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TÍTULO DO TRABALHO:

Numerical Analysis of Flow in Microchannels Using The Finite Element Method

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Resumo

Os biocombustíveis ganharam popularidade significativa por serem uma fonte de energia limpa e renovável em comparação com os combustíveis fósseis convencionais. O biodiesel é produzido a partir de ésteres monoalquílicos derivados de óleos vegetais, gorduras animais ou outros materiais compostos principalmente de triglicerídeos. Além de várias outras aplicações importantes, o biodiesel é predominantemente utilizado como combustível para veículos, sendo misturado com o diesel derivado de petróleo convencional. A tecnologia de microrreatores, um método essencial para a intensificação de processos, oferece inúmeras vantagens potenciais para as indústrias de processos. Reações bifásicas com limitações de transferência de massa podem ser efetivamente conduzidas em pequena escala em um microrreator bifásico de escoamento lento. Nesse tipo de reator, segmentos alternados e uniformes (golfadas) da mistura de reação bifásica exibem áreas de transferência de massa entre as fases e padrões de escoamento bem definidos. As circulações dentro dessas golfadas não são completamente compreendidas e requerem análises numéricas sistemáticas e o desenvolvimento de modelos matemáticos avançados para melhor entendimento e otimização. Além disso, a aplicação de microrreatores pode levar a uma maior eficiência energética e redução de resíduos na produção de biocombustíveis. Esses reatores compactos permitem um controle mais preciso das condições de reação, o que pode resultar em produtos de maior qualidade e processos mais sustentáveis. O objetivo deste trabalho é estudar o comportamento do escoamento bifásico através de um microrreator capilar para a produção de biodiesel, utilizando o modelo de escoamento homogêneo, onde as duas fases se movem a velocidades iguais e aumentam o nível de mistura, podendo assim ser tratadas como se fossem uma única fase. Uma abordagem de dinâmica dos fluidos computacional (CFD) é então utilizada para simular numericamente esse tipo de escoamento em malhas não estruturadas quadrilaterais. Os escoamentos são modelados pelas equações de Navier-Stokes bidimensionais incompressíveis, escritas utilizando a formulação função corrente-vorticidade, que são aproximadas pelo Método dos Elementos Finitos. A linguagem de programação Python foi utilizada para desenvolver o código computacional. Após a verificação do código, escoamentos característicos em microcanais foram analisados, comparando os resultados numéricos com resultados experimentais da literatura. Bons resultados foram encontrados com essa metodologia.

Palavras-chave: Biocombustível, formulação função corrente-vorticidade, Método de Galerkin, Microcanais, Transporte de massa.

Abstract

Biofuels have gained significant popularity as they are a clean and renewable energy source when compared to conventional fossil fuels. Biodiesel is produced from monoalkyl esters derived from vegetable oils, animal fats or other materials composed mainly of triglycerols. In addition to several other important applications, biodiesel is predominantly used as a vehicle fuel, where it is blended with conventional petroleum-derived diesel. Microreactor technology, an essential method for process intensification, offers numerous potential advantages for process industries. Two-phase reactions with mass transfer limitations can be effectively conducted on a small scale in a slow-flow two-phase microreactor. In this type of reactor, alternating and uniform segments (slugs) of the two-phase reaction mixture exhibit areas of mass transfer between phases and well-defined flow patterns. The circulations within these slugs are not completely understood and require systematic numerical analyzes and the development of advanced mathematical models for better understanding and optimization. Furthermore, the application of microreactors can lead to greater energy efficiency and waste reduction in biofuel production. These compact reactors allow for more precise control of reaction conditions, which can result in higher quality products and more sustainable processes. The objective of this work is to study the behavior of two-phase flow through a capillary microreactor for the production of biodiesel, using the homogeneous flow model, where the two phases move at equal speeds and increasing the mixing level, thus being able to be treated as if were a single phase. A computational fluid dynamics (CFD) approach is then used to numerically simulate this type of flow in quadrilateral unstructured meshes. The flows are modeled by the incompressible two-dimensional Navier-Stokes equations, written using the current-vorticity function formulation, which are approximated by the Finite Element Method. The Python programming language was used to develop the computational code. After checking the code, characteristic flows in microchannels were analyzed, comparing the numerical results with experimental results from the literature. Good results were found with this methodology.

