Thermal analysis of a single-cell PEM-type fuel cell with a coil as flow field architecture and its impact on cathode water formation

Análisis térmico de una monocelda de combustible tipo PEM con un serpentín como arquitectura de campo de flujo y su impacto en la formación de agua en el cátodo

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Key Handbooks

The research carried out presents crucial contributions in the field of PEM fuel cells. The analysis of the thermal effects, especially on the formation of liquid water inside the cathode, is further explored, considering variables such as temperature and tortuosity. Increasing the operating temperature in a PEM cell significantly increases the water saturation in the cathode, which can negatively impact its electrochemical performance. Cells with lower tortuosity (1.5) are more efficient in water evacuation, which reduces saturation and improves performance, especially at higher temperatures. Conversely, higher tortuosity (2.5) results in higher water accumulation, which affects reagent diffusion and overall efficiency. As temperature increases, the difference in saturation between tortuosities is amplified, highlighting the importance of optimising the porous structure to avoid water blockages that compromise cell performance.

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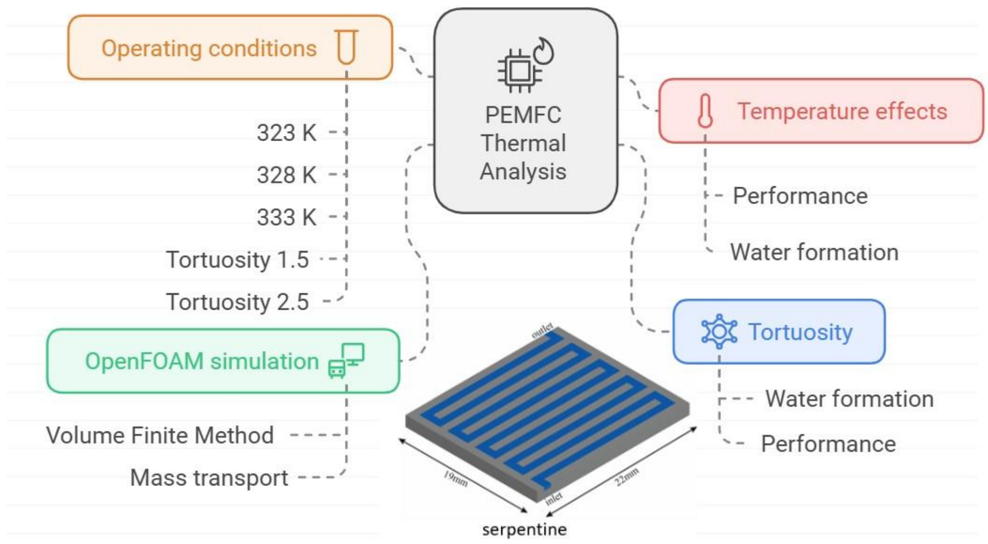
Abstract

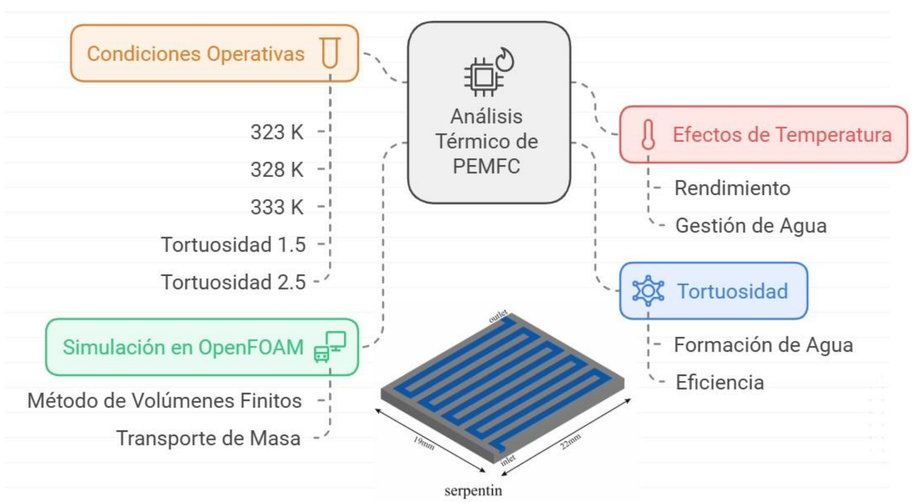
The thermal analysis of Proton Exchange Membrane Fuel Cells (PEMFC) is crucial for understanding how temperature impacts both electrochemical performance and water management, key aspects of their operation. This study focuses on evaluating the effect of thermal variations and tortuosity on liquid water formation in the cathode and its influence on overall efficiency. The thermal analysis considers the interaction between heat transfer, tortuosity due to porosity, and the presence of liquid water. To solve the governing equations of the system, the open-source software OpenFOAM, based on C++, is used with the Finite Volume Method (FVM). This approach allows for accurate modeling of thermal behavior and mass transport in the PEMFC. The study examines performance through polarization curves at three operational temperatures: 323, 328, and 333 K, combined with tortuosity values of 1.5 and 2.5. These variations help understand how tortuosity affects reactant and product transport, as well as water management and overall cell performance.



