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STUDY OF THE FLUID DYNAMIC BEHAVIOR OF THE DESALINATION PROCESS BY REVERSE OSMOSIS FOR DIFFERENT SPACER GEOMETRIES

Gilsomaro Barbosa de Melo Silva
Francisco Samuel Chaves
Diego David Silva Diniz
Jackson de Brito Simões
Federal Rural University of the Semi-Arid (UFERSA), BR 233, km 01, Sítio Esperança II, Caraúbas - RN
gilsomaro.silva@alunos.ufersa.edu.br, samuel_tab_1996@hotmail.com, diego.diniz@ufersa.edu.br, jackson.simoes@ufersa.edu.br

Abstract. *Water scarcity is a problem that has affected humanity for decades and, in recent years, has been getting worse, even more so with global warming, population growth, and droughts. Therefore, desalination processes began to be considered essential alternatives for producing drinking water worldwide. For this, several technologies are used for the desalination of brackish water; among these techniques, desalination by membrane separation processes via reverse osmosis (RO) stands out, a technology promising, considering that it is a simple process and presents low investment. However, the disadvantage that there is in its use is the sensitivity of the membrane to fouling. In this context, the objective of this work was to define a computational model capable of understanding the behavior of the reverse osmosis process. The mathematical model used for the simulations was based on mass conservation equations, movement, species transport, and Spiegler and Kedem's model. All simulations were performed using the ANSYS FLUENT 15.0 software and ICEM CFD to create the geometry and the mesh. The simulation results showed a good representation of the transfer phenomena involved in the reverse osmosis separation process; moreover, these results enabled a detailed analysis of the behavior of a fluid under the effects of turbulence promoters in the flow channel to be permeated. Finally, when analyzing these parameters in the geometries studied, it was observed that the spacers of the circular type had better process performances.*

Keywords: *Computational modeling, Desalination, Turbulence promoters.*

1. INTRODUCTION

The scarcity of water is a problem that has affected humanity for decades and, in recent years, has been getting worse with global warming, population growth, and record droughts, so that desalination processes began to be seen as essential alternatives for the production of drinking water, with the mastery of technologies of desalination, incredibly reverse osmosis, the potential exploitation of groundwater for the human consumption. The desalination process involves removing excess mineral salts, impurities, and other microorganisms found in brackish water to obtain drinking water.

Reverse osmosis is an operation in which the solvent is separated from the solution by passing it through a semipermeable membrane developed to retain salts and solutes with low molecular weights. In the osmosis process, the solvent flows through the membrane from a solution of low concentration to a more concentrated one until the elevation of static pressure ("osmotic pressure") on the side of the concentrate prevents flow. In reverse osmosis, the direction of water flow is reversed when, in the process and over the more concentrated solution, a pressure greater than the osmotic pressure is applied. In this way, water of low saline concentration moves into a saline solution. However, the downside in the use of this process of desalination by reverse osmosis is related to the useful life of the membranes semipermeable in the equipment; this disadvantage entails, throughout the process, low permeate flow rate and/or high passage of solute, thus affecting the productivity of the system and consequently reducing the useful life of the equipment.

To minimize these negative effects and increase the permeate flux, spacers promote turbulence in the feed stream and decrease the concentration layer on the membrane. In addition to increasing the permeable flow, these spacers also increase the pressure drop and, consequently, the energy used.

Because of the above, the main objective of this work is to build computational modeling capable of predicting the desalination process via reverse osmosis, using the conservation equations of mass, momentum linear, and species transport and, thus, analyze the influences of different spacer geometries on the desalination process.

2. THEORETICAL REFERENCE

2.1 Desalination

The desalination process treats brackish water, promoting the removal of dissolved minerals.

Among the various current desalination techniques, the one that has stood out the most industrially is the membrane separation process, which is superior in producing water capacity. The separation processes by membranes have shown rapid growth due to their requirements for high energy efficiency, easy maintenance, lower area occupation, quick initiation, and good cost-effectiveness, showing an influence on cost reduction global desalination rates over the last decade (Bahar, Hawlader, 2013; Werber; Deshmukh; Elimelech, 2016).

However, there are some limitations during this process, and these are linked to concentration polarization and formation of fouling., which lead to the reduction of permeate flux, increase in operating pressure, selectivity inadequate, shorter membrane life, and increased operating costs, also reducing the useful life of the equipment (Diniz, 2021).

About membrane technologies, Younos and Tulou (2005) refer to the following methods: Electrodialysis and reverse osmosis.

The electrodialysis process is an electrochemical process based on separating ions from solutions with different salinities. These ions are transferred across membranes from a less concentrated solution to a more concentrated one by applying a direct electric current. This process consists of moving salt water through electrically charged membranes, retaining salt ions dissolved in water, and allowing the extraction of fresh water (Jamaluddin et al., 1995; Rowe et al., 1995; Solt, 1971).

