Microfluidics, Lab-on-a-Chip, Rapid Mixing Processes, Ultrasound.

Introduction

The technical and digital advancements of the last decades have not only brought many interesting and new technologies, but they have also brought a miniaturization of all things technical. A well-known example is the field of microelectronics, where circuits get smaller and smaller with every development step. Another example in the field of microtechnology is microfluidics. Klaus S. Drese writes in his 2019 article [1] with respect to microfluidics: "As in microelectronics, it was found that by combining a large number of many functional units in integrated chips creates performance with disruptive potential." These chips with disruptive potential are so called "Lab-on-a-Chip" (LOC) systems. LOC-systems allow for a complete and automated lab-process in domains the size of a fingertip containing micrometer-wide fluidic channels. While producing LOC-systems may be costly, they enable a faster medical and technical lab-process where less laboratory staff must be involved, hence decreasing the operation costs dramatically [1].

Due to the small scale of its channels and the relatively low flow velocities, the fluid flow in LOC-systems is laminar. For the mixing of fluids, which is frequently required in LOC applications, this laminar nature poses a problem. Efficiently mixing two fluids which, e.g., carry different concentrations of some substance, in the laminar flow regime is challenging since the process is solely driven by diffusion, rendering it very slow. This problem, its modelling and solution are the main topic of this project.

Large parts of this project are based on the 2016 paper by Nama et al. [2] where he discusses the use of acoustically actuated sharp edges in microchannels to enhance the mixing properties of a channel segment. The concept of acoustically oscillated sharp edges would enable the mixing of two fluids in an otherwise laminar environment to achieve for example a uniform distribution of a chemical species at the end of a section of the microchannel.

The goal of this project was to build a Comsol Multiphysics model of a microchannel segment with sharp edges (based on [2]) using the new Acoustic Streaming interface of the Acoustics Module. Thereafter a parameter study was conducted, investigating the impact of geometrical and process parameters on the mixing quality. Having determined critical parameters, suggestions for optimal layouts for certain use cases are made.

Modelling of Acoustic Mixing

In this section the basic equations for modelling acoustic mixing are described, and the different orders of equations are derived which could directly be implemented in Comsol Multiphysics using the weak formulation and employing the mathematics module.

Governing Equations

The basic equations for modelling the phenomena of acoustic streaming are the conservation of mass and the conservation of momentum, which read [3] [4] respectively

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{u}) = 0$$

$$\rho\left(\frac{\partial \vec{u}}{\partial t} + \vec{u} \cdot \nabla \vec{u}\right) = -\nabla p + \mu \nabla^2 \vec{u} + \left(\mu_B + \frac{\mu}{3}\right) \nabla(\nabla \cdot \vec{u}).$$

Here ρ represents fluid density, $\vec{u}$ is fluid velocity, p is pressure and t is time. μ and μ_B are the fluid's dynamic viscosity and the dynamic bulk viscosity. To be able to model the fluid motion, these two equations are further complemented by a constitutive relation, linking pressure and density. Under the assumption that the relation is linear we can use

$$p = c_0^2 \rho$$

where c_0 is the speed of sound in the fluid at rest [2]. The concentration balance equation

$$\frac{\partial c}{\partial t} + \nabla \cdot (c \vec{u}) - D \nabla^2 c = 0$$

where c is the concentration of some species and D the diffusion coefficient completes the set of equations necessary for modelling acoustic mixing.

