

NUMERICAL SIMULATION OF A MICROMIXER COMBINING MODIFIED TESLA AND RECTANGULAR OBSTACLE GEOMETRY

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ABSTRACT:

MICROREACTOR TECHNOLOGY GAINED ON ITS MOMENTUM THROUGH DEVELOPMENT OF DEDICATED MICROMANUFACTURING TECHNOLOGIES. ONE OF THE CRUCIAL COMPONENTS OF A MICROREACTOR IS A MICROMIXER. ITS FUNCTION IS TO MIX DIFFERENT REACTANTS FOR THE PURPOSE OF CHEMICAL SYNTHESIS OR ANALYSIS.

IN THIS PAPER TWO ESTABLISHED MICROMIXER DESIGNS, NAMELY OBSTACLE AND MODIFIED TESLA MICROMIXER, ARE NUMERICALLY INVESTIGATED AT REYNOLDS NUMBER OF 0.5. POSSIBLE SYNERGIES OF INCORPORATING BOTH GEOMETRIES IN A SINGLE DESIGN WERE ALSO INVESTIGATED. THE SIMULATIONS SHOW THAT OBSTACLE DESIGN BY ITSELF PERFORMS THE BEST IN REGARDS TO MIXING INDEX AND PRESSURE DROP. ON THE OTHER HAND COMBINED DESIGNS PERFORMED BETTER THAN MODIFIED TESLA DESIGN BY ITSELF. WE CONCLUDE THAT FURTHER STUDIES ON OBSTACLES LAYOUT WITHIN THE MODIFIED TESLA DESIGN ARE SENSIBLE IN ORDER TO FULLY EXPLOIT THE MIXING PRINCIPLES OF BOTH DESIGNS.

KEY WORDS: MICROREACTOR, MICROMIXER, TESLA DESIGN, MIXING, CFD

INTRODUCTION

Miniaturization of products and their components is a common trend in various fields. Advances in micro- and nano-manufacturing technologies enable integration of small components from various materials into microdevices⁶. The research field of microreactor technologies, commonly understood as miniaturized flow through systems, is also benefiting

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⁶ Madou, Marc J. 2002. *Fundamentals of Microfabrication: The Science of Miniaturization, Second Edition: The Science of Miniaturization*. 2nd ed. CRC Press; Altung, L, F Kimura, HN Hansen, and G Bissacco. 2003. "Micro Engineering." *Cirp Annals-Manufacturing Technology* 52 (2): 635–57

from micromanufacturing systems development. Main application fields of microreactor technology are chemical and bio-chemical synthesis and analysis⁷. Related terms to microreactor technology are microfluidics and laboratory on a chip (LOC). Microreactor's advantages compared to conventional scale reactors stem from high surface/volume (S/V) ratio on microscale which enhances many physical phenomena such as heat and mass transfer. Due to small dimensions of the microreactor geometries great process control can be established, very small volumes of reactants are needed, there is less energy consumption to maintain operating conditions, they take up smaller space and can be stacked up to enhance yield and many functionalities can be integrated on a single substrate.

Micromixers are one of the key functional components of the microreactor system⁸. Their purpose is to quickly mix two or more reactants. This task is not trivial on microscale due to dominant viscous forces which determine the laminar flow characteristics of the fluids. Passive micromixers, where no additional energy aside from inlet pressure is applied, tackle this difficulty with generally four different principles: lamination, injection, chaotic advection and implementation of a droplet setup⁹.

In this paper two chaotic micromixer, namely modified Tesla design (figure 1a) and obstacle design (figure 1b, 2), are considered. The modified Tesla micromixer (TM) design was originally presented by Hong et al¹⁰ and experimentally and numerically optimized in¹¹. The principle of mixing is based on Coanda effect. Coanda effect occurs at denoted (figure 2b) diffusor like geometry and splits the whole stream into two parts. The second part of the stream continues its path along the curved shaped channel at the end of which it collides with the first part. Due to present transverse component of fluid flow mixing occurs.