2.2 Osmosis and Reverse Osmosis

Osmosis is a naturally occurring physical-chemical phenomenon when two liquids with different levels of concentration of salt in solution are separated by a semipermeable membrane (Moura et al.). During this process, the solvent from the more dilute liquid naturally diffuses through the membrane towards the more concentrated one. O The process continues until it reaches an equilibrium point when the columns of the most concentrated and dilute solution become placed one higher than the other. (Moura et al., 2008). Reverse osmosis, on the other hand, is the reversal of this natural flow. Water from the salt solution is forced through the membrane in the opposite direction by applying an external pressure above the osmotic pressure.

When pressure greater than the osmotic pressure is applied to the saltier side of the membrane, water flow is inverted and begins to flow from the salty side to the pure solution side of the membrane (Baker, 2004).

Figure 1 is a schematic representation of the reverse osmosis process, in which the application of a pump in one of the process channels, the feed channel, obtains a pressure greater than the osmotic and thus forces the flow of the water in the membrane.

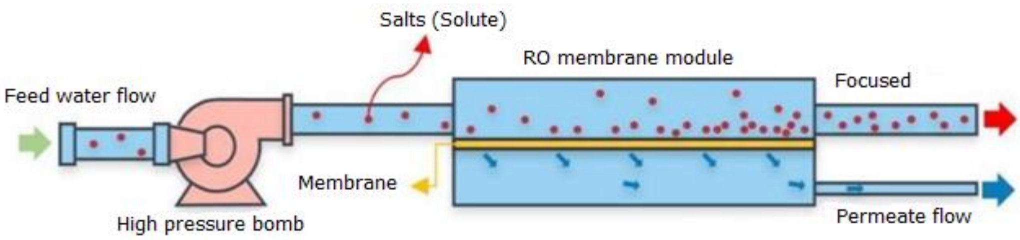

Figure 1. Schematic of a reverse osmosis process.

This type of desalination system by reverse osmosis is considered more energy efficient. Compared to other types of processes (Miller, Shemer; Semiat, 2015). However, the downside of its use is the sensitivity of the membrane to encrustations.

2.3 Membranes Semipermeable

Membranes are one of the most important elements for developing the reverse osmosis process. These membranes are versatile components whose main objective is to allow the passage of liquids and, simultaneously, prevent salts from being transported, causing these residues of salts removed from the water to remain present in the regions where the membrane is located. To reduce these adverse effects, spacers promote turbulence in the feed stream and decrease the salt concentration layer on the membrane (Proença, 2009).

These spacers are elements that make up the spiral module and directly affect the performance of the membrane. In addition, this type of component encourages an increase in mass transport, reducing the solution concentration. On the wall and fouling (Diniz, 2021). Figure 2 highlights, in a simplified way, how the desalination occurs, indicating the directions of flows within a spiral permeation module. In addition, Figure 2 presents the components present in the spiral model and the disposition of the turbulence promoters.

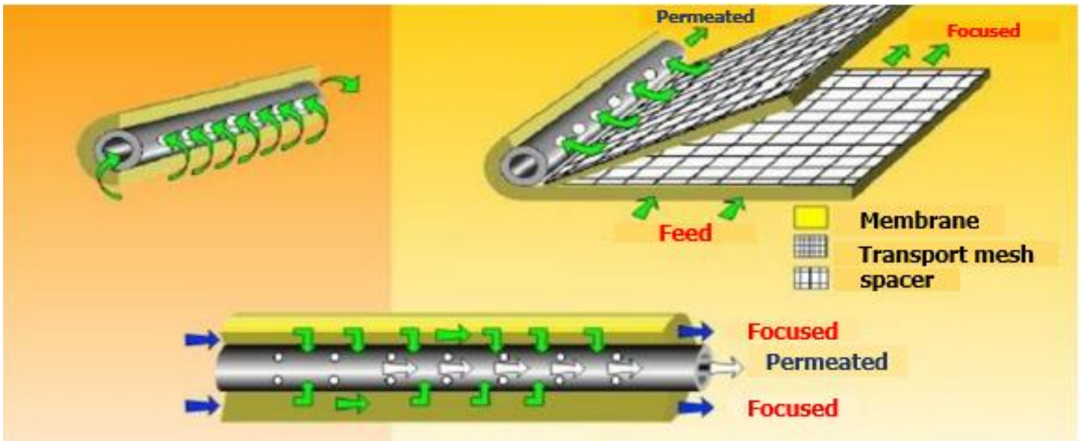

Figure 2. Spiral membrane element for reverse osmosis process.

The use of spacers as turbulence promoters allows the creation of turbulent flow, which, in addition to increasing the permeable flux, can also help to reduce the polarized boundary layers and reduce the problems of fouling.