Keywords: Biofuel, streamfunction-vorticity formulation, Galerkin method, Microchannels, species transport.

Introduction

Cutting-edge technologies necessitate that systems be compact and highly efficient. Progress in Micro Electro Mechanical Systems (MEMS) and Lab-on-a-chip technologies is crucial in meeting these needs. In numerous applications, such as drug delivery, biochemical analysis, nucleic acid synthesis, cell activation, and chemical reactions, micro-scale devices often incorporate a micromixer. When it comes to mixing operations, two primary considerations arise. Firstly, mixing efficiency should be maximized. Secondly, the flow resistance (pressure drop) must be kept low to reduce power consumption (CETKIN; MIGUEL, 2019).

Biodiesel production processes are generally categorized into batch and continuous methods. The conventional reactors utilized in biodiesel production are stirred tank reactors or batch reactors. In batch processes, a fixed quantity of reactants is processed, whereas in continuous processes, reactants are constantly supplied to the system (BART; PALMERI; CAVALLARO, 2010). Various approaches have been suggested for the process intensification of biodiesel synthesis, with microreactors emerging as the most promising option (AL-DHUBABIAN, 2005). Microreactor technology enhances chemical processes by providing benefits such as increased mass and heat transfer rates, as well as safer and more sustainable operations (HESSEL; LÖWE, 2005).

However, achieving effective mixing in microreactor flows is difficult due to the predominance of diffusion in laminar flows (LEE et al., 2016). Introducing obstacles like cylindrical pins into the microchannel can induce chaotic advection, thereby enhancing mixing, heat, and mass transfer (COSTA JUNIOR et al., 2020; SANTANA; JÚNIOR; TARANTO, 2015). While the flow around cylinders is well-studied on a macro scale (WILLIAMSON, 1996), it presents unique challenges on a micro scale, such as high blockage (the ratio between cylinder diameter and channel width) and low aspect ratio (the ratio between cylinder length and diameter) (CHEN et al., 2008). In micromixers, cylindrical obstacles face both lateral and vertical confinement, altering the flow dynamics. This confinement can inhibit vortex shedding in the flow (ZHANG et al., 2019). Nevertheless, vortex shedding can occur in these confined microchannels at sufficiently high Reynolds numbers ($\Re = U_o D/\nu$, where U_o is the mean free stream velocity in the channel, D is the cylinder diameter, and ν is the kinematic viscosity of the fluid), as shown by (ZHANG et al., 2019). This phenomenon results in periodic changes in the local flow direction. Flow vortices are highly effective at enhancing mixing due to their ability to stretch and fold the fluid streams (NGUYEN; WU, 2004).

In micro-confined cylinder flows, lateral and vertical confinements can be characterized using dimensionless parameters: $w^{\S} = W/D$ represents the lateral confinement, where W is the channel width and D is the cylinder diameter; $h^{\S} = H/D$ represents the vertical confinement, where H is the channel height.

The aim of this research is to study the behavior of two-phase flow through a capillary microreactor past a pair of cylindrical obstacles using the homogeneous flow model, where the two phases travel at equal velocities and mix well. In this model, the two phases are treated as if there is only one phase. Although this model does not allow for identification of the interface between the phases, it is possible to introduce a passive scalar representing concentration to evaluate the effect of obstacles in the microchannel section on the flow and, consequently, on the dispersion of this passive scalar along the flow.

This article is organized with an introduction to microchannel flow and the corresponding literature review, followed by the mathematical modeling used in this work, including the two-dimensional equations for fluid motion using the streamfunction-vorticity formulation and the transport equation of temperature and concentration. Next, the results section presents an important benchmark case fluid flow simulation to assess and compare the accuracy of the proposed method and eight simulations of microchannel flow to analyze the flow behavior past a pair of cylindrical pins. Finally, the article concludes with remarks in the conclusion section.

