Parametric optimization of a laminar-flow micromixer by CFD

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Abstract

Mixing is still nowadays a crucial and challenging aim in laminar, low Reynolds number microfluidic devices.

In this article, a parametric study of the geometry of a micro-channel comprising a mixing unit is studied in order to optimize the mixing process in order to have the highest mixing efficiency as possible at the channel exit. Instead of complex spatial geometries and sample strategies, simple periodic geometric features are applied to decrease the required mixing distances.

For a given 2D geometry studied in a previous article [?] consisting of a "T"type inlet channel and a mixing unit in which there are two bars forming known and fixed angles α and β with respect the channel walls, it will be shown how the values of alpha and beta affect the efficiency of the resulting mixing at the outlet section of the channel as well as the pressure requirements to run the channel.

After the optimization process, an optimal combination of the angles α and β has been found for which the mixing efficiency is as high as possible and the pressure at the inlet section is as minimum as possible. Other angle values have been also found to have either the highest efficiency (regardless the pressure drop) or the lowest pressure drop (regardless the mixing efficiency). Following [?], the mixing cost (a ratio between the efficiency and the pressure drop) of each configuration has been also calculated and discussed. The configuration with the lowest cost is also presented.

Keywords: Mixing unit, CFD, microchannel, response surface, optimization.

1. Introduction

The fluid mixture at low Reynolds number appear in many processes of industrial processes, chemical or medical field. Any industrial process should lead to the optimization of his time and to the increase of its efficiency.

Those processes in which the mixture is produced in conditions of laminar flow can be improved by optimizing the different mixing units. There are several principles already available to achieve mixing in microchannels, mainly based upon complex geometries, clever simple strategies or external fields. The optimization of the different mixing units can be done by modifying the different geometric parameters, such as its length, width or, as in the case is discussed in this paper, the angles formed by the bars with respect to the channel walls.

Many researches have carried out studies in many different geometries looking for an improvement in the mixing process. In particular, Kim et al. [?], chose to calculate the correlation between the different geometric parameters of a particular mixing unit through the advanced-RSM technique to obtain the optimum value of each parameter that allows to obtain the maximum mixing. On the other hand, Fang et al. [?], studied the variation of a coefficient denoted by MP depending on the length of the mixing device. This MP coefficient indicates the degree of mixing between two fluids. In this paper, a modification of the geometry proposed by these authors will be used.

2. Problem description

The previously mentioned geometry consist in a microchannel device that contains a "T" type inlet channel and a mixing unit in which there are two bars forming known and fixed angles alpha and beta with respect the channel walls. Figure 1 shows the geometry proposed by [?], this geometry will be modify in order to perform our optimization study. Basically these changes consist in the increase of the distance between the two bars and between each bar and the channel walls (Figure 2).

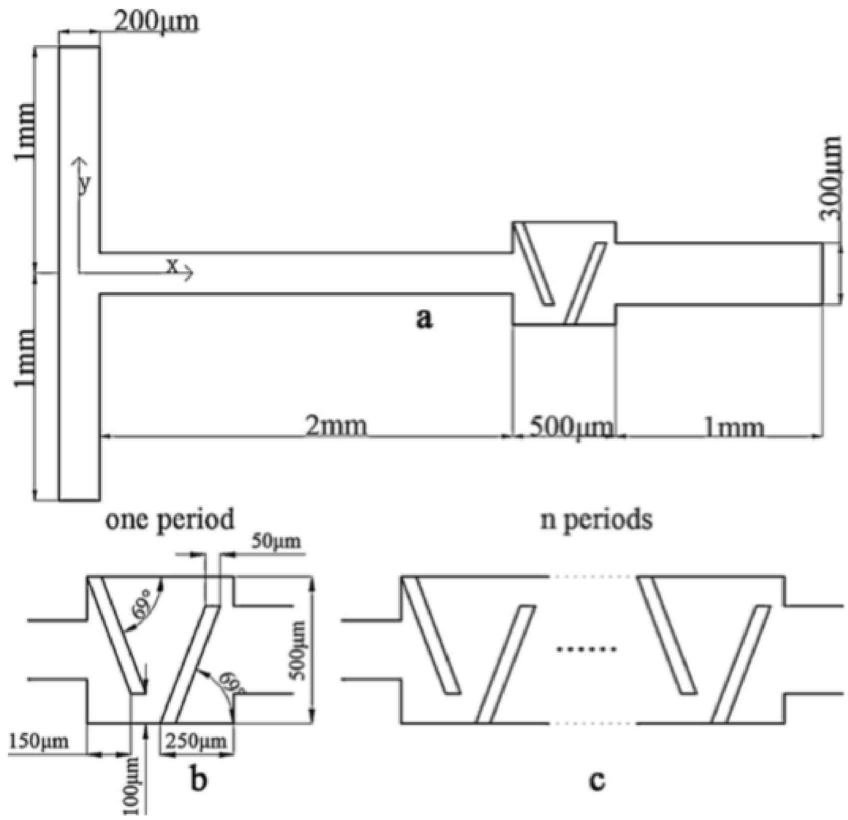


Figure 1: Geometry of the mixing unit proposed by [2].