3. METHODOLOGY

With the development of technology, numerical modeling emerged as a very interesting possibility, as it dramatically reduces the costs, time, and operational risks of repeat experiments.

The research of this work is linked to the modeling and simulation of a domain of study that can represent the physical phenomena occurring in a permeation module with a reverse osmosis membrane. The software used was ANSYS ICEM CFD for building domains and their meshes and ANSYS FLUENT for the numerical solution of models and analysis of results.

3.1 Geometry of the feed channel domains

The adopted geometries were built in the ANSYS ICEM CFD software, where you can draw, dimension the domains of study, and characterize each region or zone of interest. In this study, a geometry was constructed with an empty channel (without a spacer) and two channels with different spacer geometries with submerged type arrangement to carry out the simulations.

The geometries with spacers were built with the main dimensions of 69 mm in length and 2 mm in height of feed channel with 5 spacers for each case. Furthermore, another geometry without the spacers was created with the same dimensions to perform comparisons of results. Figure 3 is a schematic illustrative of a geometry without a spacer used for fluid dynamic analysis; in this scheme, the black arrow represents the flow direction.

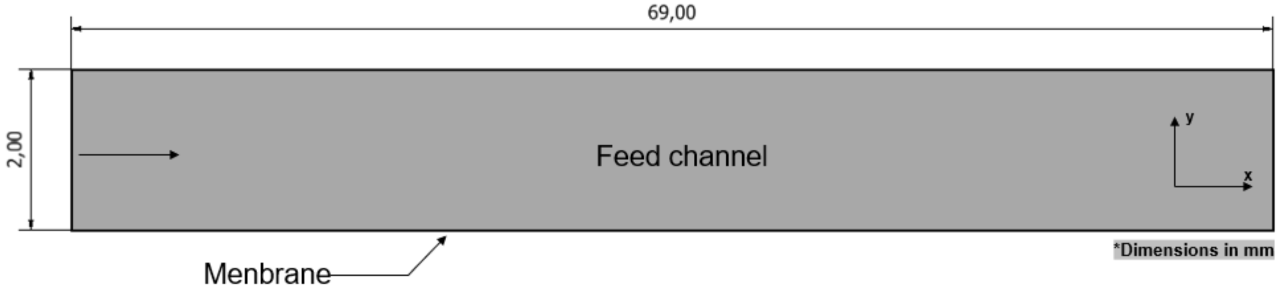

Figure 3. The geometry of the channel without spacer.

The proposed constructions were based on dimensionless relationships between channel size values and their spacer dimensions. Can find relationships found in the works of Amokrane et al. (2016), Keir (2012), Schwinge, Wiley e Fletcher (2002), and Fimbres-Weihs.

Based on the work of Diniz (2021) and the relations of the dimensions, were built with the values of the distance between the beginning of the feeding channel and the centroid of the first filament of 12 mm, the distance between the centroids of the spacers of 8 mm and the distance between the centroid of the last filament and the end of the feed channel of 25 mm, as shows Figure 4.

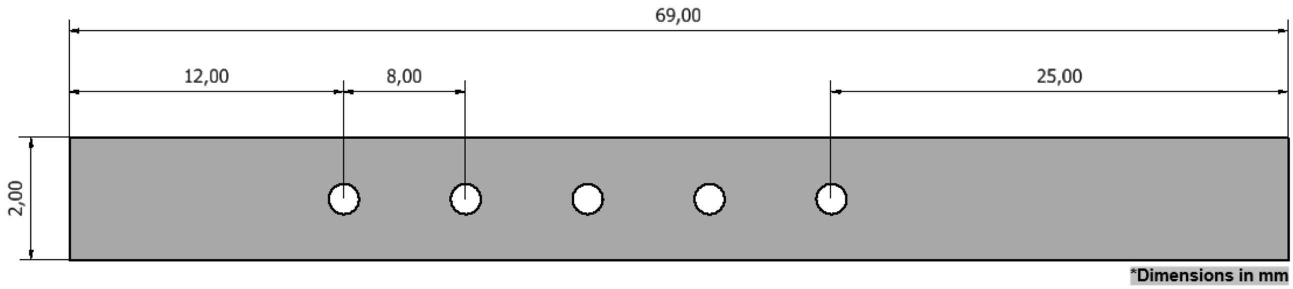

Figure 4. Geometry with circular type spacers.

The two different types of spacers used are circle and square shapes, the internal dimensions of which are shown in Figure 5.