Methodology

To characterize the flow field, the Poisson equation, derived from the Navier-Stokes equations as outlined by (TEZDUYAR et al., 1990), was numerically solved using the finite element method with two-dimensional linear arbitrary quadrilateral elements. For the vorticity and species transport equation, the non-dimensional variables (with superscript §) in Eq.1 are defined by some reference parameters, that are the characteristic length D, characteristic velocity U_0, characteristic diffusion coefficient Di_0 and characteristic concentration of a chemical specie c_0.

$$t^{\S}=\frac{U_0 t}{D}, \quad x^{\S}=\frac{x}{D}, \quad y^{\S}=\frac{y}{D}, \quad v^{\S}=\frac{v}{U_0}, \quad Di^{\S}=\frac{Di}{Di_0}, \quad c^{\S}=\frac{c}{c_0} \tag{1}$$

Using the non-dimensional variables, the non-dimensional vorticity transport equation is defined as follows (dropping the § for simplicity of notation):

$$\frac{\partial \zeta_z}{\partial t}+v\cdot\nabla\zeta_z=\frac{1}{\Re}\nabla^2\zeta_z \tag{2}$$

where $\Re$ is the Reynolds number as commonly defined in the literature.

The Poisson equation for the non-dimensional streamfunction and the recovery of the velocity field are written, respectively, as follows (dropping the § for simplicity of notation):

$$\nabla^2\psi+\zeta_z=0, \quad v_x=\frac{\partial\psi}{\partial y}, \quad v_y=-\frac{\partial\psi}{\partial x} \tag{3}$$

Additionally, the non-dimensional species transport equation is defined as follows (dropping the § for simplicity of notation):

$$\frac{\partial c}{\partial t}+v\cdot\nabla c=\frac{1}{\Re Sc}\nabla^2 c \tag{4}$$

where $Sc=\nu/Di_0$ is the Schmidt number.

The numerical code, written in Python, has been carefully crafted using state-of-the-art techniques with the Finite Element Method to discretize the fluid and species equations (ANJOS; MANGIAVACCHI; THOME, 2020). The convective term was also treated with the Galerkin method. Although this term can cause instability at high Reynolds numbers, the simulations conducted in this research were at low Reynolds numbers, remaining within the laminar regime. The numerical algorithm is solved on an unstructured quadrilateral mesh generated by Gmsh (GEUZAINE; REMACLE, 2009), with refined zones near the regions of interest (adjacent to the channel and cylindrical pin walls). The 'lgmres' solver, from the 'scipy' library, was used to solve the linear systems resulting from the discretization of the vorticity and concentration transport equations, the streamfunction equation, and the velocity field computation (BAKER; DENNIS; JESSUP, 2006; VIRTANEN et al., 2020).

The mesh boundary conditions for the microchannel walls and the cylindrical pins were set to enforce the no-slip condition, constraining the velocity in both horizontal and vertical directions. At the inlet, a parabolic profile for the horizontal component of the velocity was applied, while the vertical component was set to zero. At the outlet, a zero-gradient boundary condition was set for the velocity, streamfunction, and concentration.

Results

Validation: Lid-Driven Cavity for moderate Reynolds number

In Fig.2, one can observe the numerical solution for the velocity field of an important benchmark in fluid dynamics namely Lid-Driven cavity flow. Good accuracy was found for this simulation (Fig.1) where the chosen parameters were $\Re=100$ with Δt intervals of 0,0014s, for 7000 iterations. The simulation's mesh used 2-dimensional linear quadrilateral elements. This simulation was realized using 10000 nodes and 10197 elements, with dimensions of 1m x 1m, in

1927s of computational time. This case was simulated using the 'SuperLU' solver (LI, 2005), on a computer with an $Intel$ $Core$ i7-4790 CPU @ 3.60 GHz.