Perturbation Technique

In acoustic streaming modelling it is customary to divide the fields into three components: a background field called zeroth order, a first order and a second order with the latter being generally referred to as acoustic streaming. To do so Nyborg's perturbation technique is applied where the fluid velocity, density and the pressure have the following form [2]

$$\begin{aligned} \vec{u} &= \overrightarrow{u_0} + \varepsilon \overrightarrow{\widetilde{u_1}} + \varepsilon^2 \overrightarrow{\widetilde{u_2}} + O(\varepsilon^3) + \cdots \\ p &= p_0 + \varepsilon \widetilde{p_1} + \varepsilon^2 \widetilde{p_2} + O(\varepsilon^3) + \cdots \\ \rho &= \rho_0 + \varepsilon \widetilde{\rho_1} + \varepsilon^2 \widetilde{\rho_2} + O(\varepsilon^3) + \cdots \end{aligned}$$

where ε is a non-dimensional smallness parameter which is usually chosen to be a ratio between two process parameters, in the case of [2] the ratio of the amplitude of the first-order velocity and c_0^2. As Nama et al. [2] further states: “Usually, the zeroth-order velocity field [...] is assumed to be zero, thereby precluding the presence of a background flow. However, in the case of the [...] micromixer, there is an additional background flow imposed, which needs to be considered [...].”

Using the notation

$$\begin{aligned} &\overrightarrow{u_1} = \varepsilon \overrightarrow{\widetilde{u_1}}, \quad p_1 = \varepsilon \widetilde{p_1}, \quad \rho_1 = \varepsilon \widetilde{\rho_1} \\ &\overrightarrow{u_2} = \varepsilon^2 \overrightarrow{\widetilde{u_2}}, \quad p_2 = \varepsilon^2 \widetilde{p_2}, \quad \rho_2 = \varepsilon^2 \widetilde{\rho_2} \end{aligned}$$

for the different orders, the perturbation equations are inserted into the mass and momentum equations, followed by a separation of terms by their order in ε. Terms carrying ε^3 and higher can be neglected due to their smallness caused by the high power of the smallness parameter ε.

This procedure results in three pairs of mass and momentum balance equations in three different orders. [2]

Zeroth Order:

$$\frac{\partial \rho_0}{\partial t} + \rho_0 (\nabla \cdot \overrightarrow{u_0}) = 0$$

$$\begin{aligned} \rho_0 \frac{\partial \overrightarrow{u_0}}{\partial t} + \rho_0 (\overrightarrow{u_0} \cdot \nabla) \overrightarrow{u_0} &= -\nabla p_0 + \mu \nabla^2 \overrightarrow{u_0} \\ &+ \left(\mu_B + \frac{\mu}{3}\right) \nabla(\nabla \cdot \overrightarrow{u_0}) \end{aligned}$$

First Order:

$$\frac{\partial \rho_1}{\partial t} + \nabla \cdot (\rho_0 \overrightarrow{u_1} + \rho_1 \overrightarrow{u_0}) = 0$$

$$\begin{aligned} \rho_0 \frac{\partial \overrightarrow{u_1}}{\partial t} + \rho_1 \frac{\partial \overrightarrow{u_0}}{\partial t} + \rho_0 (\overrightarrow{u_1} \cdot \nabla) \overrightarrow{u_0} + \rho_0 (\overrightarrow{u_0} \cdot \nabla) \overrightarrow{u_1} \\ + \rho_1 (\overrightarrow{u_0} \cdot \nabla) \overrightarrow{u_0} \\ = -\nabla p_1 + \mu \nabla^2 \overrightarrow{u_1} \\ + \left(\mu_B + \frac{\mu}{3}\right) \nabla(\nabla \cdot \overrightarrow{u_1}) \end{aligned}$$

Second Order:

$$\left\langle \frac{\partial \rho_2}{\partial t} \right\rangle + \nabla \cdot \left(\langle \rho_0 \overrightarrow{u_2} \rangle + \langle \rho_2 \overrightarrow{u_0} \rangle + \langle \rho_1 \overrightarrow{u_1} \rangle \right) = 0$$

