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A CFD study on different configurations of spacer-filled membrane distillation system using OpenFOAM

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KEY WORDS

Membrane distillation, Computational fluid dynamics, OpenFOAM, Spacer

ABSTRACT

Circular economy initiatives like the EC funded iWAYS project (grant agreement: 958274) promote the reuse of waste heat in industrial sites. This presents opportunities and challenges for technological adaptation. Membrane distillation (MD) is a thermally driven process for water treatment that can use waste heat. However, effectively treating complex industrial wastewater requires adapting MD units to achieve reliable and efficient performance. Filament spacers within the MD units play a key role in structural maintenance and flow mixing. CFD simulations can help to characterize filament spacer configuration impacts on the hydrodynamic of feed and permeate channels, which affects both trans-membrane temperature gradient and membrane fouling control. Here, we performed a CFD study on a direct contact membrane distillation (DCMD) sub-unit with the goal of evaluating impact on robustness and performance of a set of designed filament spacer configurations. The modeled membrane distillation system has an overall length of 200 mm, width of 10 mm and height of 4.1 mm, containing two layers of filaments in each of the feed and permeate channels. The diameter of the filaments was 1 mm, and they had a 45° degree angle to the flow direction in the channels. Variations of this standard filament configuration were also tested and simulated to optimize their mixing performance. The numerical simulations to approximate in a 3D solution of Navier-stokes equations for steady state conditions were performed using OpenFOAM code. The computational domains were meshed using OpenFOAM snappyHexMesh utility, and finite-volume based simulation relying on the chtMultiRegionFoam solver was executed in parallel over 40 CPU cores. Comparing the CFD analysis of different filaments' configurations lead to an assessment of an improved spacer structure. The selected configuration is to be 3D printed for laboratory-scale experimental confirmation of the validity of the CFD model and the optimal configuration finding.

1. INTRODUCTION

Membrane separation technology is considered one of the efficient ways of wastewater treatment due to its smaller footprint and higher energy efficiency compared to other technologies [1], [2]. In Membrane distillation (MD) systems, the driving force is the partial pressure difference of water vapor across membrane pore caused by the temperature difference, therefore they do not show drawbacks including the osmotic-pressure constraint, especially for super saline wastewaters [3]. In MD systems the feed and permeate are in contact with a layer of hydrophobic membrane which repels the aqueous solution from entering the pores of the membrane [4].

There are different forms of MD configurations, but the most studied one is DCMD (Direct Contact Membrane Distillation) in which feed and permeate are in touch with the membrane [1]. DCMD has already been used for treatment of industrial wastewater in textile, radioactive, pharmaceutical and rubber industrial context, and the results revealed that this technology can be an appropriate substitute or complement for conventional wastewater treatment methods [5]. However, constraints such as temperature/concentration polarization effects, which will lead to flux decline and membrane fouling/wetting [6] are limiting this technology implementation at broad operational levels. Therefore, the essence of addressing each one of these drawbacks for using the MD system on an industrial scale is inevitable.

The use of spacers in the feed and permeate channels has been deemed to promote mixing and enhance the mass and heat transfer, with the aim of reducing concentration and temperature polarization [7]. Many studies have investigated the use of spacers for improving the performance of the MD system. For instance, in Tan et al.'s study [8], the energy efficiency in DCMD system was investigated using CFD simulations and performing experiments, while different metallic spacers with different thermal conductivities were installed in the system. El Kadi's research group in 2020, conducted a CFD study on membrane distillation process to evaluate the performance of a spacer-filled module in terms of temperature profiles, heat and mass flux, thermal efficiency, and temperature polarization coefficient (TPC) [9]. In another study, the effect of various factors such as filament orientation and inlet velocity in a spacer-filled channel has been investigated by 3D CFD simulations in MD modules [10]. In 2013, Al-Sharif et al., using CFD simulation by OpenFOAM software, studied the effect of different geometries of the spacers on the DCMD performance, especially the fluid dynamics and temperature profiles [11]. Mojab et al., [12],