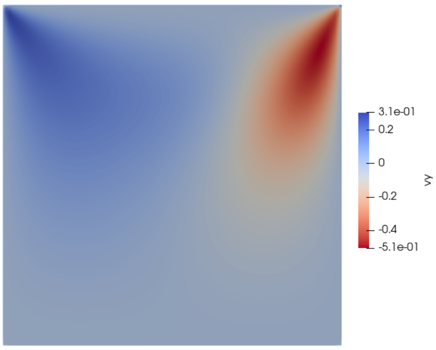

Figure 2: 2-dimension Lid-Driven cavity solution for vertical v_y velocities using the streamfunction-vorticity formulation.

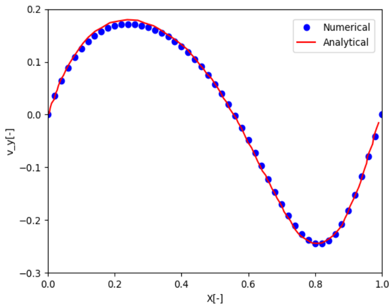

Figure 1: Comparison between numerical data and analytical velocity profile for the Lid-Driven cavity flow.

Despite the low Reynolds numbers, the current code is ready to simulate laminar flows with accuracy. The numerical results obtained for the Lid-Driven example have a maximum relative error of 6.3% when compared to its analytical solution (SHIH; TAN; HWANG, 1989).

Flow dynamics past confined microfluidic cylinders

Eight simulations were elaborated, using quadrilateral finite element meshes to reproduce a microchannel with a pair of cylindrical pins on its cross section. The boundary conditions and dimensions, relative to the pin diameter D , for the mesh utilized for the fluid flow simulations can be observed in Fig.3. The darker region on the centre of Fig.3 is due to the mesh refinement on the region near cylinders wall and where the vortex-shedding is expected to occur. To evaluate the interface between mixing fluids, at the inlet, a theoretical dye, with $Sc=1.0$, is inserted at the upper half of the channel. The longitudinal pitch ratio, L/D , (where L is the centre-to-centre longitudinal spacing), ranged from 2.5 to 6.5 , and the dimensionless cylinder diameter is $D=1$.

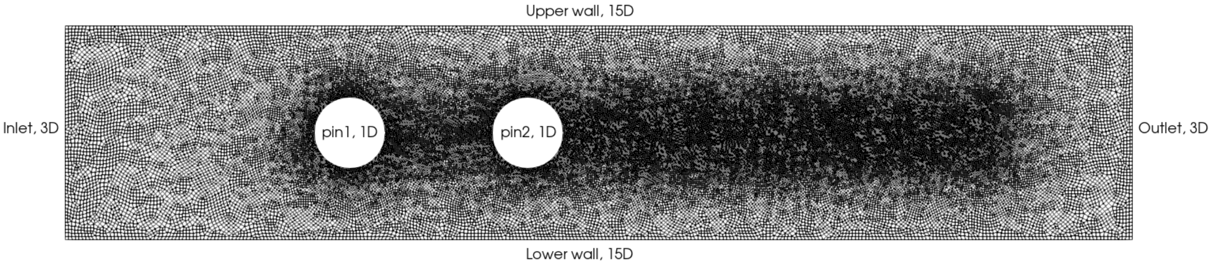

Figure 3: Detailed schematic diagram of microchannel simulations.

The information concerning the meshes and simulations' parameters can be consulted in Tab.1.

Table 1: Mesh information.

Mesh	Number of nodes	Number of elements	Physical time (s)	Computational time(s)	Time step (s)
L/D=2.5	51675	52196	45	43200	0.0005
L/D=3.5	49487	50008	45	38100	0.0005
L/D=4.5	48357	48878	45	39623	0.0005
L/D=6.5	54649	55170	45	46800	0.0005

Vorticity and concentration fields for $\Re=70$

Figures 4-11 present selected instantaneous vorticity fields (ζ_z) and concentration contours (c) for tandem flow configurations at $\Re$ equal to 70 , with L/D ratios ranging from 2.5 to 6.5 .