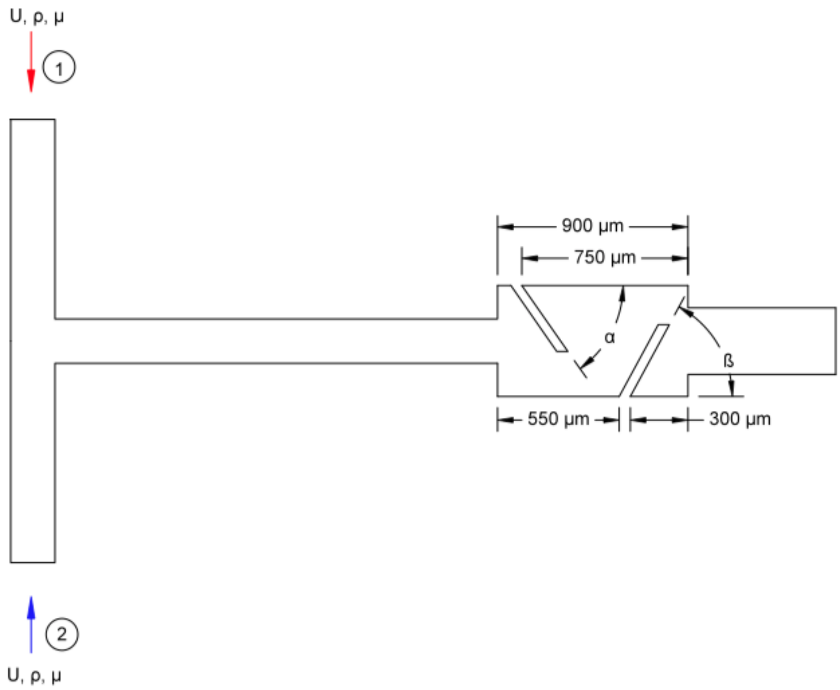


Figure 2: Geometry of the modified mixing unit.

In computer simulations, a two-dimensional (2D) model was set up instead of the three-dimensional (3D) model. The reason to apply 2D model is because the characteristic diffusion time along the width, defined as $T_D = L^2/D$, where L is the diffusion length and D is the diffusion coefficient, is two orders of magnitude larger than that along the depth. Therefore, the mixing of two identical fluids will take place along a 2D channel, the fluid injected to both inlets will be identical but labeled by different names, 1 and 2, whose concentrations were set 1 and 0, respectively.

The problem is governed by the Reynolds number (Re), defined as $Re = \frac{UH}{\nu}$, it measures the ratio of the inertial effects to viscous effects, the Schmidt number (Sc), defined as $Sc = \frac{\nu}{D}$, it represents the ratio of momentum diffusivity (viscosity) and mass diffusivity, and the Peclet number (Pe), defined as $Pe = ReSc$, which represents the ratio between the characteristic diffusive time and the characteristic inertial time. These three important dimensionless parameters in fluid mechanics were introduced to characterize the flow in the system.

Therefore, in order to show how the values of alpha and beta affect the efficiency of the resulting mixing at the outlet section of the channel as well as the pressure requirements to run the channel, the value of the standard deviation sigma of the mass fraction m of one of the liquids at the outlet section and the pressure value at the inlet sections will be calculated for every simulation.

$$\sigma = \sqrt{\sum_{i=1}^{n} \frac{(m_i - \bar{m})^2}{n}}$$

where m_i is the mass fraction in the ith cell, n is the number of cells, and is the average mass fraction across the section. Notice that the standard deviation of the equation above is such that $0 \leq \sigma \leq 0,5$ where 0 is obtained for full mixing and 0,5 occurs in the case of no mixing. Many authors usually normalize the standard deviation to represent the mixing performance by a coefficient denoted by MP, such that no mixing yields a value of 0 and a complete mixing a value of 1.

$$MP = (1 - \frac{\sigma}{\sigma_{max}}) \times 100$$

3. Numerical considerations

The evaluations were conducted by computational fluid dynamics (CFD) using ANSYS Fluent. To check the validity of our model, we will compare the value of MP obtained on our simulations, using the geometry proposed by the article, with the value of MP obtained on [?]. To do so, the 2D model was discretized with structured quad meses with most of the cells having 10 μm long. The solver was set pressure based. Laminar, steady and species transport model without reaction were applied. In the Solution Controls, the mass fraction was set Second Order Upwind scheme and the other schemes were set default value. The base flow from both inlets is set 0,04167 m/s, the mass diffusivity is set constant $D = 10^{-10} m^2/s$ and the kinematic viscosity is set $\nu = 10^{-6} m^2/s$.