conducted a mixed experimental and numerical study for investigating the hydrodynamic conditions of the flow in a spiral-wound membrane channel filled with spacers. In this work, two sets of parallel spacers were placed with 45° angle with respect to the flow direction, and the flow characteristics within a range of different Re numbers were studied. Anqi's research group in 2020 [13] studied how adding filaments in the feed channel in a vacuum membrane distillation (VMD) system can increase momentum mixing, and therefore the overall performance of VMD systems. So, they developed 3D transient CFD simulations for the fixed membrane properties while changing the flow properties. Their results showed that addition of filaments is highly recommended because of the great effects it has on the water permeate rate [13].

Based on the previous studies, the addition of spacers in the MD module can improve the mixing process which will lead to lower concentration and temperature polarization. Hence, the objective of this study is to test different novel geometries and configurations of the spacers to decrease the temperature polarization which will also lead to less fouling and wetting.

2. MODELLING PROCEDURE

In this work, CFD simulations of three different spacers' configurations have been developed. The overall procedure of CFD simulation for numerical solution is presented in Figure. 1. First a 3D geometry of the desired configuration is prepared using Salome software [14]. The generated geometry file will be exported to the OpenFOAM [15] to create the mesh, and then after selecting the suitable solver and defining boundary conditions and physical properties, the numerical calculation will be performed, and finally the case will be ready for post processing using Paraview [16].

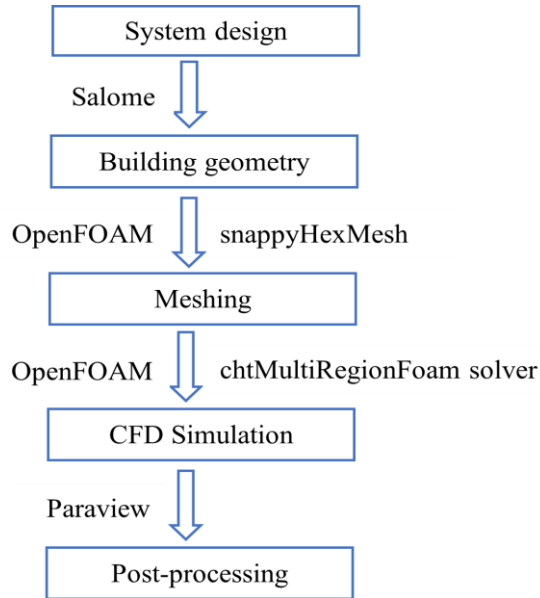


Figure. 1: Overall flowchart of the CFD procedure for our numerical simulations.

2.1. Mathematical Modeling

To study the thermal and velocity distributions in the system, a mathematical 3D model was developed using OpenFoam. A suitable solver, in this case chtMultiRegionFoam [17], that can solve heat transfer problems in multi region cases, is used for simulation. However, mass transfer phenomenon in membrane is disregarded here, since it will not have an impact on hydrodynamic behavior of the MD system. Table. 1 shows the initial boundary conditions of momentum and energy transport for feed and permeate channels. The properties of the feed and the permeate channels are defined as fluid, and membrane is defined as a porous solid. To reduce the computational cost, following simplifying assumptions have been implemented:

1. The operation is on steady-state mode, and the flow for feed and permeate channel is considered laminar.
2. No chemical reaction is taking place in the system.

The incompressible fluid flow in both channels of the MD system is governed using continuity and Navier-Stokes equation:

$$\nabla(\mathcal{J}_f \mathbf{U}) = 0 \quad (1)$$

$$\mathcal{J}_f \frac{D\mathbf{U}}{Dt} = -\nabla P + \mu_f \nabla^2 \mathbf{U} + \mathcal{J}_f \mathbf{g} \quad (2)$$

And for the heat transfer in both channels convective-diffusive equation is used [18]:

$$\rho_f C_p \frac{DT}{Dt} = \nabla(k\nabla T) \quad (3)$$

The spacer performance is also studied in terms of temperature polarization index ϕ . The definition used here is:

$$\phi = \frac{T_h - T_c}{T_{hm} - T_{cm}} \quad (4)$$

In Eq. (4) T_h and T_c are input temperatures of feed and permeate flows respectively, and T_{hm} and T_{cm} are the temperatures at the membrane surface on hot and cold sides respectively.