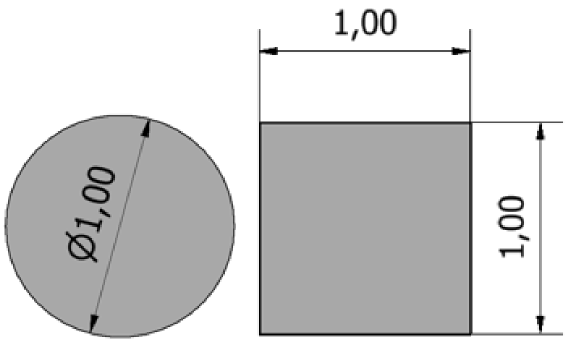

Figure 5. Spacer geometries.

3.2 Generation of numerical meshes

The computational domain models were built using the ANSYS ICEM CFD 15.0 software since when using finite volumes as a discretization method to solve equations; it becomes necessary to construct a mesh numeric for each domain under study. After modeling the geometries, defined the entry and exit zones of the fluid, walls, and interface with the membrane conditions, and then blocking, pre-meshing, and performed conversion from the file mesh output element to ANSYS FLUENT.

For the construction of the meshes, an increase in the density of cell numbers close to both the surface of the membrane and the spacers due to the presence of factors that cause a greater gradient in the process variable constituents, such as concentration polarization. According to Geraldes (2001), the concentration factor in a desalination process is a measure that indicates how many times the water has been concentrated in solutes during the process. It is the value of the concentration at the membrane, that is, the amount of salt accumulating on the membrane along the channel. The higher the concentration factor, the greater the concentration of salts in the rejected water, which may require additional treatment or proper disposal. This fact is reported in the works of the authors Ahmad et al. (2005a), Amokrane, Sadaoui, and Dudeck (2015), and Keir (2012). Ahmad *et al.* (2005-2007) recommend that the height of the first cell closest to the surfaces should have magnitudes less than $2{,}5x10^{-7}$ meters.

In addition, refined the mesh in the regions near the spacers with the intention that the values found for the study were closest to the analytical values. Then, an assessment of the quality of the meshes, using the ICEM CFD quality criterion, concluded that the meshes showed values above 0.8, considered satisfactory, as seen in Diniz (2021). Figure 6 highlights the refinement regions of the mesh in nearby places to the area where the membrane effect was modeled.

Figure 6. Mesh refinement close to the membrane area.

3.3 Modeling the physical properties of the solution and the boundary conditions

The study states that a solution flows in the feed channel and in the membrane, where this solution is composed of water and sodium chloride solution (NaCl). The physical properties of this solution vary depending on the fraction solute mass (m_a) at a temperature of 25 ± 0.5 ºC. Thus, Geraldes, Semião, and De Pinho (2001) suggested equations that represent the density (ρ), viscosity (μ), and diffusivity (D_{AB}) of the solution in a density for a mass fraction of (Nacl) less than 0.09 kg/kg. Such values are highlighted in Table 1.

Table 1. Polynomial functions describing density, viscosity, and diffusivity values.

Property	**Equations**
Density (ρ)	$\rho = 997{,}1(1 + 0{,}696 m_a)$
Viscosity (μ)	$\mu = 0{,}89(1 + 1{,}63 m_a)10^{-3}$
Diffusivity (D_{AB})	$D_{AB} = \begin{cases} 1{,}61(1 - 14 m_a)10^{-9}, & m_a < 0{,}006 \\ 1{,}45x10^{-9}, & max < 0{,}006 \end{cases}$

The *inlet* boundary condition is defined by entering a fully developed flow with a certain mass fraction of sodium chloride. Where $\bar{u}$ is the average velocity at the entrance, where it was calculated with a Reynolds number of 70 for all domains studied, with laminar flow, for this case, a value of the mass fraction of NaCl in the input of m_a = 0.002 kg/kg was chosen, such value was taken as the basis of the works by Diniz (2021), Amokrane et al. (2016) and (2015) and Fletcher and Wiley (2004). For the output conditions (*outlet*), a pressure outlet was adopted, wherein a pressure (^{outlet}) applied was the atmospheric pressure with the condition of the fully developed flow. For the walls, it was considered the fact that there was no slipping and that the walls were waterproof. For geometries with spacers, surfaces were defined as impermeable and without slip.

Finally, for this case, the modeling adopted for the membrane was like a semipermeable wall, without sliding, based on the modeling presented by Ahmad and Lau (2007). The equations used to describe the Membrane effects were from the Spiegler and Kedem model and the film theory. Following the work of Amokrane, Sadaoui, and Dudeck (2015) obtained data for an aqueous solution of NaCl in an empty membrane channel, as $\Delta p = 8.103\times10^{5}$ Pa and a mass fraction of 0.002 kg/kg. Values are from salt rejection R = 0.99 and resistance constant of the membrane $Rm = 1.562\times10^{14}$ m^{-1}. Table 2 highlights in a simplified way the equation applied to the inlet, wall, membrane, and outlet conditions.

To implement the equations in ANSYS FLUENT, it was necessary to implement and develop a code structure in C language (UDFs).