The velocity-pressure coupling was set up by Coupled algorithm, this algorithm solves the equations of velocity and pressure simultaneously, which implies that for each iteration takes longer but is compensated by a faster convergence of residuals.

Once we check the validity of our model, we proceed to perform a mesh convergence analysis by the Grid Convergence Index (GCI). The Grid Convergence Index is a method to indicate the degree of convergence of the numerical solution in studies where multiple meshes are used. Thus, the GCI is a measure, in percent, of the difference between the calculated value and the asymptotic value. A small value of GCI indicates that the numerical solution is within the asymptotic region and differs little from that which would be obtained with the new refined mesh.

To calculate an estimation of the exact solution we will use the standard Richardson extrapolation, which will provide a correction to the solution obtained in the fine mesh for a mesh size toward zero.

Mesh	Element size (μm)	Standard deviation (σ)	MP	r
Mesh 1	2,9629629	0,45084912	0,0983	1,5
Mesh 2	4,44444	0,4444351	0,1111298	1,5
Mesh 3	6,66667	0,4219282	0,1561436	1,5
Mesh [2]	10	0,386	0,228	

Table 1: Mesh used for the study of convergence.

$$\sigma_{exact} \approx \sigma_1 + \frac{\sigma_1 - \sigma_2}{r^p - 1} \approx 0,4534,$$

$$GCI_{3,2} = \frac{3}{r^p - 1} \mid \frac{\sigma_3 - \sigma 2}{\sigma_2} \mid = 0,057,$$

$$GCI_{2,1} = \frac{3}{r^p - 1} \mid \frac{\sigma_2 - \sigma 1}{\sigma_1} \mid = 0,015,$$

$$\frac{GCI_{3,2}}{r^p GCI_{2,1}} = 1,0144 \approx 1.$$

In Figure 3. are shown the values obtained with 4 different meshes with its corresponding values of sigma and GCI, as well as the value of sigma obtained by the Richardson extrapolation. Also it is shown the relation between the time it takes each mesh to perform 500 iterations with the time it takes a coarse mesh to do the same.

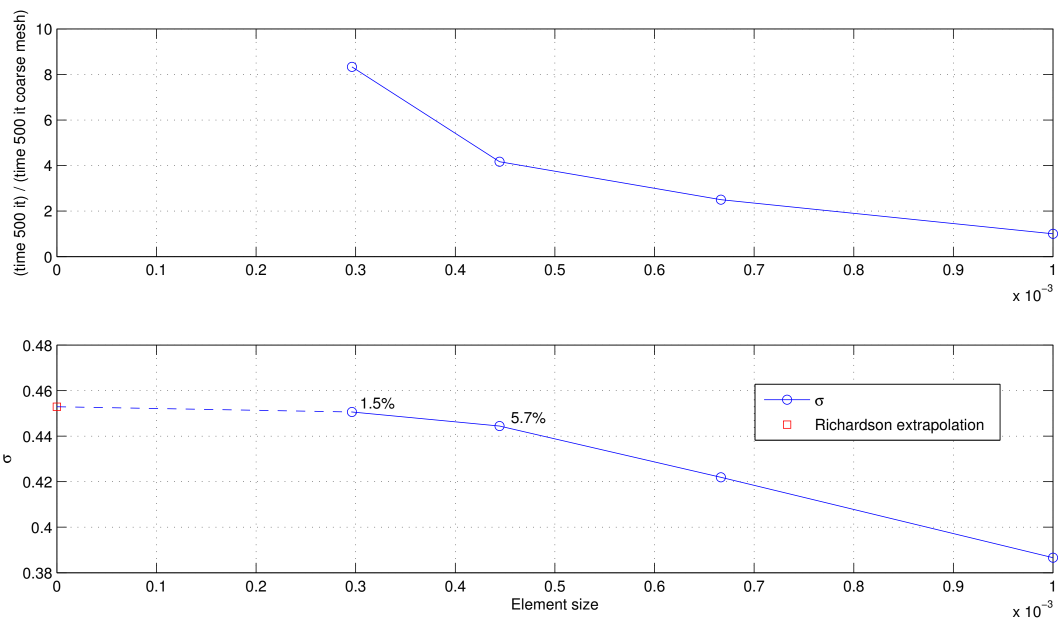


Figure 3: Convergence mesh. In % is indicated the error of the corresponding mesh.