Table. 1: Initial boundary conditions for the numerical simulation

Parameters	Value
Inlet temperature in feed channel, °k	333
Inlet temperature in permeate channel, °k	293
Inlet velocity in feed and permeate channel, m/s	0.05

The simulations were run in parallel, using 40 cores in cluster. The obtained simulation time in such a configuration was about eight hours.

2.2. Spacers' Configuration and Mesh Generation

A schematic of different membrane distillation modules with different spacers' orientations has been presented in Figure. 2. The details of each case are: (a) *Standard case*: two rows of cylindrical filaments with a 45 degree to the entering flow are placed in each channel. For the case (b), *Cylindrical case*, there are three rows of cylindrical filaments that the filaments on the upper and lower parts of the channels are placed with a 45 degree to the entering flow while the middle row of filaments is perpendicular to the entering flow. And finally for the last case (c), *Triangular case*, there are three rows of filaments like the Cylindrical case, however, the middle row has a triangle shape instead of cylinder shape. In all the cases, the hot flow runs in the bottom channel along the x direction, and the cold flow runs on the upper channel and has a counter-current flow to the hot flow. The overall parameters and dimensions of the MD system is presented in Table. 2. Also, specific dimensions of the spacers in different configurations are described in Table. 3.

Table. 2: Overall geometric parameters and dimensions of the MD system. Dimensions are in m.

Parameter	Value
Block length	0.2
Block width	0.01
Block height	0.0041
Hot channel height	0.002
Cold channel height	0.002
Membrane thickness	0.0001
Membrane material	PTFE
Membrane porosity	0.8

Table. 3: Geometric parameters and dimensions of the spacers in different configurations. Dimensions are in m.

Configuration	Angle	Diameter/ Triangle base	Spacing	Quantity
(a) Standard	45°, -45°	0.001, 0.001	0.01	11, 11
(b) Cylindrical	45°, 90°, 45°	0.0005, 0.001, 0.0005	0.01, 0.0071, 0.01	11, 21, 11
(c) Triangular	45°, 90°, -45°	0.0005, 0.001, 0.0005	0.01, 0.0071, 0.01	11, 21, 11