$$\begin{aligned}\left\langle \rho_0 \frac{\partial \overrightarrow{u_2}}{\partial t} \right\rangle + \left\langle \rho_2 \frac{\partial \overrightarrow{u_0}}{\partial t} \right\rangle + \left\langle \rho_1 \frac{\partial \overrightarrow{u_1}}{\partial t} \right\rangle + \langle \rho_0 (\overrightarrow{u_1} \cdot \nabla) \overrightarrow{u_1} \rangle & \\ + \langle \rho_0 (\overrightarrow{u_0} \cdot \nabla) \overrightarrow{u_2} \rangle & \\ + \langle \rho_0 (\overrightarrow{u_2} \cdot \nabla) \overrightarrow{u_0} \rangle & \\ + \langle \rho_1 (\overrightarrow{u_0} \cdot \nabla) \overrightarrow{u_1} \rangle & \\ + \langle \rho_1 (\overrightarrow{u_1} \cdot \nabla) \overrightarrow{u_0} \rangle & \\ + \langle \rho_2 (\overrightarrow{u_0} \cdot \nabla) \overrightarrow{u_0} \rangle & \\ = -\nabla \langle p_2 \rangle + \mu \nabla^2 \langle \overrightarrow{u_2} \rangle & \\ + \left(\mu_B + \frac{\mu}{3} \right) \nabla (\nabla \cdot \langle \overrightarrow{u_2} \rangle) &\end{aligned}$$

where $\langle k \rangle$ denotes the time average off the quantity k over a full oscillation period.

The different orders of mass and momentum balance equations and the concentration balance equation could now be transformed into their weak form and implemented in Comsol Multiphysics using the Weak Form interface of the Mathematics module.

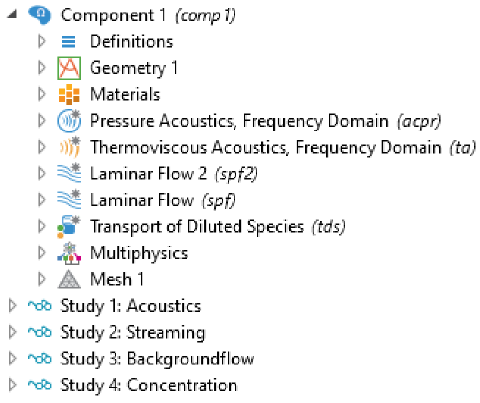
This was done in [2] and serves as a reference for the results obtained in this paper using the Acoustic Streaming interface of the Acoustics Module.

Acoustic Mixing Implementation in Comsol Multiphysics

The Acoustic Streaming interface is part of the Acoustics Module of Comsol Multiphysics and enables the combined use of pressure acoustics and thermoviscous acoustics, both in the frequency domain, and fluid flow interfaces.

In addition to the acoustic steaming interfaces a second Laminar Flow interface was used for the mentioned background flow as well as a Transport of Diluted Species interface to simulate the concentration of some species in the fluids.

The necessary coupling is done using the Multiphysics node. Figure 1 show the model tree of the simulation built using the Acoustic Streaming interfaces. Furthermore, the four studies conducted to solve the model are shown.



- Component 1 *(comp1)*
  - Definitions
  - Geometry 1
  - Materials
  - Pressure Acoustics, Frequency Domain *(acpr)*
  - Thermoviscous Acoustics, Frequency Domain *(ta)*
  - Laminar Flow 2 *(spf2)*
  - Laminar Flow *(spf)*
  - Transport of Diluted Species *(tds)*
  - Multiphysics
  - Mesh 1
- Study 1: Acoustics
- Study 2: Streaming
- Study 3: Backgroundflow
- Study 4: Concentration

Figure 1. Model tree of the simulation built using the Acoustic Streaming interfaces.

The studies are:

- Study 1: The two acoustics interfaces are solved in the frequency domain using a fixed signal frequency.
- Study 2: The Laminar Flow 2 interface and the Multiphysics node are solved to obtain the stationary solution of the velocity fields based on the results of the previous step.
- Study 3: The stationary background velocity field is calculated.
- Study 4: Based on the combined velocity field of the previous study steps, the stationary solution of the concentration field is calculated.