After studying Figure 3, it can be concluded that the most appropriate mesh for our study is that with a size of elements of 4.4444 μm because it does not compensate the error reduction that offers the following finer mesh with the increased time of calculation.

Once the mesh convergence analysis has been performed with the geometry proposed in 2, we continue our study modifying the geometry in order to perform the optimization of our mixing unit. After changing the distance between the bars and the distance from each to the channel walls, for the combination of angles provides in [?], that is, for $\alpha = 69$ ° and $\beta = 69$ °, the coefficient MP has been modified from 0,08183 to 0,11113. The ratio worsens with the new geometry because the distance between obstacles is now larger so the curvature experienced by the streamlines, and therefore the gradients, are less pronounced and do not benefit the mixture. As in this paper only the optimization of the angles α and β is studied, the distance required to perform this optimization study is used, allowing for a future work to study the optimization of this distance.

To optimize the mixing unit is used the integrated application in Workbench, Goal Driven Optimization, that leverages the constant and automated power of ANSYS Workbench for parametric analysis. Goal Driven Optimization describes the relationship between the design variables α and β, and the product performance, in our case the standard deviation of the mass fraction of one of the fluids at the outlet channel and the average pressure of the two fluids at the inlet channel, using the design of experiments combined with the response surfaces.

For the design of the different combinations of the design variables α and β necessary for obtaining the response surfaces may be used different methods. In this paper we have chosen the Central Composite Design method, which is the default method offered by ANSYS. The location of the input parameters generated with this method, if the number of the design variables is 2, consists in: a central point, 4 axial points and 4 factorial points.

Once we have chosen the method to obtain the design points necessary to build the response surfaces, the maximum and minimum values that will take α and β, which will be 90°and 30° respectively, and the output parameters to be obtained for each design point are introduced. These output parameters are the standard deviation of the mass fraction of one of the fluids at the outlet channel and the average pressure of the two fluids at the inlet channel, since we want to get the geometry that provides the best mixture with the lowest pressure requirements to run the channel.

As a result of the design of experiments, the design 9 points shown in Table 2. are obtained.

Design points	α	β
1	60	60
2	30	60
3	90	60
4	60	30
5	60	90
6	30	30
7	90	30
8	30	90
9	90	90

Table 2: Design of experiments (Central Composite Design).

Once the design points are obtained, we proceed to perform the simulation of each in order to obtain the response surfaces. Response surfaces are functions of different nature where output parameters are described in terms of input parameters. They are built from the design of experiments to provide approximate values of output parameters at all points in the design space to be analyzed without having to make a simulation of each point. The accuracy of a response surface depends on several factors: complexity of the variation of the solution, the number of point of design and the choice of the type of response surface. ANSYS DesignXplorer provides tools to estimate and improve the quality of response surfaces.

The three methods of construction of the response surface that will be studied in this paper are:

- Standard Response Surface 2nd-Order Polynomial: This is the algorithm Ansys offers by default, it creates a standard response surface. This method is effective when the variation of the output parameters is soft with respect to the input parameters.

- Kriging: This algorithm is efficient in many cases, it is recommended for highly nonlinear responses and not noisy results, as Kriging is an interpolation that matches exactly the design points. For this method does not work look at the Goodness of fit, because it matches the response surface with the design points, so the goodness of fit will be perfect. To verify the goodness of fit of this method it should be used verification points.

- Non-Parametric Regression: This algorithm is recommended for non-linear responses and noisy results.

In order to compare these three methods, in addition to the 9 design points, we have used 8 refinement points and 2 verification points. In Tables 3. and 4. the values of each method are discussed about the Goodness of fit for both output parameters.

Goodness of fit	**Standard**	**Kriging**	**Non-Parametric**
Coefficient of Determination (Best value=1)	0,98497	1	1
Maximum Relative Residual (Best value= 0 %)	0,49548	0	0
Root Mean Square Error (Best value = 0)	0,0012082	$6,7277 \times 10^{-11}$	$9,840 \times 10^{-10}$
Relative Root Mean Square Error (Best value=0 %)	0,26094	0	0
Relative Maximum Absolute Error (Best value = 0 %)	22,812	0	0
Relative Average Absolute Error (Best value = 0 %)	9,5248	0	0
Goodness of fit of verification points			
Maximum Relative Residual (Best value = 0 %)	0,21057	0,09657	0,28762
Root Mean Square Error (Best value = 0)	0,00082971	0,00039581	0,0009353
Relative Root Mean Square Error (Best value = 0 %)	0,18268	0,087828	0,2096
Relative Maximum Absolute Error (Best value = 0 %)	9,5766	4,2668	12,708
Relative Average Absolute Error (Best value = 0 %)	8,0953	3,9097	7,9847

Table 3: Goodness of fit of the different methods for the standard deviation of the mass fraction of one of the fluids at the outlet channel.