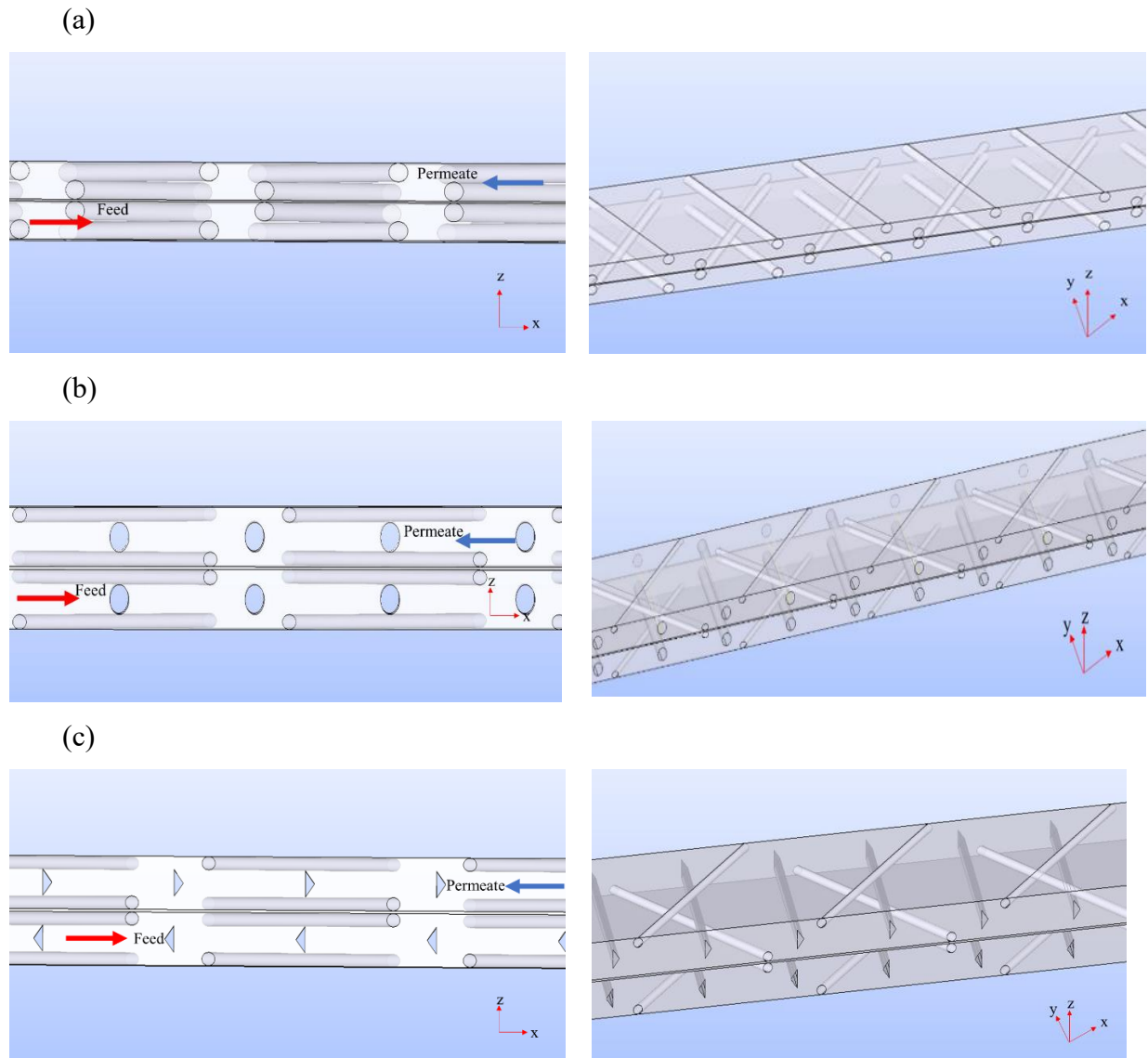


Figure. 2: schematic of different membrane distillation modules with different spacers' orientations (a) Standard case, (b) Cylindrical case, (c) Triangular case

After finalizing the 3D geometries of the desired configurations, the STL files (Salome software geometry file extension) of each configuration were exported to OpenFOAM for mesh generation using snappyHexMesh tool. SnappyHexMesh is an implemented meshing tool in OpenFOAM that its base mesh comes from the blockMesh tool and creates high-quality hex-dominant mesh for improving numerical accuracy. The number of generated computational cells for all the cases was around 3.5 million hexahedra cells and around 245000 polyhedral cells. The

meshed computational domain of the 3D model for each configuration has been represented in Figure. 3.