In obstacle micromixer (OM) design (figure 2) transvers fluid flow is generated by placing obstacles in the flow path¹². Placing obstacles inside the microchannel stirs the fluids creating lateral mass transport which enhances fluid mixing.

⁷ Cvjetko, Marina, Izidor Sabotin, Ivan Radoš, Joško Valentinčič, Tomislav Bosiljkov, and Mladen Brnčić. 2013. "A Comparative Study of Ultrasound-, Microwave-, and Microreactor-Assisted Imidazolium-Based Ionic Liquid Synthesis." *Green Processing and Synthesis* 2 (6): 579–90. doi:10.1515/gps-2013-0086

⁸ Hessel, V, H Lowe, and F Schonfeld. 2005. "Micromixers - a Review on Passive and Active Mixing Principles." *Chemical Engineering Science*, 2479–2501; Nguyen, Nam-Trung. 2008. *Micromixers: Fundamentals, Design, and Fabrication*. 1st ed. William Andrew

⁹ Sabotin, Izidor, Gianluca Tristo, Mihael Junkar, and Joško Valentinčič. 2012. "Two-Step Design Protocol for Patterned Groove Micromixers." *Chemical Engineering Research and Design*. Accessed October 30. doi:10.1016/j.cherd.2012.09.013

¹⁰ Hong, Chien-Chong, Jin-Woo Choi, and Chong H Ahn. 2004. "A Novel in-Plane Passive Microfluidic Mixer with Modified Tesla Structures." *Lab on a Chip* 4 (2): 109–13. doi:10.1039/b305892a

¹¹ Asgar, A, S Bhagat, and I Papautsky. 2008. "Enhancing Particle Dispersion in a Passive Planar Micromixer Using Rectangular Obstacles." *Journal of Micromechanics and Microengineering*; Hossain, S, MA Ansari, A Husain, and KY Kim. 2010. "Analysis and Optimization of a Micromixer with a Modified Tesla Structure." *Chemical Engineering Journal*, 305–14

¹² Asgar, A, S Bhagat, and I Papautsky. 2008. "Enhancing Particle Dispersion in a Passive Planar Micromixer Using Rectangular Obstacles." *Journal of Micromechanics and Microengineering*; Bhagat, Ali Asgar S., Erik T. K. Peterson, and Ian Papautsky. 2007. "A Passive Planar Micromixer with Obstructions for Mixing at Low Reynolds Numbers." *Journal of Micromechanics and Microengineering* 17 (5): 1017. doi:10.1088/0960-1317/17/5/023; Tseng, Li-Yu, An-Shik Yang, Chun-Ying Lee, and Chang-Yu Hsieh. 2011. "CFD-Based Optimization of a Diamond-Obstacles Inserted Micromixer with Boundary Protrusions." *Engineering Applications of Computational Fluid Mechanics* 5 (2): 210–22. doi:10.1080/19942060.2011.11015365