In the microchannel with an L/D ratio of 2.5 and 3.5 (Fig.4-7), the shear layers originating from the first pin reattach onto the second pin. Downstream of the second cylinder, the shear layers gradually converge towards the wake centerline instead of rolling up into vortices. This interaction between the shear layers and the neighboring walls generates vorticity with opposite signs. While there is always some positive vorticity at the upper wall and negative vorticity at the lower wall due to the boundary layers, the vorticity in these regions increases significantly when the shear layers from the cylinder form, starting from $x \approx -1$ and reaching a peak at $x \approx 3.5$, for $L/D = 2.5$, and $x \approx 5.0$, for $L/D = 3.5$ (where $x = 0$ on the first cylinder centre). Beyond this point, the vorticity magnitudes of all four shear layers are approximately equal.

For a L/D ratio of 4.5 (Fig.8,10), the shear layers originating from the first pin start to develop into vortices, and the resulting waviness propagates downstream to the wake of the second pin, causing vortex shedding in its near wake. This improves mixing on the region between cylinders and downstream the second one. When L/D is increased to 6.5 (Fig.9,11), the shear layers from the first pin develop without causing unsteadiness. A similar behavior is observed behind the second cylinder. The changeable effect of L/D on the occurrence of vortex shedding and the interaction between the wall-formed shear layers and those generated by the cylinder indicate that the wake dynamics are highly sensitive to the position of the second cylinder and the confinement of the channel.

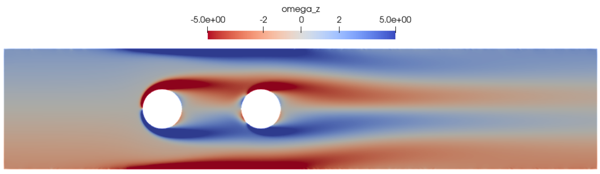

Figure 4: Vorticity contour, L/D=2.5, R=70.

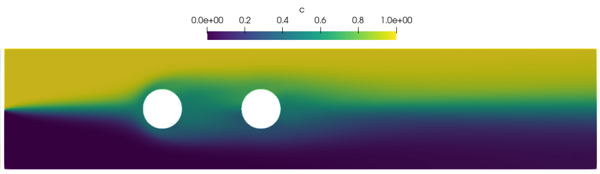

Figure 5: Concentration contour, L/D=2.5, R=70.

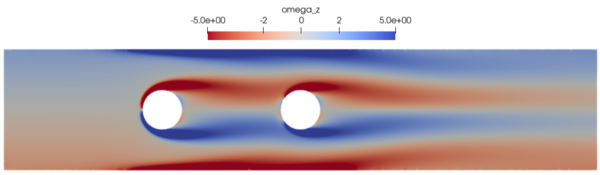

Figure 6: Vorticity contour, L/D=3.5, R=70.

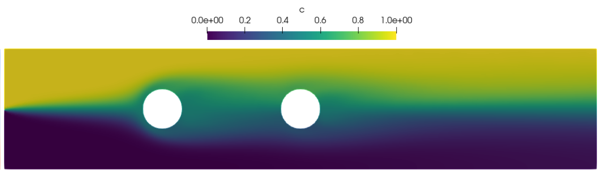

Figure 7: Concentration contour, L/D=3.5, R=70.

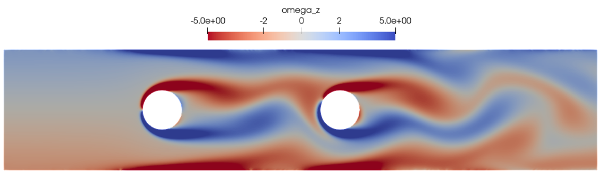

Figure 8: Vorticity contour, L/D=4.5, R=70.