The numerical solution methods adopted in the proposed studies were the Least Squares Cell-Based methods for the determination of the gradient and discretization of the pressure, the Second-Order Upwind for moment equations, and the First-Order Upwind method for the discretization of the species equations. Finally, the SIMPLE algorithm (Semi-Implicit Method for Pressure Equations) was used to perform the pressure-velocity coupling.

Table 2. Equation adopted for zone conditions.

Zon	**Boundary condition**
Inlet	$u = 6\bar{u}\frac{y}{h}\left(1-\frac{y}{h}\right), \quad v = 0, \quad m_a = m_a^{inlet}$
Wall	$u = 0, \quad v = 0, \quad \frac{\partial m_a}{\partial y} = 0$
Membrane	$u = 0, \quad v = J_w = \pm\frac{1}{R_m \mu}(\Delta p - \sigma\Delta\pi), \quad m_a = m_a^{sp}$
Outlet	$\frac{\partial u}{\partial x} = 0, \quad \frac{\partial v}{\partial x} = 0, \quad \frac{\partial m_a}{\partial x} = 0, \quad p_A = p_a^{outlet}, \quad p_B = p_{atm}$

Regarding mathematical modeling, all domains performed in this study were treated permanently, considering an isothermal and adiabatic process, and the effect of gravity was neglected. In the simulations, the initial conditions in the solution were with initial velocity values adopted for the cells in the feeding zone and the mass fraction of NaCl with a value of zero and the chosen number of iterations of 10000 and a convergence criterion from 1×10^{-7}, where it showed good results.

4. RESULTS

This chapter addresses the analyses and results of the simulations; in addition, it presents the comparison between the results obtained with the geometry without a spacer and with the geometry with circular and square spacers. And subsequently, the effects of the spacers in the fight against the polarized layer and their efficiency during the reverse osmosis process.

The results obtained in the simulations for a two-dimensional domain with spacers arranged in an arrangement of the type submerged, with a diameter of 1 mm, are presented in Figures 8 and 9. In the following figures, it is possible to highlight that the presence of spacers influences the flow behavior and the mass distribution. Figures 7 and 8 show the velocity field and mass fraction present in the feeding channels.

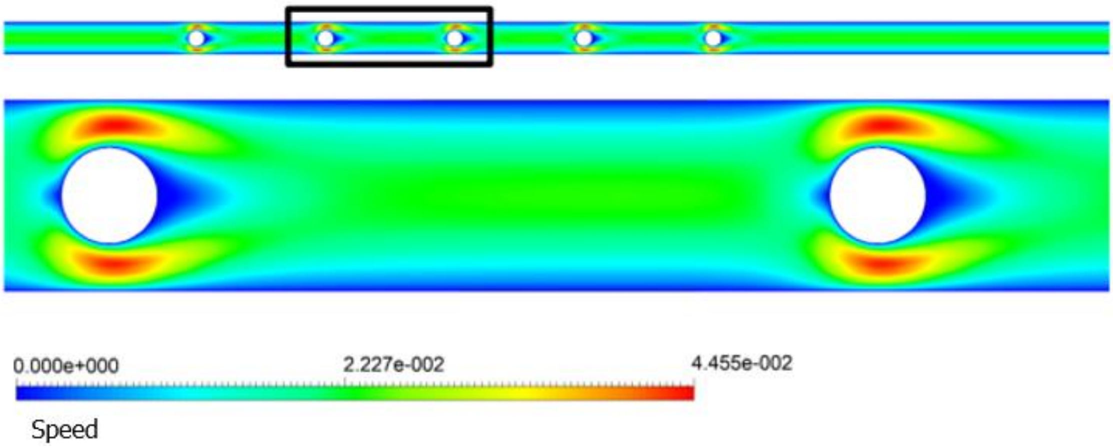

Figure 7. Velocity field in m/s for a domain with circular spacer.

In Figure 7, it is possible to observe that the presence of spacers directs the flow to the membrane and the wall of the domain, resulting in a high-velocity local field that increases the drag force of the solution on the surroundings of the surface of the membrane and, as a result, causes its cleaning. However, due to the low pressure and the shape of the flow that forms immediately after the spacer, the flow tends to line up in the middle of the channel, forming a "comet tail," slowing it down and reducing the effect of drag near the membrane. This effect stimulates the accumulation of the solution between the filaments in the next region of the membrane, which increases the thickness of the concentration layer polarized. Such effects can also be observed in the work of Diniz (2021) and Amokrane et al. (2016).