Goodness of fit	Standard	Kriging	Non-Parametric
Coefficient of Determination (Best value=1)	0,99846	1	1
Maximum Relative Residual (Best value= 0 %)	6,1251	0	0
Root Mean Square Error (Best value = 0)	3,2708	$6,5087 \times 10^{-7}$	$1,0084 \times 10^{-7}$
Relative Root Mean Square Error (Best value=0 %)	2,416	0	0
Relative Maximum Absolute Error (Best value = 0 %)	8,4616	0	0
Relative Average Absolute Error (Best value = 0 %)	3,1086	0	0
Goodness of fit of verification points			
Maximum Relative Residual (Best value = 0 %)	2,1587	2,5743	1,2544
Root Mean Square Error (Best value = 0)	5,6499	6,0119	2,9403
Relative Root Mean Square Error (Best value = 0 %)	2,1154	1,8795	0,92649
Relative Maximum Absolute Error (Best value = 0 %)	8,1321	9,6977	4,7253
Relative Average Absolute Error (Best value = 0 %)	6,2229	5,5382	2,7569

Table 4: Goodness of fit of the different methods for the average pressure at the inlet channel.

Comparing the three methods can be seen that the algorithm Standard Response Surface 2nd-Order Polynomial is the one with the worst goodness of fit. Of the remaining two methods, should be noted that for the algorithm Kriging, the Goodness of fit of the design points does not indicate anything, but nevertheless for Non- Parametric Regression algorithm it indicates a perfect goodness of fit. It is also noted that although the goodness of fit of verification points for the standard deviation is better in Kriging, the goodness of fit of verification points for the average pressure at the inlet is better in Non-parametric regression.

Finally, because of the goodness of fit of the design points as well as the verification points, the Non-parametric regression algorithm is chosen. In Figures 4. and 5. are shown the response surfaces constructed with each method for each output parameter. According to the goodness of fit, the Non-parametric regression algorithm is the one that best represents the variations of the output parameters in terms of the input parameters.

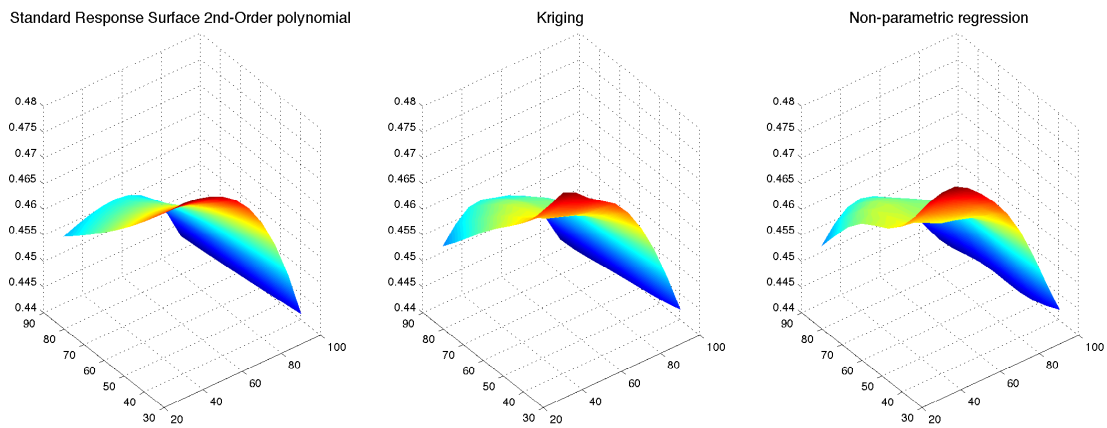


Figure 4: Response surface of the standard deviation at the outlet channel.