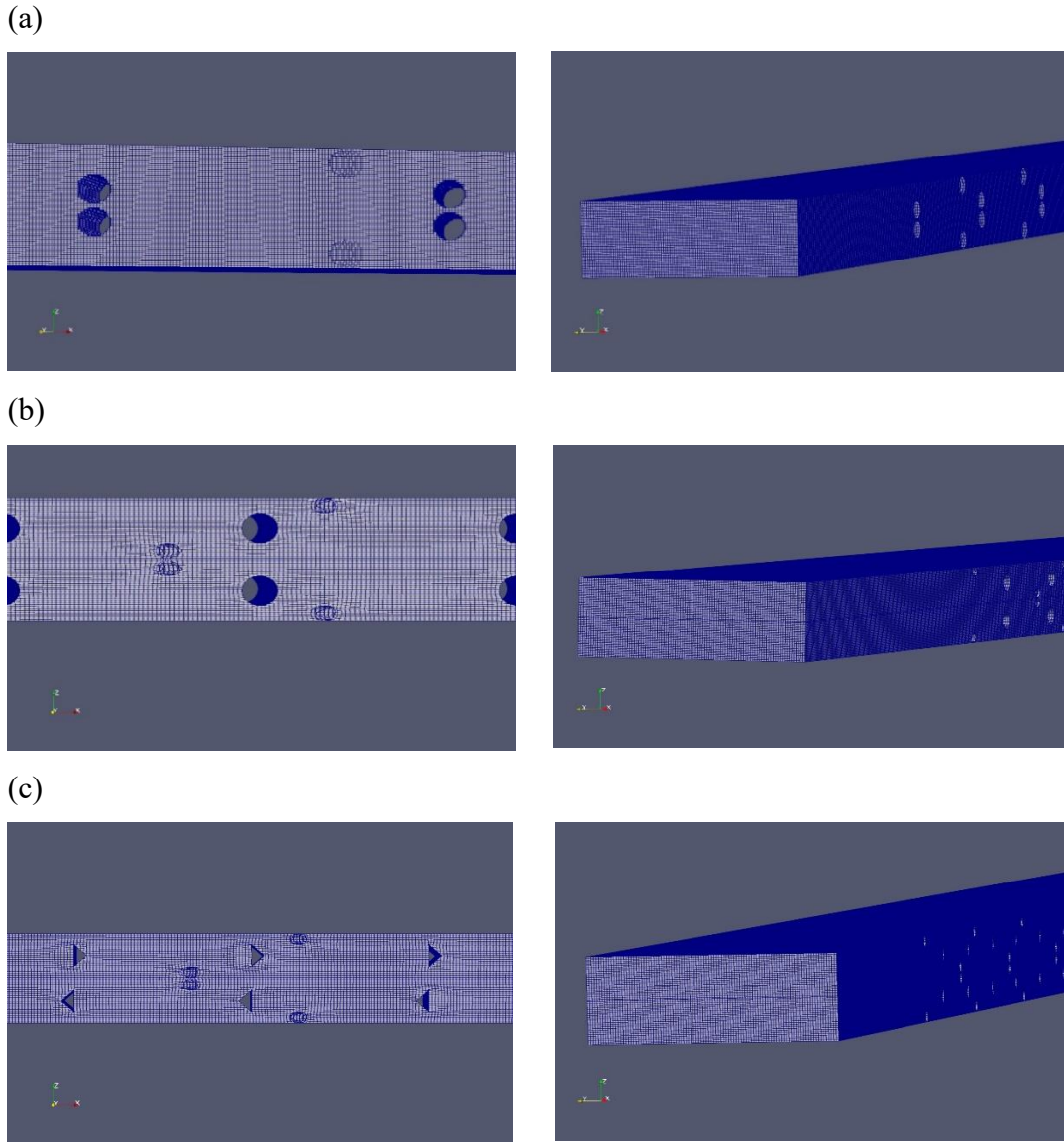


Figure. 3: 3D meshed computational domain constructed by snappyHexMesh for configurations (a) Standard case, (b) Cylindrical case, (c) Triangular case

3. RESULTS AND DISCUSSION

The overall thermal behavior of feed and permeate flows in each channel is studied to compare the system for the three feed-spacer configurations. Figure. 4 shows the thermal distribution in both channels along the x direction. These longitudinal thermal profiles data have been extracted at two different locations in each channel of the MD system: (i) at 50 μm from the surface of the

membrane, (ii) exactly in the middle of each channel. As shown in the figure. 4, for feed channel there is a temperature decrease along the x direction, however for the area close to the membrane this decrease is greater than the one in the middle of the channel which is due to its contact with the cold channel. For the permeate channel, as the flow passes through the channel along the x direction, the temperature gradually increases from 293°k to 302°k for the longitudinal thermal profile at 50 μm from the surface of the membrane, while for the middle of the channel the temperature only increases from 293°k to 295.5°k, showing logically a lesser longitudinal thermal gradient with an increased distance between permeate channel and membrane surface in touch with hot flow of feed.