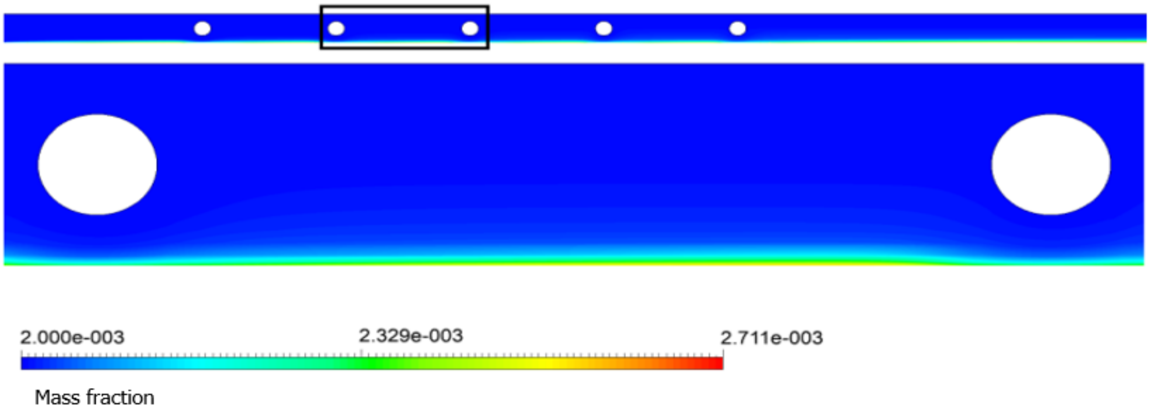

Figure 8. Mass fraction for a domain with circular spacer.

Figure 9 compares the polarization concentration factor (Γ) of the domain with and without spacers as a function of the dimensionless length along the surface of the membrane.

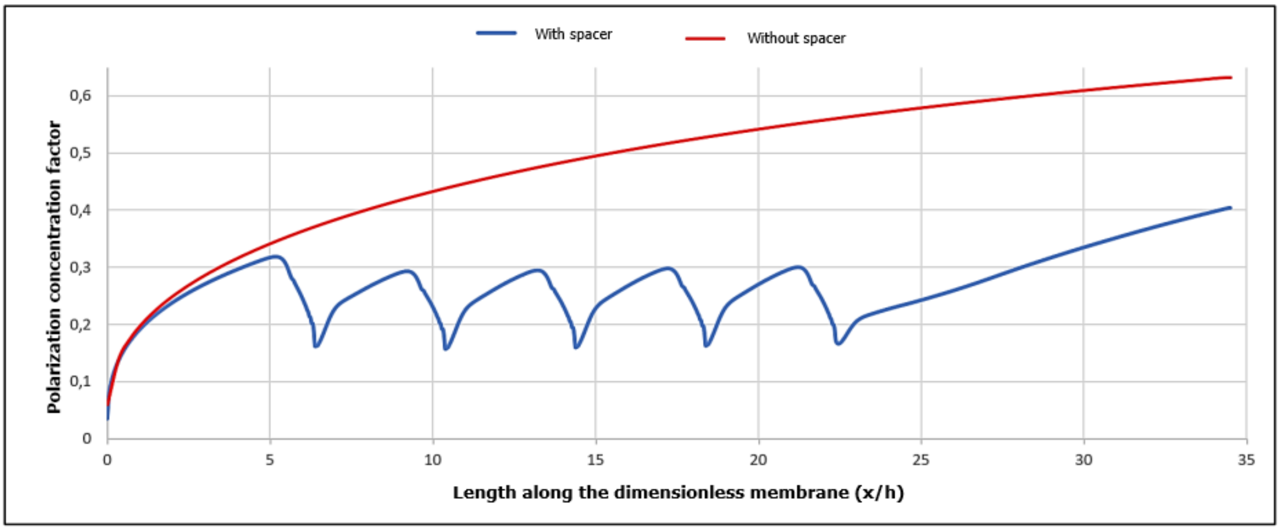

Figure 9. Γ factor curves for a domain with and without spacer.

It is possible to observe, by comparing the curves, the effect of the spacers causing a change in the behavior flow mass and causing a decrease in the polarization concentration factor, inducing a decreased concentration of the solute in the membrane. Ahmad, Lau, and Abu Bakar (2005) observe such behavior, and the results are similar to those obtained in the works of Diniz (2021).

With the use of the mean polarization concentration factor metric for cases with circular spacers, it was possible to quantify the capacity of the spacer in the reduction of the polarization film. Thus, the metric produced median values of 0.010650 for the curve with spacer and 0.017757 for the curve without using spacers, obtaining a 40% reduction in Γ_{medium} values along the surface. Already, concerning loss pressure per unit length (P/L) caused by the presence of spacers, the value is 138.58 Pa/m, which corresponds to 3.38 times the value without the use of spacers.

For the case with spacers with square geometry, Figures 10 and 11 illustrate the velocity fields and the mass fraction distribution, respectively.