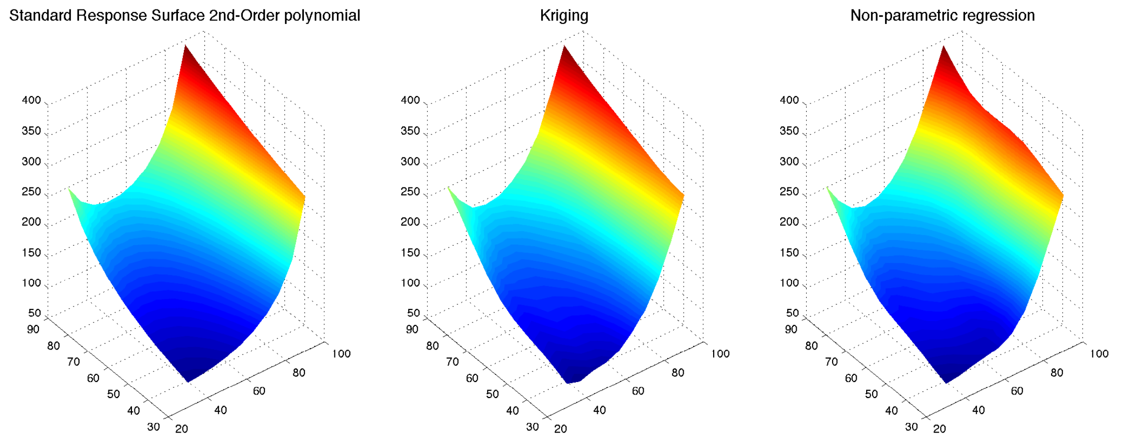


Figure 5: Response surface of the average pressure at the inlet channel.

Once the response surface is built, we are going to continue doing the last step of the optimization process. An optimization of the response surface gets its information from the response surface itself, so that it is dependent on the quality of this.

There are four methods available for optimization: Screening, MOGA, NLPQL and MISQP, of these four methods will only be studied two of them, Screening and MOGA, since they are the only ones who perform optimization with multiple objectives and our optimization problem is such that the objectives are to minimize both the standard deviation of the mass fraction of one of the fluid at the outlet channel as the average pressure of the two fluids at the inlet channel.

Screening option is a non-iterative approach available for all input parameters. Screening method is normally used for a preliminary design, which can lead to apply later the method MOGA to more refined optimization results. The option MOGA (Multi-Objective Genetic Algorithm) is an iterative approach available for all input parameters and allows to obtain a more refined approach than Screening. However, this algorithm has a higher computational cost.

In order to check whether the additional computational time spent using MOGA is necessary with respect to the results obtained by Screening, we will obtain the optimal combination of alpha and beta with both methods. To do so, we configure both methods with 1000 initial samples. The initial samples are the number of samples to be generated for the optimization, these are generated by the response surface. In the MOGA method the number of samples per iteration is set as 10. All other parameters in both methods have been left by default.

4. Results

Once we have configured both methods for the optimization process, we proceed to obtain the optimal combination of alpha and beta.

	Screening				MOGA			
Candidate	α	β	σ	**Pa**	α	β	σ	**Pa**
A	54,39°	54,757°	0,46239	136,48	54,39°	54,757°	0,46239	136,48
Verification A			0,46001	144,53			0,46001	144,53
B	58,47°	51,475°	0,46304	131,85	58,47°	51,475°	0,46304	131,85
Verification B			0,45984	148,31			0,45984	148,31
C	45,27°	59,796°	0,46293	134,05	44,31°	57,921°	0,46326	131,46
Verification C			0,46335	133,51			0,46207	134,54

Table 5: Candidates for the optimal combination of the angles α and β.

As we can see in Table 5. the first two candidates are exactly the same for both methods, while the candidate C is slightly different but almost the same. Thus the Screening method is finally chosen due to it is faster in finding the different candidates and provides the same results as the MOGA method.

After choosing the best method for our optimization study, in order to minimize the standard deviation of the mass fraction of one of the fluids at the outlet channel and the average pressure at the inlet channel, it can be done in three ways: not prioritizing any of those objectives (this has been the procedure for choosing the appropriate method and previously discussed), prioritizing the standard deviation or prioritizing the pressure requirements. In this paper, we will present the solutions to these three cases since, as we can see in Figures 4. and 5., when the standard deviation is low, the pressure is high, so it is interesting to know the optimal values of the angles alpha and beta when we give greater priority to the minimization of one another.

The results in Table 6. correspond to the optimization of the device when it is prioritized minimize the standard deviation of the mass fraction of one of the fluids at the outlet channel and the results from Table 7. correspond to the optimization of the device when it is prioritized minimize the average pressure at the inlet channel.

	Screening			
Candidate	α	β	σ	**Pa**
A	89,79°	39,346°	0,44499	319,42
Verification A			0,44633	308,17
B	73,65°	85,167°	0,4521	236,12
Verification B			0,45321	231,87
C	83,01°	78,487°	0,44844	282,65
Verification C			0,44967	262,08

Table 6: Candidates for the optimal combination of the angles α and β prioritizing minimizing the standard deviation of the mass fraction of one of the fluids at the outlet channel.