Comparing the obtained results for the thermal behavior in channels for all the configurations shows that regardless of the spacers' configuration, all the cases have almost the same thermal behavior along x direction in both channels.

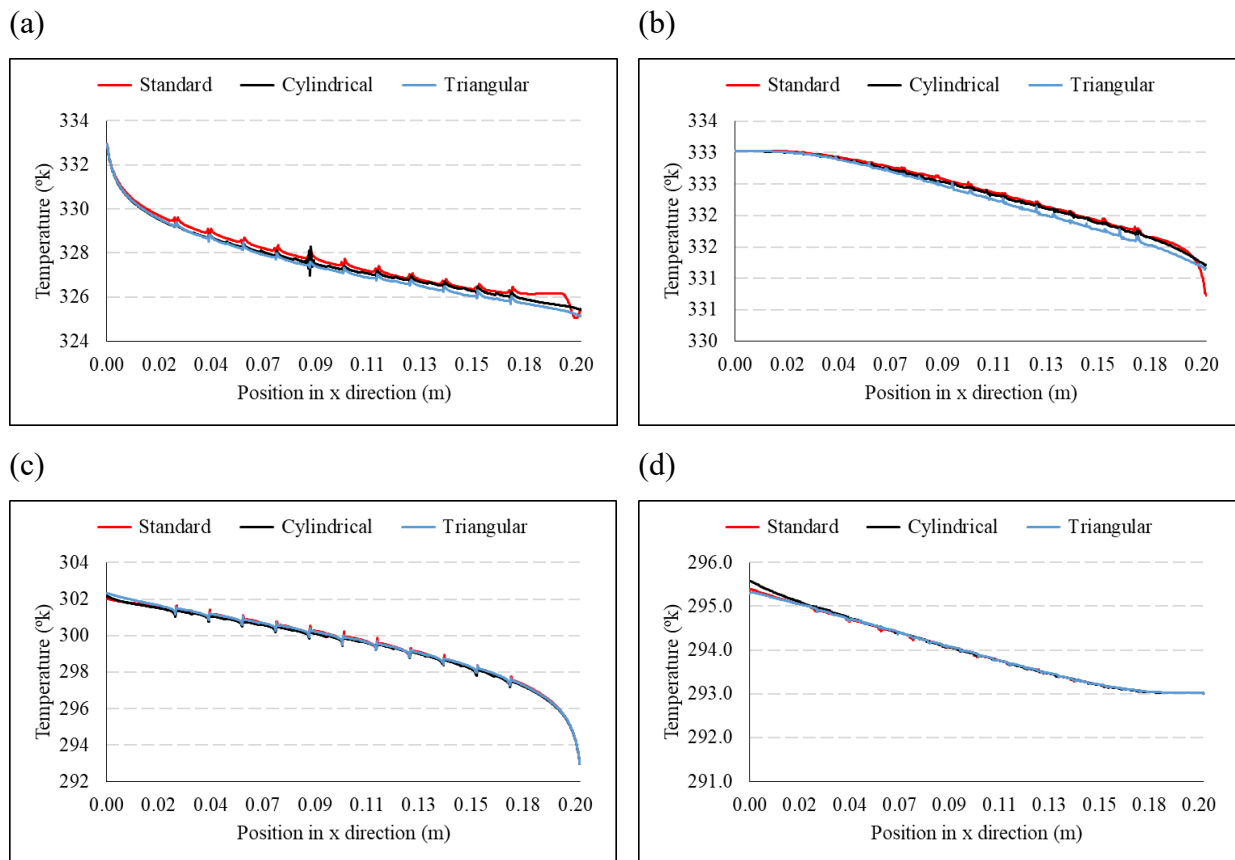


Figure. 4: Thermal distribution along x direction, near the membrane in feed channel (a), in the middle of the feed channel (b), near the membrane in permeate channel (c), in the middle of the permeate channel (d)

Analyzing U_z vertical component factor has been done to investigate the turbulence near the surface of the membrane in both channels. Figure 5. shows the obtained results with 50 μm distance from the membrane in both channels.