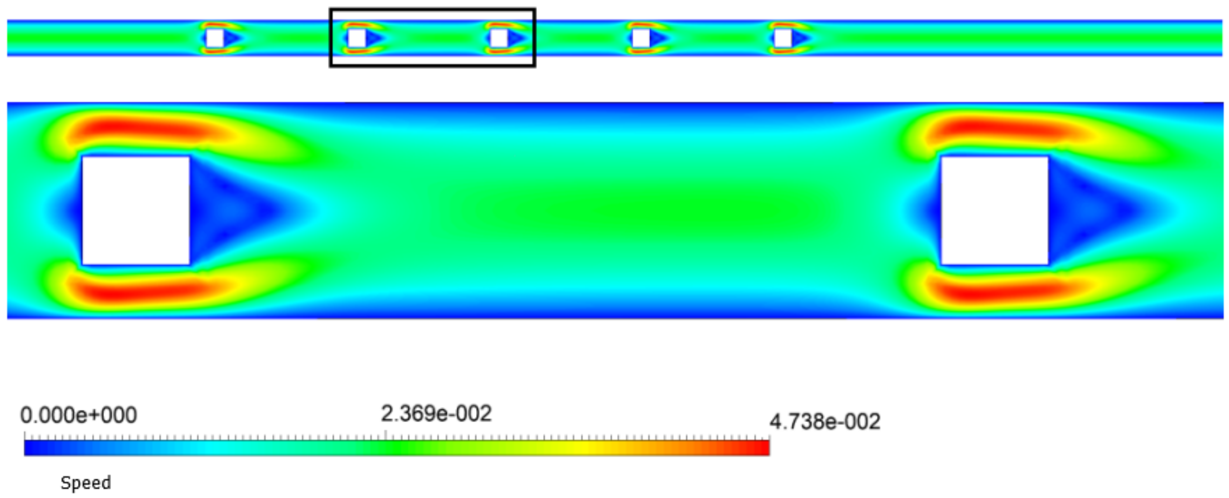

Figure 10. Velocity field in m/s for quadrilateral spacer domain.

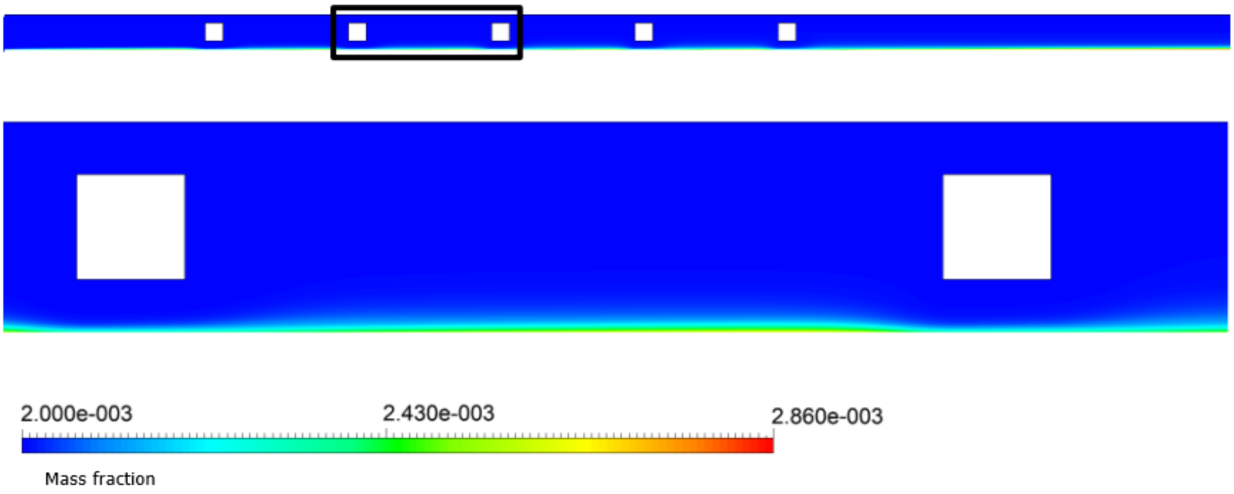

Figure 11. Mass fraction for a domain with quadrilateral spacer.

Figure 12 compares the polarization concentration factor with and without a square spacer along the membrane length in the feed channel.