General Setup

As mentioned in the introduction the general problem is the mixing of two identical fluids carrying different concentrations of a diluted species in a microchannel. Due to the small dimensions of such microchannels the fluid flow is laminar, and the mixing is purely diffusion driven, making the process inefficient and slow. Figure 2 shows an exemplary microchannel with two inlets (upper half, lower half) on the left side. The laminar flow through the channel segment causes little mixing of the two fluids, resulting in an inhomogeneous concentration profile at the outlet as depicted in figure 3.

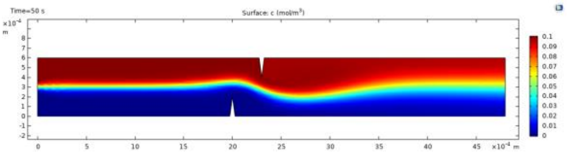


Figure 2. Exemplary microchannel with two inlets and little mixing due to laminar flow

The concentration profile confirms that the laminar flow leads to a very slow, diffusion dependent mixing process and highlights the need for enhancing the process.

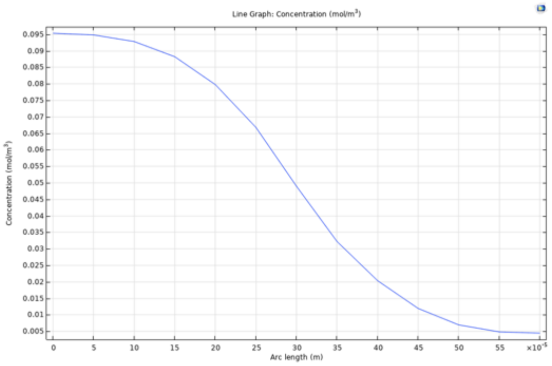


Figure 3. Concentration profile at channel outlet for diffusion driven mixing.

The investigated microchannel with added sharp edges can be seen in figure 4. In comparison to the channel segment shown in figure 2, the new channel has three pairs of actuated sharp triangular tips. Over the length of the channel three measuring cross sections are defined to evaluate the mixing quality at these positions.

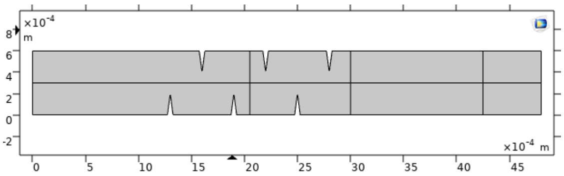


Figure 4. Investigated microchannel segment with three pairs of sharp triangular tips.

The geometrical dimensions of the channel segment are listed in Table 1 and are based on [2].

Table 1. *Geometrical dimensions of microchannel segment*

Parameter	**Value / Unit**
Length of channel	4800 µm
Height of channel	600 µm
Height H of tips	200 µm
Distance L between tips	300 µm
Position first tip	1300 µm
Tip angle α	15 °

The fluids are assumed to be water and the transported species are massless.

The two fluid inlets feature uniform flow profiles with identical velocity u_{in}. The relevant process parameters are listed in Table 2 and refer to an ambient temperature of 25°C [2].

Table 2. *Process Parameters*

Parameter	**Symbol**	**Value / Unit**
Speed of sound	c_0	1497 m/s
Density	ρ	997 kg/m^3
Dynamic viscosity	µ, η	1 mPas
Dyn. bulk viscosity	μ_B, η_B	1 mPas
Diffusion coefficient	D	0.4 nm^2/s
Inlet velocity	u_{in}	417 µm/s

To fully resolve the simulated physics properly the domain must be especially densely meshed and refined around the sharp edges. This can be seen in figure 5 where the fully meshed domain is depicted. Overall, the mesh consists of about 24000 elements.