For the Standard case in both channels there are eleven large peaks which represent the turbulence of the flow around the intersection of two rows of eleven filaments in each channel. While for the Cylindrical and Triangular cases, ten smaller peaks are also represented which is due to the presence of third row of filaments in these cases. The higher turbulence in areas close to the membrane can signify promoted mixing which will enhance heat transfer and thus reducing thermal and concentration polarization. Figure. 5 also reveals that the extra peaks generated for the Cylindrical and Triangular cases are quite bigger for the feed channel compared to the permeate channel which is related to higher temperature of the fluid in the feed channel. In other words, fluid with higher temperature in the feed channel has lower viscosity which will result in relatively higher recirculation and turbulence in this channel [19].

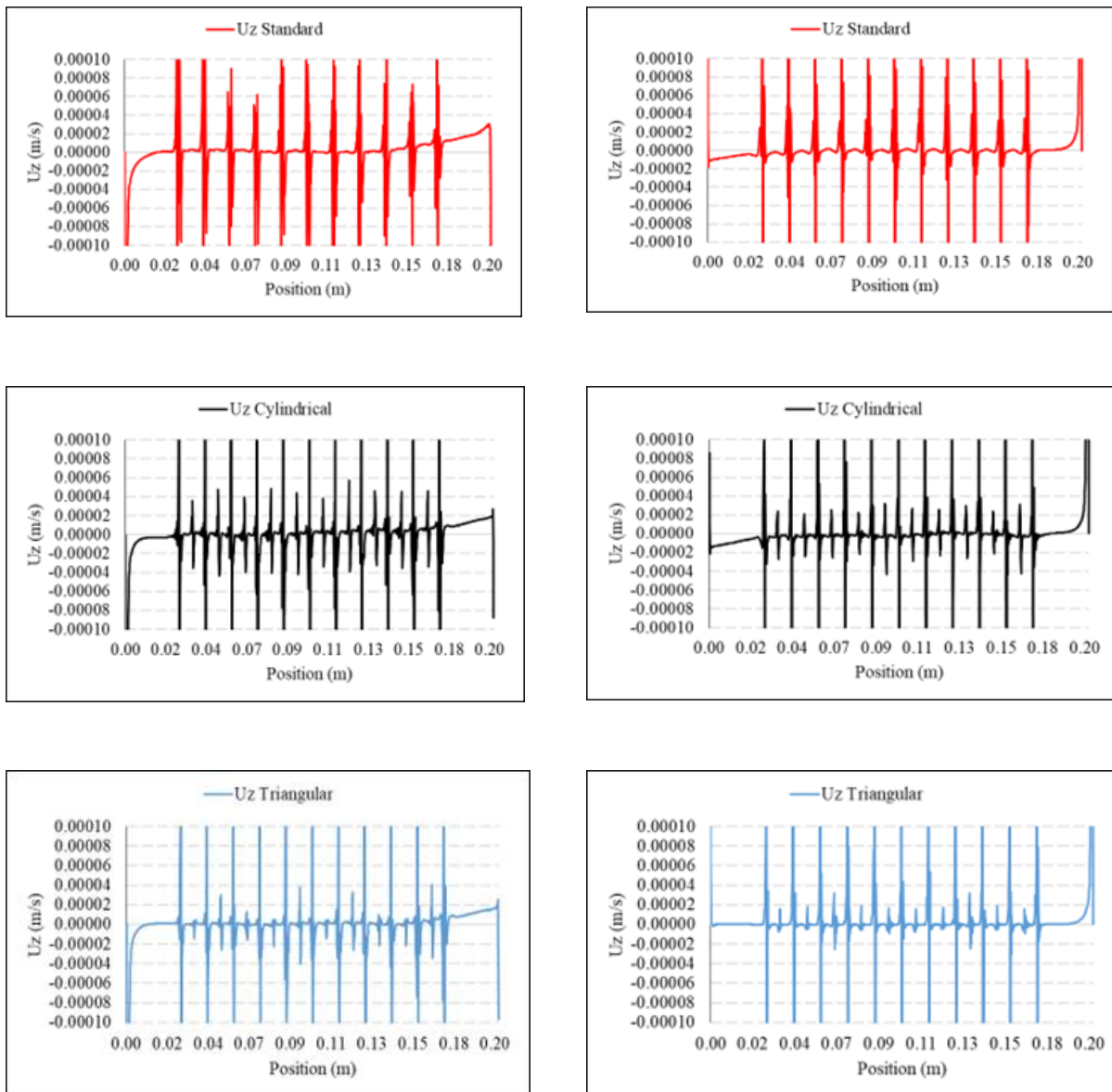


Figure. 5: U_z velocity component distribution near the membrane in feed channel (left), and permeate channel (right)

Results of temperature polarization index for each configuration in the x direction are presented in Figure. 6. Overall no big difference is observed for the three configurations, however standard case shows relatively lower temperature polarization comparing to the others, which may be due to the bigger recirculation regions created around the filaments in touch with membrane surface. The presence of filaments in MD systems creates recirculation regions which boosts the

heat and momentum transfer in those areas. However, it can also generate stagnant zones which increases temperature polarization that results in lower driving force for heat transfer [20].