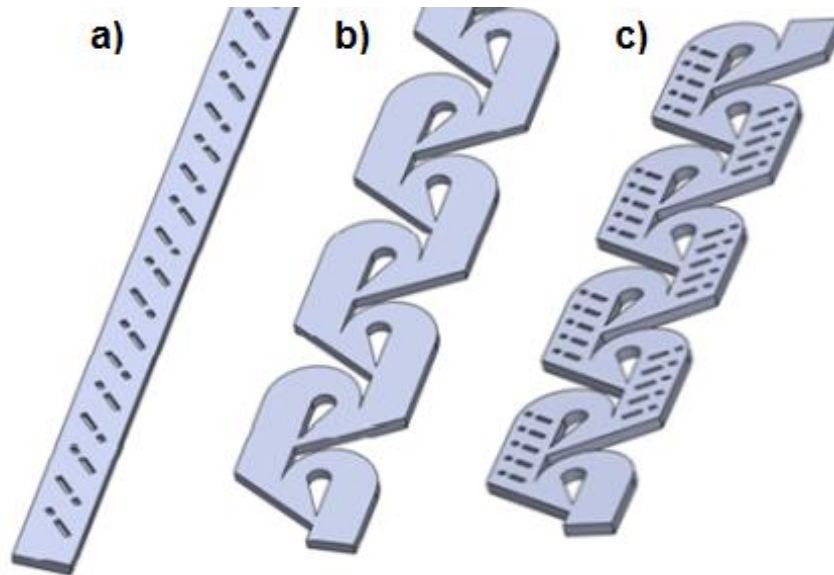


Figure 11. a) Obstacle micromixer design (OM), b) modified Tesla micromixer (TM) design and c) combined (TM+OM) design representation.

In this paper we present preliminary results of possible synergies between both designs combined into a single micromixer design (figure 1c). Both original designs are readily made by soft lithography¹³, thus combined design (TM+OM) does not represent additional difficulties to manufacture combined design. The investigation is based upon using CFD simulation software and coefficient of variance is used as the mixing criterion.

MATERIALS AND METHODS

Geometry of micromixers

The basic geometries of TM and OM design were adopted from Bhagat et al¹⁴ and are shown in figure 2. The main difference was in channel cross section where we used the width of the channel $w = 0.2$ mm and depth of the channel $d = 0.05$ mm whereas Bhagat et al used $w = 0.1$ mm at the same channel depth. All the other functional geometries were scaled to our width of the channel. The inlet length before the start of the first functional geometry was set to be 0.1 mm.

At combined TM+OM designs functional geometries of the particular design remained the same. This means that the basic geometry of the TM was taken in which we implemented obstacles as they were in the basic OM design. Since this is a preliminary research only three variations of the TM+OM design were investigated (figure 5):

1. insertion of obstacles before the diffuser – TM+OM var1;
2. insertion of obstacles after the diffuser – TM+OM var2;
3. insertion of obstacles on the both ends of the diffuser – TM+OM var3.

¹³ Bhagat, Ali Asgar S., Erik T. K. Peterson, and Ian Papautsky. 2007. "A Passive Planar Micromixer with Obstructions for Mixing at Low Reynolds Numbers." *Journal of Micromechanics and Microengineering* 17 (5): 1017. doi:10.1088/0960-1317/17/5/023; Asgar, A, S Bhagat, and I Papautsky. 2008. "Enhancing Particle Dispersion in a Passive Planar Micromixer Using Rectangular Obstacles." *Journal of Micromechanics and Microengineering*

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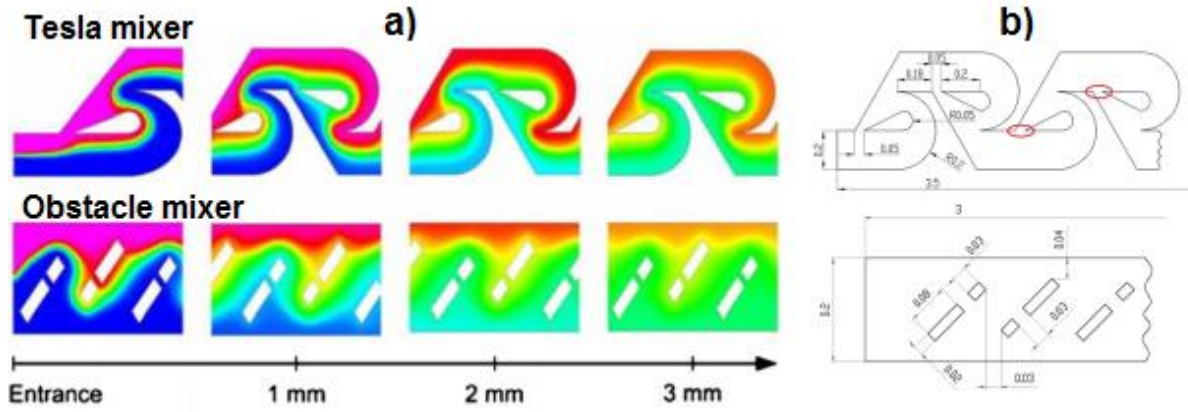


Figure 12. a) Presentation of modified Tesla micromixer and Obstacle micromixer mixing mechanism (Asghar, Bhagat, and Papautsky 2008). b) Applied geometry for TM and OM design.