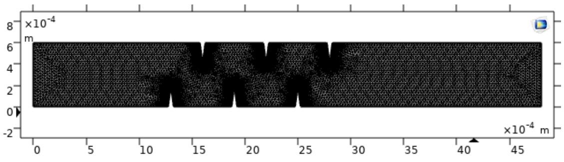


Figure 5. Fully meshed simulation domain with especially fine mesh around the sharp edges

Actuation Signal

The actuation of the sharp edges is modelled according to [2] and is a function of the position along the channel height. Nama et. al [2] have determined an expected sharp edge displacement of

$$d_{exp}(z) = 25.3\ d_0\ \left[1.22\left(\frac{z}{H}\right)^2 - 0.29\left(\frac{z}{H}\right)\right]$$

from measurement data where z is the position along the channel height and H is the total tip height. d_0 is a size parameter chosen to be 1 µm. This displacement in turn is the amplitude of the vibration signal.

$$s(t) = \sin(2\pi f t) + \cos\,(2\pi f t)$$

Resulting in the actuation signal

$$ac(t, z) = d_{exp}(z) s(t)$$

To improve the numerical behavior of the simulation the signal is ramped up slowly over time. Figures 6 and 7 show the actuation signal over time as a function of the position along the channel height for the bottom sharp edes and the top sharp edges respectively.

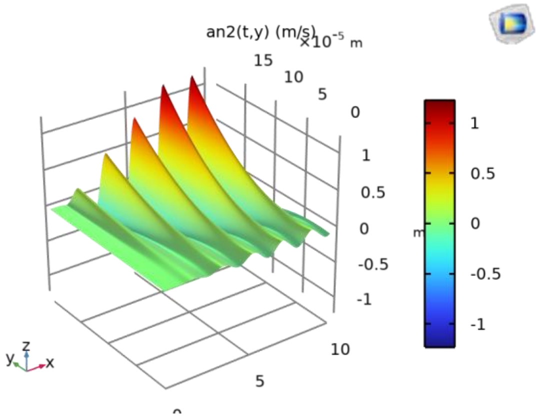


Figure 6. Actuation signal for the bottom sharp edges, dependent on time and position along the channel height

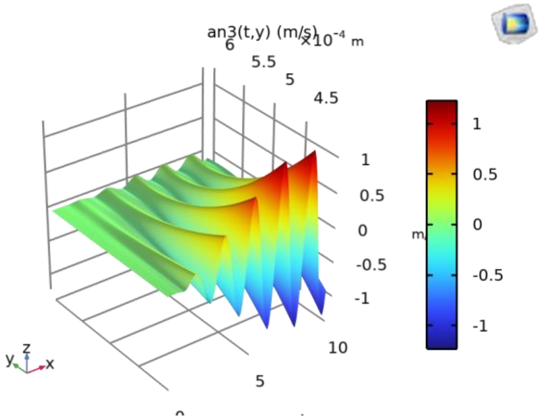


Figure 7. Actuation signal for the top sharp edges, dependent on time and position along the channel height

Acoustic Streaming Interfaces

As shown previously in figure 1 the model developed for the acoustic streaming simulation consist of several different interfaces. First the pressure and thermoviscous acoustics are combined with a laminar flow interface. Those three interfaces are used to simulate the acoustic streaming phenomena. The boundary conditions are the actuation signals on the sharp edges and no-slip conditions on the side walls.

Subsequently, another Laminar Flow interface is added to simulate the background flow using standard boundary conditions, e.g., no-slip conditions on the side walls, the specified inlet velocity, and an outlet pressure.

Last, the Transport of Diluted Species interface is used to simulate the distribution of species concentration within the fluid. The velocity field used for the simulation of the concentration field is the sum of the acoustic streaming velocity field and the laminar background flow. As boundary conditions individual concentrations are set at the two inlets, 1 mol/m^3 at the top inlet and 0 mol/m^3 at the bottom inlet.