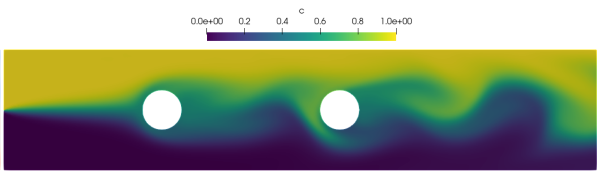

Figure 10: Concentration contour, L/D=4.5, R=70.

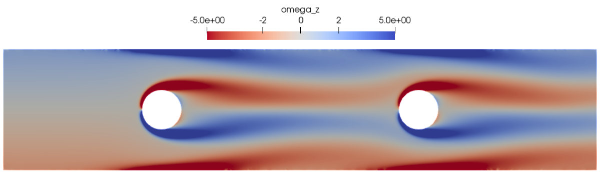

Figure 9: Vorticity contour, L/D=6.5, R=70.

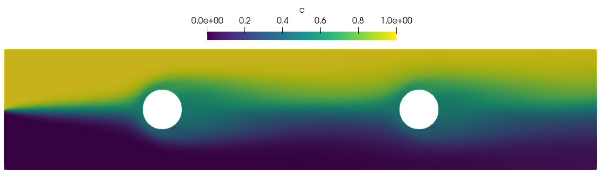

Figure 11: Concentration contour, L/D=6.5, R=70.

Vorticity and concentration fields for $\Re = 150$

As can be seen in Fig.12-19, the flow becomes more unstable when the $\Re$ is increased to 150 . In the microchannel with an L/D ratio of 2.5 and 3.5 (Fig.12-15), no vortex shedding is observed behind the first cylinder. The shear layers remain nearly parallel until they reattach to the second cylinder. Nevertheless, behind the second cylinder, one can observe the vortex-shedding after approximately $20\,s$ of physical time of simulation. This behavior is observed until the end of the simulation ($45\,s$ of physical time). On the region between the cylinders, mixing was still diffusion dominated, as it was for the lower $\Re$ simulations.

There is significantly greater mixing when the longitudinal pitch ratio is set to be $L/D=4.5$ and $L/D=6.5$. Fig.17 and 19 show that vortex shedding from the first pin results in greatly enhanced mixing between the fluid layers. The impingement of the shed vortices on the second pin leads to asymmetric vertical component flow in its wake and very effective mixing between the fluid layers, with the interface region (where $c\approx0.5$) extending across the entire width of the channel.

When compared to the results reported on the experimental work performed by (ZHANG et al., 2023) the behavior observed for the flow with $\Re=70$ and $\Re=150$ were more similar to Reynolds number of 150 and 300, respectively. This suggests that the lateral and vertical confinement on a microchannel impacts the $\Re$ from which the vortex-shedding can be observed. When only the lateral confinement is taken into account, as was the case of the present research, this decreased significantly.

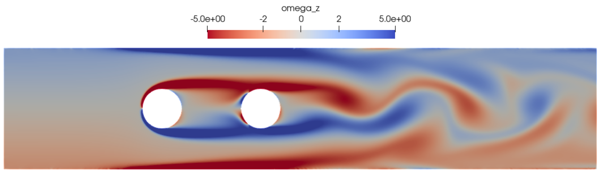

Figure 12: Vorticity contour, L/D=2.5, R=150.

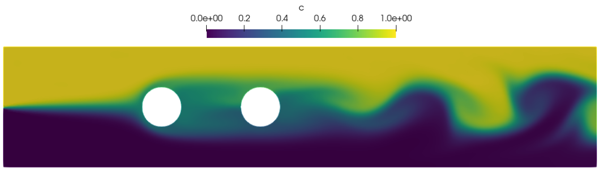

Figure 13: Concentration contour, L/D=2.5, R=150.

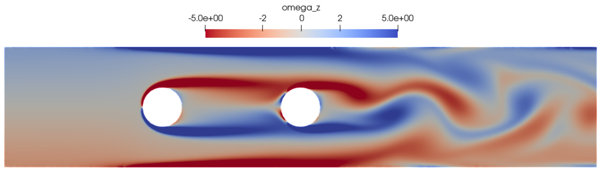

Figure 14: Vorticity contour, L/D=3.5$, R=150.