Simulation tool

CFD modeling was performed using Comsol Multiphysics 4.1 which implements the finite element method (FEM) for numerical computation of physics governing equations. The numerical simulation was used to solve Navier-Stokes equations for incompressible fluid and convection-diffusion equations at steady state. The governing equations that describe the physical phenomena of mixing are as followed: Navier-Stokes (NS) equations,

$$\rho(\mathbf{v} \cdot \nabla)\mathbf{v} - \nabla \cdot \eta(\nabla\mathbf{v} + (\nabla\mathbf{v})^T) + \nabla p = 0, \quad (1)$$

$$\nabla \cdot \mathbf{v} = 0,$$

and convection-diffusion (CD) equations,

$$D\nabla^2 c - \mathbf{v} \cdot \nabla c = 0. \quad (2)$$

In equations 1 and 2 ρ denotes density [kg/m^3], \mathbf{v} is the velocity vector [m/s], η denotes viscosity [$\text{Pa}\cdot\text{s}$], p equals pressure [Pa], D denotes the diffusion coefficient [m^2/s] and c represents the concentration [mol/m^3].

Meshing of simulated geometries was implemented by the software applying free mesh elements that can easily adapt to the structure of the channel. The tetrahedral free meshing method was applied. Briefly, the computation of NS and CD equations was decoupled in order to reduce the computational power needed. Maximum mesh element size for the main channel of the mixer was set to $25 \mu\text{m}$ in order to reliably capture the fluid dynamics and diffusion of the species. Minimum element size was set to 0.002 mm , element growth rate to 1.3, mesh curvature factor to 0.3 and the resolution of the narrow region to 1. The laminar flow terms were discretized using P2+P1 scheme; second order elements for the velocity field and first order elements for pressure. For transport of diluted species quadratic discretization was employed.

The fluid properties were set to the ones of water at 20°C ; density $\rho = 998.2 \text{ kg/m}^3$ and viscosity $\eta = 1.002 \text{ mPa}\cdot\text{s}$. The diffusion coefficient of the solute was set to $D = 10^{-9} \text{ m}^2/\text{s}$ since this is a typical value for most ions in aqueous solution. The inlet flows were set as inflows with average linear fluid velocity $v = 0.0063 \text{ m/s}$ corresponding to Reynolds number $Re = 0.5$ and Peclet number $Pe = 630$.

The boundary condition for the outflow was set to 0 Pa (pressure, no viscous stress) and flow velocity at the walls to a no-slip condition ($v = 0 \text{ m/s}$). Fluid concentration of one half of the channel was set to 1 mol/m^3 (color coded red) and the other half to 0 mol/m^3 (color coded

blue) respectively. The post processing and visualizations of simulated results were obtained using the associated functions in Comsol and Matlab.

Coefficient of variance was used as a criterion of mixing efficiency which is commonly applied to static mixers¹⁵,

$$CoV_x = \frac{\sqrt{\frac{1}{N} \sum_{n=1}^N (c_{xn} - \bar{c})^2}}{\bar{c}} \quad (3)$$

where CoV_x denotes the coefficient of variance in yz -cut plane at channel length x , c_{xn} denotes the concentration at a point in the cut plane, N denotes the number of concentration points considered in the cut plane and \bar{c} denotes complete mixing, which is 0.5 mol/m^3 in our case. Concentration data at each cut plane was exported in a uniform grid with $2.5 \mu\text{m}$ spacing ($N = 1600$ points). A value of CoV_x closer to 0 corresponds to better mixing performance.