2D Test Simulation

The 2D test simulation with the beforementioned boundary conditions and parameters showed that the model can be used to simulate the acoustic streaming phenomena in the microchannel. The result was verified with [2]. Figure 8 shows the result of the test simulation. It can be seen very well that the two fluid streams and their respective concentrations are mixed very rapidly by the actuated sharp edges as compared to the slow, diffusion driven mixing previously shown in figure 2. The counter-rotating circular motion of the fluid between pairs of sharp edges, induced by the acoustic streaming phenomena and responsible für the enhanced mixing, can be seen in figure 8.

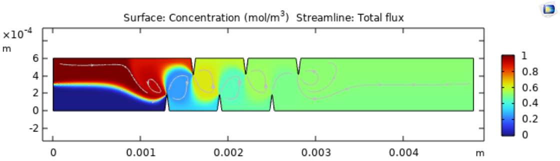


Figure 8. Concentration field of 2D test simulation with the Acoustic Streaming interface

3D Test Simulation

In addition to the 2D test simulation a 3D test model was built using the same parameters and boundary conditions. The 2D domain was simply extruded to the third dimension and a symmetry condition was applied to the top surface to reduce the overall domain size. All other boundary conditions and parameters remained unchanged. Figure 9 shows the concentration field in 3D. The same observations as for the 2D simulations can be made. Figure 10 in addition shows slices of the velocity field along the channel. As expected, the velocity is highest at the center of the channel and reduces to zero at the side walls. This validates the simulation model and shows the capabilities of the new interface.

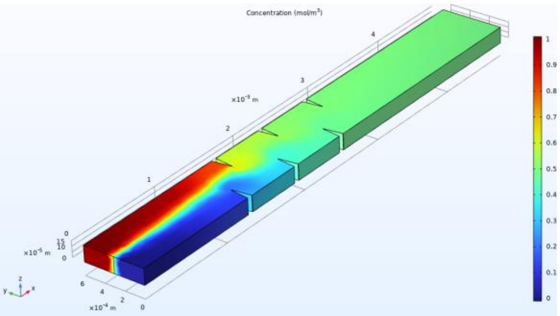


Figure 9. Concentration field of 3D test simulation with symmetry condition on the top surface

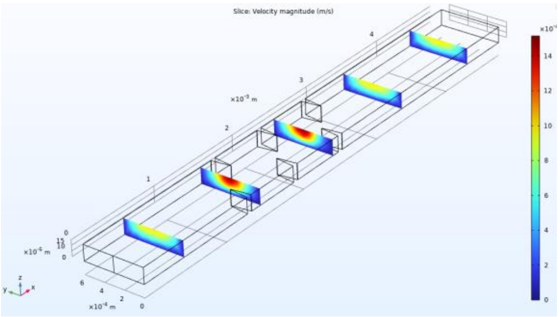


Figure 10. Velocity field slices of 3D test simulation

Parameter Study

The parameters, which are of interest for the parameter study, are of two types, geometrical and process parameters. For the geometrical aspect parameters associated with the tips are investigated. They are "tip angle" (the angle at the tip of the sharp edge), "tip height" (the height of the sharp edge from tip to side wall) and "tip distance" (the distance from one tip to the next tip on the other side of the channel of the sharp edge pair). The investigated process parameters are the inlet velocity of the fluid and the actuation frequency of the ultrasound signal on the sharp edges.

The default configuration of the model parameters is chosen according to [2] and listed in Table 3.

Table 3. *Parameter study default configuration*

Parameter	**Symbol**	**Value / Unit**
Inlet velocity	u_{in}	556 µm/s
Tip angle	α	15°
Tip height	H	200 µm
Tip distance	L	300 µm
Frequency	f	5.5 kHz

For the parameter study the individual parameters are shifted up or down in their value, while all other parameters remain the same as in the original configuration. This way the parameter space around the original configuration is explored and the sensitivity of the mixing results for the evaluated parameters is assessed.

Effects of Geometrical Changes

Tip height: When changing the tip height, meaning the individual height of each tip, the mixing quality increases with the increased tip height. The simulated heights are 160, 200 and 240 µm. Figure 11 shows the concentration fields for the different parameter values. Apparently, the smaller the tips get, the longer it takes the two fluids to mix. This can also be seen in figure 12, where the concentration profiles at the end of the microchannel section are shown.