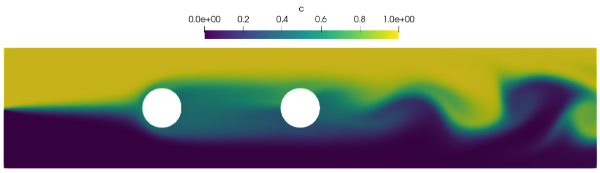

Figure 15: Concentration contour, L/D=3.5, R=150.

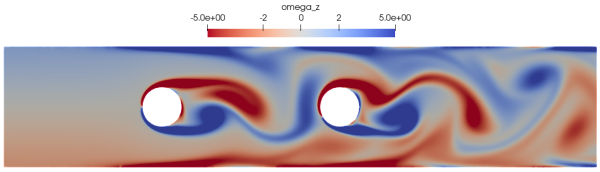

Figure 16: Vorticity contour, L/D=4.5, Re=150.

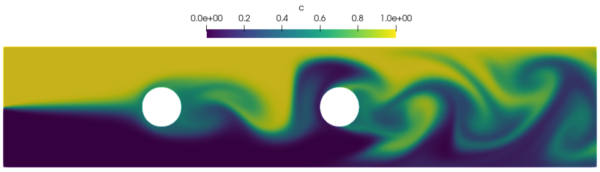

Figure 17: Concentration contour, L/D=4.5, R=150.

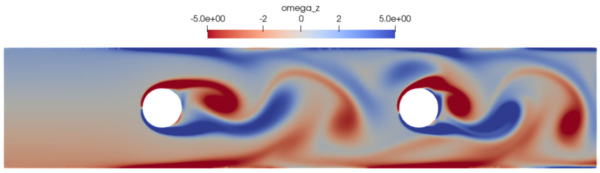

Figure 18: Vorticity contour, L/D=6.5, Re=150.

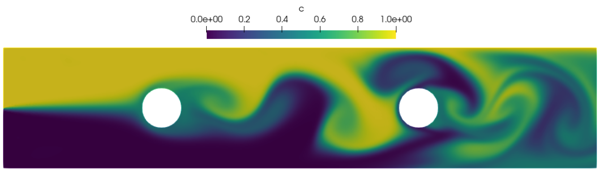

Figure 19: Concentration contour, L/D=6.5, Re=150.

Conclusion

Numerical simulations have been used to investigate the mixing of two fluid streams in microchannels featuring a pair of confined cylindrical obstacles (pins). A range of longitudinal pitch ratios were explored to analyze their impacts on the mixing dynamics. When the value of L/D was 2.5 and 3.5, the shear layers from the first cylinder attached to the second one, without vortex-shedding on the region between cylinders, regardless of Reynolds number. When L/D was equal to 4.5 and 6.5, the flow behavior on the region between cylinders was strongly affected by $\Re$. Vortex-shedding was observed on this region for both $\Re=70$ and $\Re=150$, with $L/D=4.5$. With $L/D=6.5$, vortex-shedding was only observed when $\Re=150$. Improved mixing was found for $L/D=4.5$ at $\Re=70$ and $\Re=150$, and for $L/D=6.5$ at $\Re=150$.

Limitations and Further Development

Cylindrical obstacles in micromixers experience both lateral and vertical confinement, which modifies the flow dynamics. This confinement can suppress vortex shedding in the flow. This effect was not observed in the simulations performed during this research. Which can be related to fact that the simulations are made for a 2-dimensional domain, i.e the third dimension is considered to be much higher than the other two dimensions. As a consequence, the velocity profile used in this research is also different from the one reported on the literature for microfluidic devices. This demands a much more detailed 3-dimensional simulation. We aim to consider such factors in future simulations and new results will be presented.

Acknowledgments

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