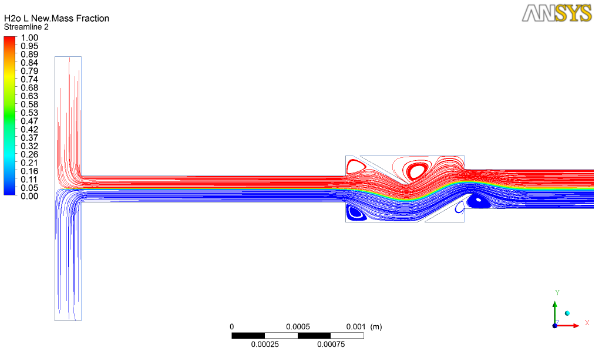
	Screening			
Candidate	α	β	σ	**Pa**
A	58,95°	46,788°	0,46459	122,92
Verification A			0,46381	137,86
B	35,67°	58,624°	0,46442	124,13
Verification B			0,46308	131,01
C	54,63°	51,007°	0,46335	130,18
Verification C			0,45953	142,34

Table 7: Candidates for the optimal combination of the angles α and β prioritizing minimizing the average pressure at the inlet channel.

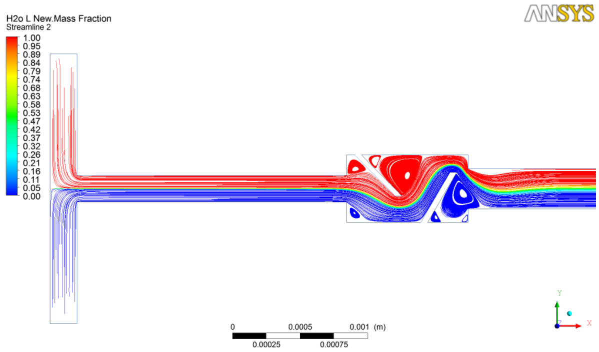
Finally, noting the error between each candidate and each verification, we will choose one for each type of optimization. In case we want to minimize both equally, the candidate C is chosen as it is the one with less error observed with respect to the response surface, giving the optimal values of $\alpha = 45,27°$and $\beta = 59,796°$. On the other hand, if we prefer to prioritize minimizing the standard deviation from the pressure, the chosen values are $\alpha = 73,65°$and $\beta = 85,167$ °. While if we prefer to prioritize minimizing the pressure against the standard deviation, the chosen values are $\alpha = 35,67°$and $\beta = 58,624°$.

To better understand why the three cases mentioned above are optimal, it has been included for each geometry the streamlines and isocontours of pressure and mass fraction. To understand the difference between the different combinations of angles we are going to compare each of the optimal cases with the most unfavorable case respect to the homogeneity of the mixture, i.e. the case when $\alpha = 30°$and $\beta = 30°$. In Figure 6 we can see the streamlines of the two fluids in the mixing unit. We can observe that depending on the combination of angles, the streamlines are more or less disturbed, and vortices are generated at the corners. So, in the worst case of mixing both fluids are hardly disturbed by obstacles and therefore there is poor mixing. However, in the optimized geometry of the mixing unit for $\alpha = 73,65°$and $\beta = 85,167$ °, Figure 6 (c), which it is the candidate in case you prefer to prioritize minimizing the standard deviation from pressure, can be observed as compared to the other, that the fluids are considerably disturbed by obstacles so that is why it is obtained more mixture.

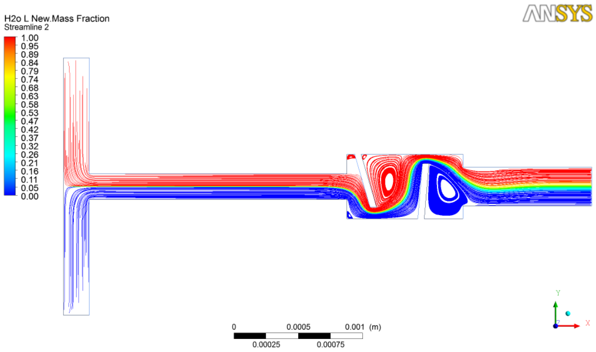
As we saw with the response surfaces, the greater the disturbance suffered by fluids due to obstacles, the higher the pressure is at the inlet channel. Thus, in Figure 7, as can be seen in the worst case respect to the homogeneity of the mixture, the pressure is much lower than in the other candidates, since fluids barely have to overcome any obstacle to move. The same happens in the optimized geometries of the mixing unit for $\alpha = 45,27°$and $\beta = 59,796°$, Figure 7 (b), and $\alpha = 35,67°$and $\beta = 58,624°$, Figure 7 (d), which are the candidates in the case we want to minimize equally both, standard deviation and pressure, and in case we prefer to prioritize minimizing pressure against the standard deviation respectively, as in both cases we have minimized the pressure. However, in the optimized geometry of the mixing unit for $\alpha = 73,65°$and $\beta = 85,167°$, Figure 7 (c), which is the candidate in case we prefer minimizing the standard deviation against pressure, we can observe as we obtained more mixture, the pressure increases significantly, since fluids are very disturbed by the presence of obstacles.