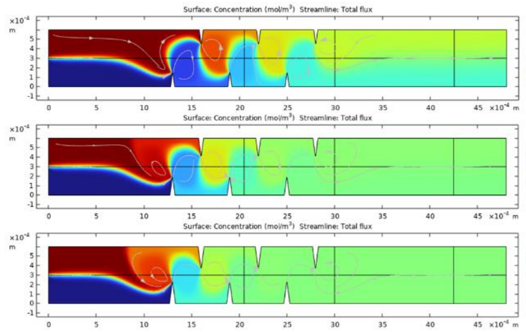


Figure 11. Concentration fields for different sharp edge heights (160, 200, 240 µm top to bottom).

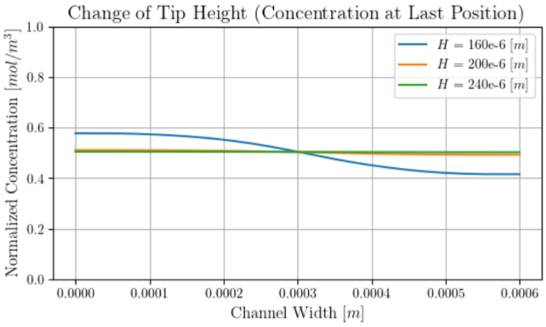


Figure 12. Concentration profiles at end of channel section for different sharp edge heights.

On the other hand, an increased tip height also leads to a higher flow resistance, which increases the required input pressure.

Tip angle: The simulated tip angles of 12, 15 and 18 degrees showed no significant influence on the mixing quality in the model.

Tip distance: The simulated distances between two opposing sharp edges of the same tip pair showed no significant differences in the mixing quality, except when approaching distances close to zero. In that case, the mixing quality dropped. The corresponding concentration fields are shown in figure 13.

The drop in mixing quality when decreasing the tip distance to zero can also be seen in figure 14 in the corresponding concentration profiles at the end of the channel.

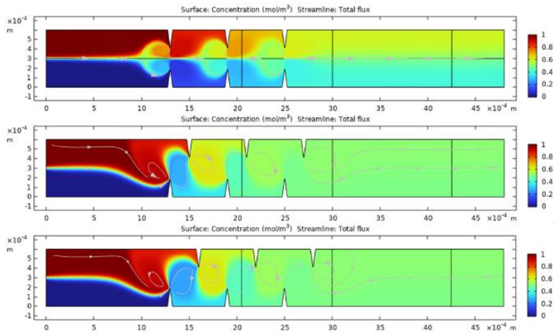


Figure 13. Concentration fields for different tip distances (0, 200, 300 µm top to bottom).

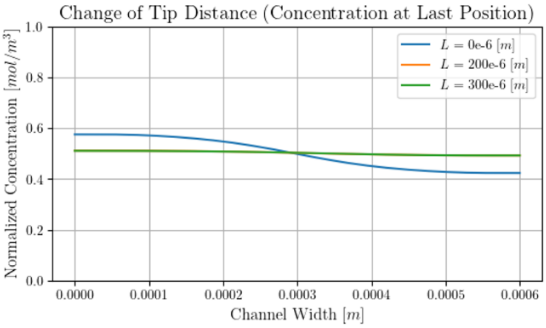


Figure 14. Concentration profiles at end of channel section for different tip distances.

Effects of Changing Process Parameters

Inlet velocity: The inlet velocity is the first of the process parameters to be studied. The simulated velocities where 417, 556, 834 and 1112 µm/s. The resulting concentration fields are shown in figure 15 where the velocity increases from top to bottom. The mixing quality decreases as the inlet velocity increases. This is due to the reduced residence time of the fluid in the section with sharp edges. The reduced quality of mixing can also be seen in figure 16 where the concentration profiles at the end of the channel are depicted.