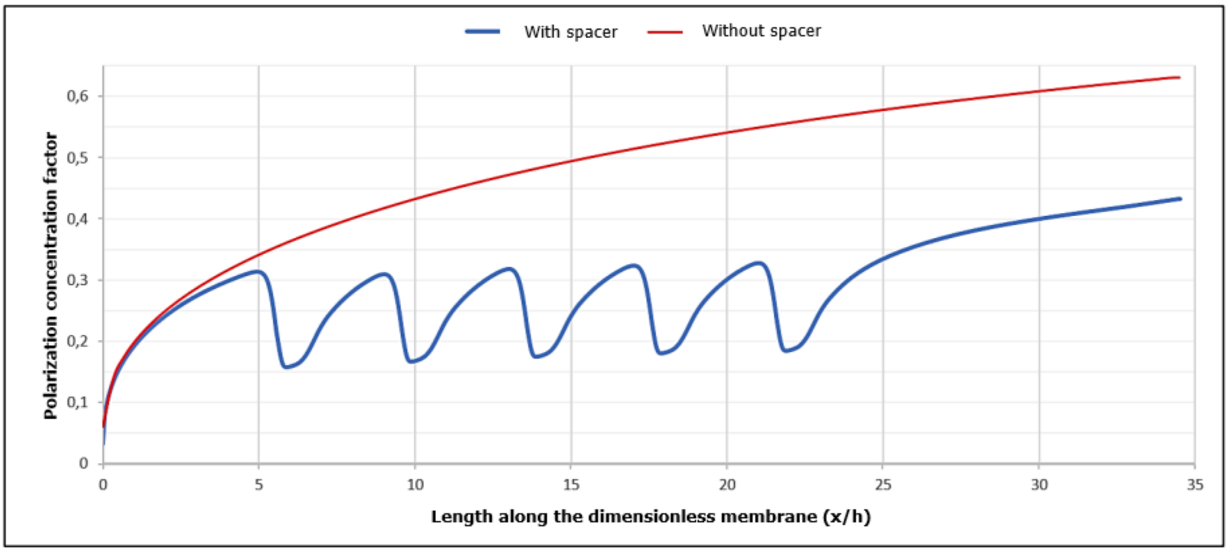

Figure 12. Γ factor curves for a domain with and without spacer.

As for cases of square-type spacers, the metric of the polarization concentration factor was valued equivalent to 0.0125729, which corresponds to only a 29% reduction in Γ values across the surface compared without the spacers. The presence of the spacers causes their pressure loss per unit length (P/L); the value is 217.4 Pa/m, which is 5.30 times the value without the spacers.

To analyze the performance of the arrangements and geometries of the spacers, the metrics of the Ratio of Spacer Performance (SPMP), which is calculated using Equation 1, was used to quantify the comparison between cases, according to Schwinge, Wiley, and Fletcher (2002). Where ΔC represents the concentration difference of the mass fraction, and ΔP is the pressure difference between the outlet and inlet of the feed channel. A spacer is said to be more efficient when it presents the highest SPMP value among the analyzed promoters.

$$SPMP = \frac{\Delta \text{Cspacer} \;/\; \Delta \text{C without spacer}}{\Delta \text{Pspacer} \;/\; \Delta \text{P without spacer}} \tag{1}$$

Based on this, Table 3 shows the values of the mass fraction difference, the pressure loss per unit of length (P/L) found, and the SPMP calculated for each case:

Table 3. SPMP values for cases with submerged arrays.

Geometry	**Δc**	**ΔP/L**	**SPMP**
Without spacer	$6{,}38\text{x}10^{-3}$	41,03	-
Circular	$2{,}44\text{x}10^{-3}$	138,58	0,11341
Square	$1{,}65\text{x}10^{-3}$	217,43	0,04880

When comparing the data obtained by the SPMP parameters, it is possible to observe that the geometry of the type spacer circular obtained the most satisfactory values.

5. CONCLUSION

The results of the simulations with the model used in this study were adequate for the research. It was possible to evaluate the hydrodynamic and mass behavior of the concentrate channel, being able to predict the formation of the polarization layer by concentration; it is a phenomenon typically present in the membrane desalination process.

A good representativeness of the phenomena involved in the separation process by reverse osmosis was verified. In addition, it was possible to analyze in detail the behavior of fluid under the effects of turbulence promoters in the flow channel to be permeated. By the general analysis of the results of this research, it was possible to conclude that the spacers promote a change in the velocity field and, consequently, also in the distribution of the mass fraction of the salt. The presence of spacers causes an increase in local velocity since there is a choke at the place where these turbulence promoters are present; at that moment, the flow of the fluid is forced to change its conduction towards the membrane and the wall, causing a high-speed local field.

In addition, due to the low pressure and the formation of the wake region after the spacer, the flow tends to align in the middle of the channel, decreasing its speed and the effect of drag near the membrane. This effect promotes an accumulation of the solute in the subsequent region between the filaments, which consequently increases the thickness of the polarized concentration layer.

Finally, based on the values obtained by the SPMP parameter, the geometries with the best results are those with the best balance between head loss and the production capacity of the final product. Therefore, the geometries with circular spacers were the ones that presented the best SPMP values among the geometries studied in this paper.

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7. RESPONSIBILITY NOTICE

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8. ACKNOWLEDGMENT

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