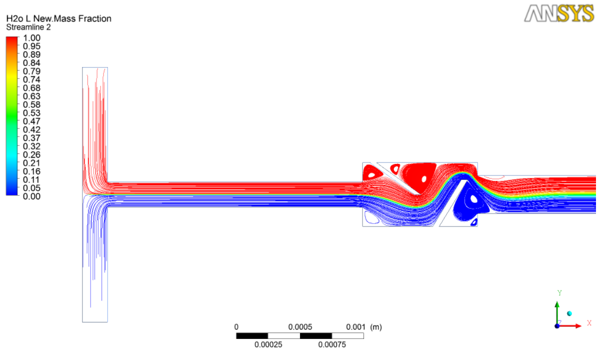
(a) Streamlines for $\alpha = 30$ y $\beta = 30$.



(b) Streamlines for $\alpha = 45,27$ y $\beta = 59,796$.

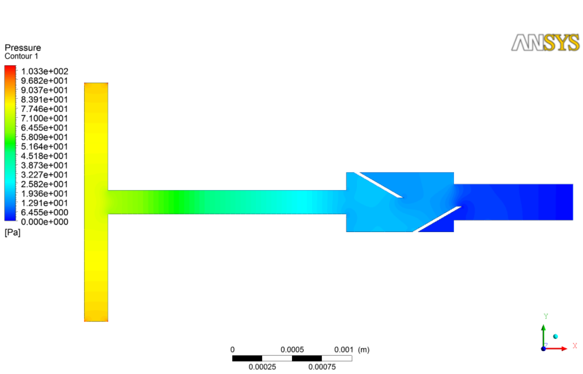


(c) Streamlines for $\alpha = 73,65$ y $\beta = 85,167$.

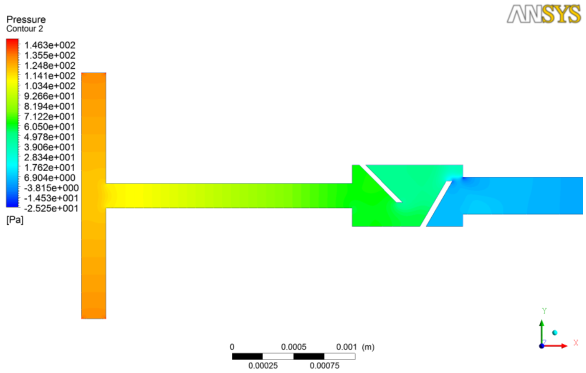


(d) Streamlines for $\alpha = 35,67$ y $\beta = 58,624$.

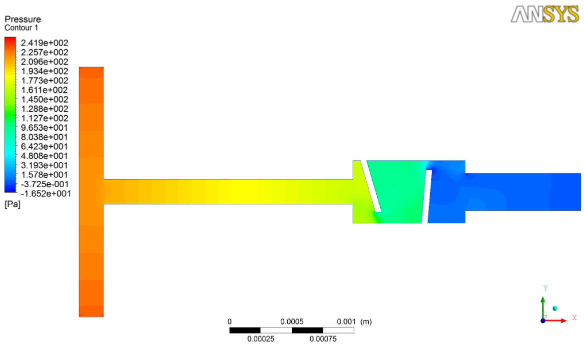
Figure 6: Streamlines of the "T" inlet channel and the one-period mixing unit. The color indicates the mass fraction.



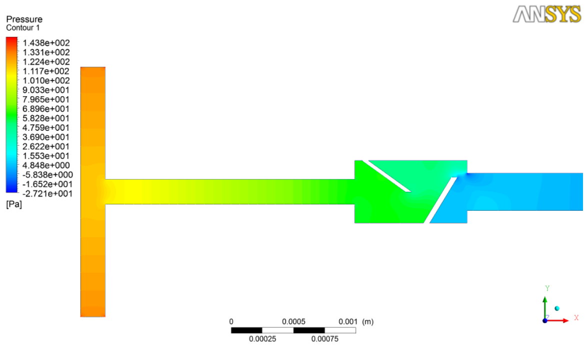
(a) Isocontour of the pressure for $\alpha = 30$ y $\beta = 30$.



(b) Isocontour of the pressure for $\alpha = 45,27$ y $\beta = 59,796$.



(c) Isocontour of the pressure for $\alpha = 73,65$ y $\beta = 85,167$.



(d) Isocontour of the pressure for $\alpha = 35,67$ y $\beta = 58,624$.

Figure 7: Isocontour of the pressure in the mixing unit.