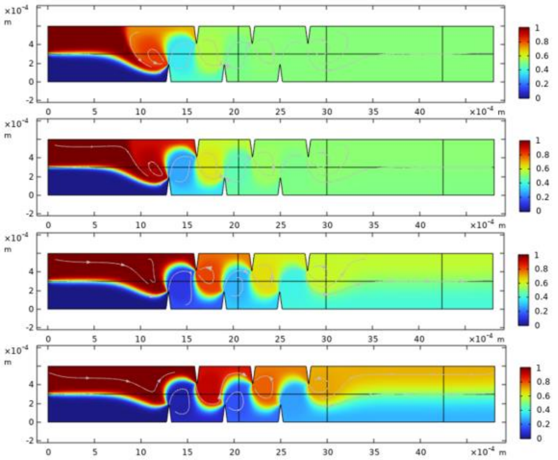


Figure 15. Concentration fields for different inlet velocities (417, 556, 834, 1112 µm/s top to bottom).

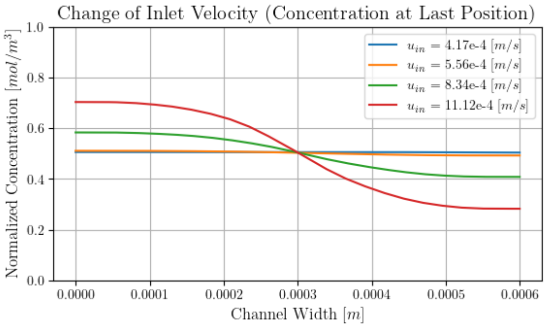


Figure 16. Concentration profiles at end of channel section for different inlet velocities.

A higher inlet velocity requires a higher inlet pressure. A smaller velocity on the other side would reduce the throughput of the system significantly. This is also discussed in the next section "Optimal Layouts".

Frequency: The tested frequencies, ranging from 4 to 6 kHz showed no significant influence on the simulation results. This could be due to the confined parameter space which could be extended in a subsequent, larger parameter study.

Optimal Layouts

The findings from the parameter study allow for the derivation of optimal layouts for certain scenarios. In general, the following points apply based on the findings of the parameter study:

- The inlet velocity has a strong influence on the mixing-quality. The lower the inlet velocity, the more homogeneous the concentration is after the microchannel. On the other hand, the lower the inlet velocity, the lower the throughput of the channel.
- The tip angle has no perceivable influence on the mixing quality in the investigated value range.
- The height of the tips has a strong influence on the mixing results. The higher the sharp edge, the better the mixing-quality becomes. But an increase of tip height requires an increase of the input pressure to maintain the same input velocity.
- The tip distance only has an impact on the mixing process, when reducing it towards zero, thereby deteriorating the mixing efficiency. At larger tip distances, the mixing quality is basically inert to changes in tip distance.
- The actuation frequency has no influence on the mixing-quality in the investigated range.

In a scenario where high throughput is required and medium mixed quality is sufficient, one would therefore choose a medium inlet velocity, e.g., 834 µm/s, and a medium to low tip height, e.g., 160 µm or 200 µm. The other parameters are of secondary importance.

If perfect mixing quality is needed and throughput is less important one would choose a low inlet velocity and medium to high sharp edges.

Conclusions

The modelling with the Acoustic Streaming interface proved to be quite straight forward and provided a fast and efficient path to setting up and running simulations. The parameter study therefore was also efficient and would lend itself for a further extended parameter space to investigate. This would bring further insights into the sensitivity of the mixing process for certain parameter variations.

The results of the simulations showed the potential of inserting acoustically actuated sharp edges into lab-on-a-chip systems to enhance the mixing efficiency within the channel. Although the topic has been part of several papers throughout the last years, modelling the system using the new Acoustic Streaming interface provided a new and user-friendly way to explore the topic and gain new insights into the influences of the geometrical and process parameters.

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