RESULTS AND DISCUSSION

Investigation of basic TM and OM design

Firstly, basic TM and OM designs were used for mixing simulations. Figure 3 qualitatively presents the performance of both designs. TM designs shows $CoV = 0.68$ at the end of the 4 mixer segments and the pressure drop of 265 Pa. OM designs performs better with the values of $CoV = 0.50$ at the end of the main channel and the pressure drop of 148 Pa. From the figure depiction of the cut plane at the end of both mixers (figure 3) it can be seen, that OM design was able to disperse both fluid components laterally whereas the TM design failed to do so.

Figure 4 shows the course of mixing for both simulated geometries along the x -axis. It is clearly visible, that OM propagates mixing faster than TM. At this stage it should be noted, that the literature reports modified Tesla design to be more effective at higher flow rates (Re above 5). Thus, low mixing performance of the TM is also a consequence of less suitable operating conditions defined by Re . This fact also suggests, that adding features to TM should be oriented in enhancing mixing for low Re regimes ($Re < 5$).

¹⁵ Kukuková, Alena, Benjamin Noël, Suzanne M. Kresta, and Joelle Aubin. 2008. "Impact of Sampling Method and Scale on the Measurement of Mixing and the Coefficient of Variance." *AIChE Journal* 54 (12): 3068–83. doi:10.1002/aic.11639

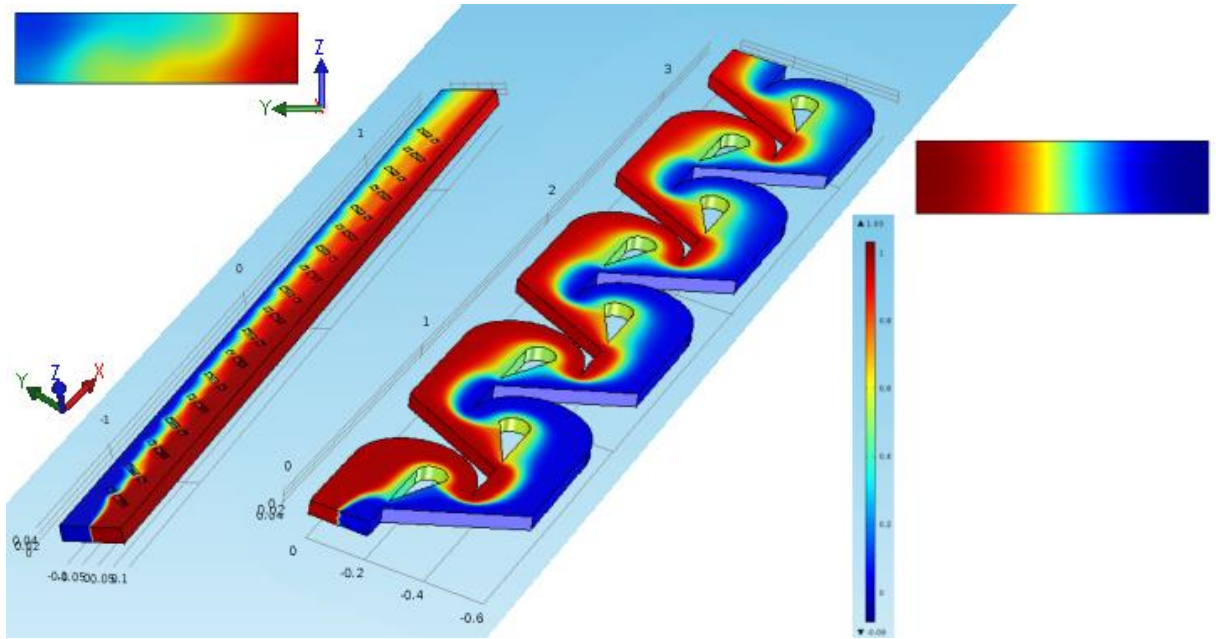


Figure 13. Simulation of basic TM and OM designs at $Re = 0.5$. Mixing along the channel length is presented. In the upper parts the exit cut-plane concentration profiles are presented for each design.