For the standard case as it is shown in Figure. 2, the diameter of the filaments that are in touch with the membrane are two times bigger than that of the Cylindrical and Triangular cases. Therefore, the presence of bigger filaments can create larger recirculation regions which will decrease the temperature polarization index. While for the Cylindrical and Triangular cases, due to the presence of smaller filaments in touch with the membrane surface, the recirculation effect is not as great as for the Standard case and therefore the stagnant zones created around the filaments had higher negative impact regarding the temperature polarization phenomenon.

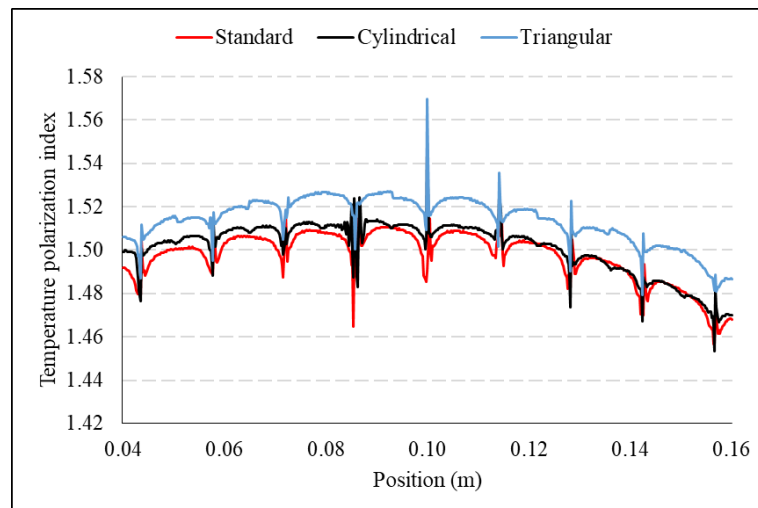


Figure. 6: Thermal polarization index for all the cases in x direction

4. CONCLUSIONS AND FUTURE WORK

The impact of three different configurations of spacers in the MD system has been studied in this work. The obtained results from this study show that the addition of third row of the filaments in MD modules increases the turbulence near the membrane which results in enhanced mixing and therefore an improved heat transfer. However, regarding the temperature polarization index, no big difference was observed among all the cases, although the Standard case showed slightly better performance due to the creation of larger recirculation regions in the area near the membrane.

Based on the obtained results, there was an improvement in generating more turbulence in areas in touch with membrane surface but still regarding the temperature polarization index, more

detailed investigation such as particle tracking technique is required to have a better understanding of the impact of different spacers' configuration on MD system performance.

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