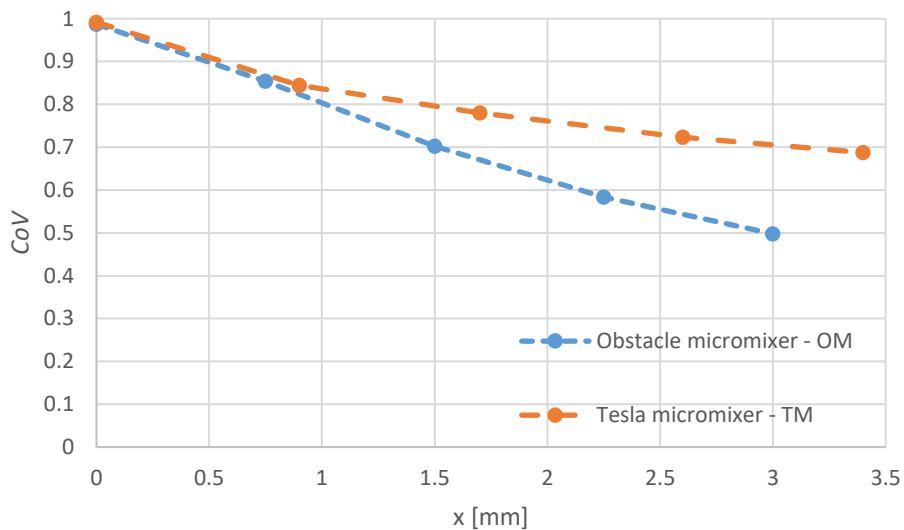


Figure 14. The course of mixing along the x -axis for OM and TM.

Investigation of combined TM+OM design

As mentioned under previous subsection three variations of the combined Tesla and obstacle design were investigated. The qualitative presentation of mixing performances can be observed on figure 5. It can be seen that only TM+OM var1 and TM+OM var3 enhance the mixing process due to the interface surface between both fluids is being trapped within the obstacles. The corresponding lateral displacement of the interface enhances mixing. As seen from the figure 5 mainly the obstacles placed before the diffusor influence mixing. Later observation is especially obvious at inspection of the TM+OM var2. Very little difference in mixing dynamics can be seen in comparison to pure TM design (figure 3).

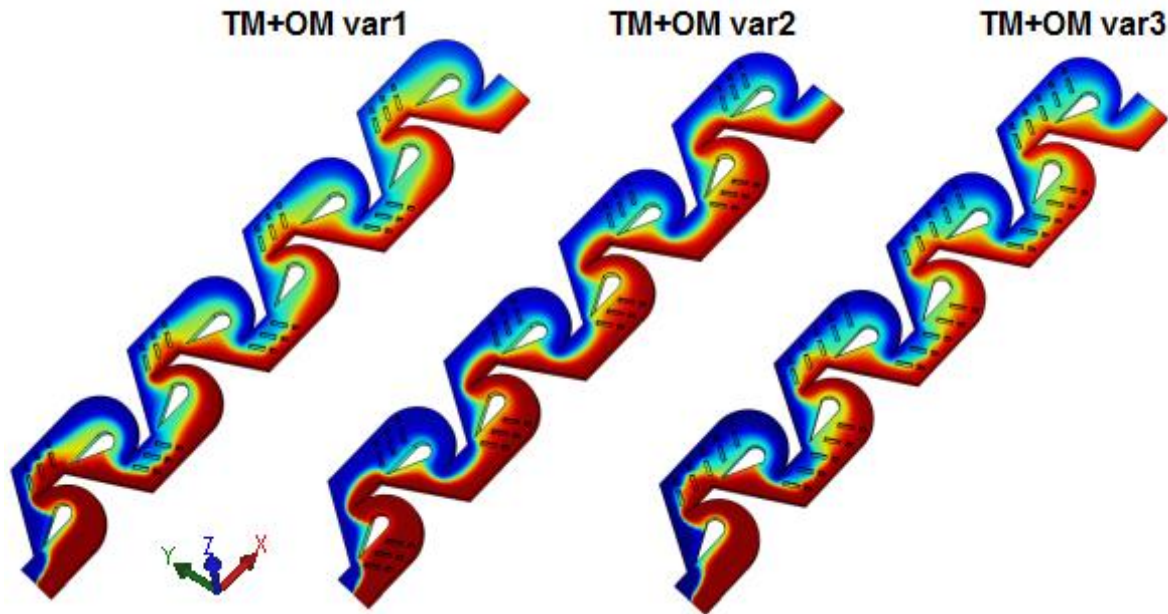


Figure 15. Mixing performance of combined TM and OM designs.

Quantitative evaluation of the hybrid designs is presented in figure 6. The best performing TM+OM designs are var1 and var3 with $CoV = 0.57$ (at pressure drop of 323 Pa) and $CoV = 0.59$ (at pressure drop of 329 Pa) respectively. Mentioned variation perform better then original modified Tesla design. On the other hand, from the comparison of mixing performance with original OM design it can be concluded that the OM outperforms all of the variation of combined designs. This is due to acting of obstacles along the whole channel length on lateral displacement of the fluid. Once the both fluids interface is trapped within the small opening between one obstacle segment, this further increases the surface of the interface in thus mixing.

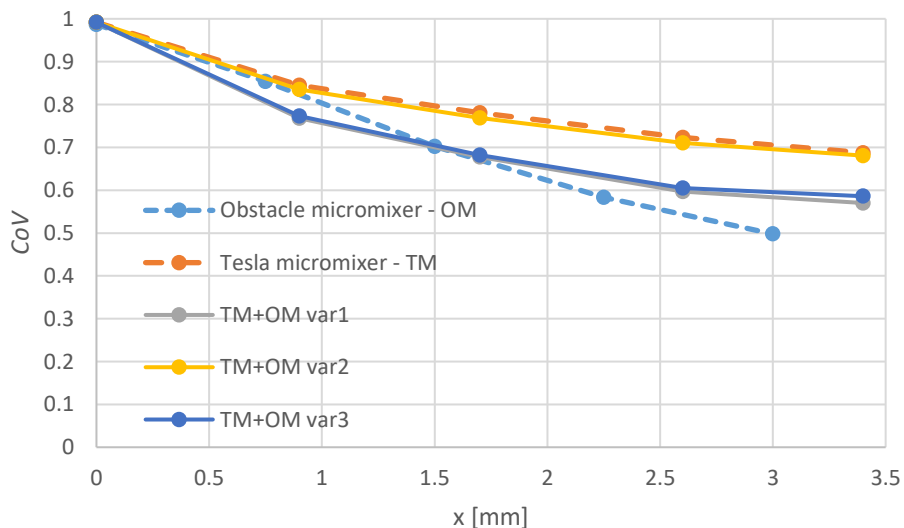


Figure 16. The course of mixing along the x -axis for all simulated designs.

The reason for smaller effectiveness of obstacles placed into the modified Tesla design is due to 1 phase of the fluid quickly escaping the obstacles through the diffuser and thus leaving the second phase almost exclusively flow around the curved part of the Tesla shaped segment. In order to enhance mixing the interface area must be enlarged and since mainly 1 phase is present at particular place of the Tesla segment this phenomenon is hindered.

CONCLUSION

In the presented paper possible synergies between obstacle and modified Tesla micromixer geometries were briefly investigated. The simulations show, that the enhancement of mixing by adding obstacles in modified Tesla design is not achieved successfully since the OM by itself performs better than any of the tested combined variations.

On the other hand, combined designs performed better than original TM. The results show, that the obstacles enhance mixing only if placed before the diffuser segment. This finding implicates, that there should be a more favorable obstacles configuration which would adapt the Tesla design mixing principle in more synergetic way. Thus, further studies on obstacle geometry in combination with modified Tesla design should be performed.

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