PEMFC, OpenFOAM, Tortuosity

Resumen

El análisis térmico en celdas de combustible tipo PEM (PEMFC) es crucial para entender cómo la temperatura afecta tanto el rendimiento electroquímico y la gestión de agua, un aspecto clave en su operación. Este estudio se enfoca en evaluar el impacto de las variaciones térmicas y la tortuosidad en la formación de agua líquida dentro del cátodo de la PEMFC y su efecto en su eficiencia global. Este análisis térmico considera la interacción entre la transferencia de calor, la tortuosidad debido a la porosidad y la presencia de agua líquida por su formación en el cátodo. Para resolver las ecuaciones gobernantes del sistema, se utiliza OpenFOAM (Open Field Operation and Manipulation), un software de código abierto basado en C++, empleando el Método de Volúmenes Finitos (FVM, por sus siglas en inglés). Este enfoque permite modelar con precisión el comportamiento térmico y el transporte de masa dentro de la PEMFC. El estudio analiza rendimiento de una PEMFC descrito por las curvas de polarización obtenidas bajo tres temperaturas operativas: 323, 328 y 333 K, combinadas con valores de tortuosidades de 1.5 y 2.5. Estas variaciones permiten entender cómo la tortuosidad afecta el transporte de reactivos y productos, así como el manejo del agua dentro de la celda, y su rendimiento global.



PEMFC, OpenFOAM, Tortuosidad

Introduction

The search for sustainable and clean energy sources has led to a growing interest in proton exchange membrane fuel cells (PEMFCs). These cells represent one of the most promising technologies for the highly efficient conversion of chemical energy from fuel into electrical energy, with low pollutant emissions and the ability to operate at relatively low temperatures. However, to maximise the performance of a PEMFC, it is crucial to thoroughly understand the factors that affect its operation, including thermal management and water dynamics within the system (Shiva Kumar & Himabindu, 2019).

Thermal analysis in PEMFCs is critical, as temperature has a significant impact on electrochemical performance. Improper temperature control can lead to problems such as decreased system efficiency, water accumulation in unwanted locations and, in extreme cases, damage to cell components. It is therefore critical to analyse how thermal variations affect not only the electrochemical reaction itself, but also water management, which is a crucial aspect for the optimal operation of these cells (Yu et al., 2009).

One of the key characteristics influencing the performance of PEMFCs is the tortuosity of the porous medium of the catalyst and diffuser layers. Tortuosity refers to the complexity of the path that the reactants and products must follow through the pores of the material, which affects the diffusion and, consequently, the efficiency of the electrochemical reactions. In this study, we seek to assess the impact of different levels of tortuosity on liquid water formation and overall cell efficiency. Understanding how tortuosity affects the transport of reactants and products is vital to improve water management, which in turn influences overall system performance (Ceballos et al., 2022).

The present study focuses on the use of OpenFOAM, an open source simulation software based on C++. This program is widely used in the scientific community to solve complex fluid and heat transfer problems through the Finite Volume Method (FVM). The choice of OpenFOAM allows accurate modelling of thermal behaviour and mass transport within the PEMFC. Using this approach, different scenarios considering both thermal variations and different tortuosity levels can be simulated, thus providing a robust framework for the analysis of cell performance.

In the research, simulations are carried out at three operating temperatures: 323 K, 328 K and 333 K. These temperatures represent a typical operating range for PEM fuel cells. The choice of these temperatures allows us to observe how the performance of the cell is affected by thermal changes, as well as by variations in tortuosity, which is analysed at two levels: 1.5 and 2.5. This work is based on a previous study (Ceballos et al., 2024), from which key information has been extracted for the methodology used in this analysis. In the previous work, the quality of the mesh was verified, all governing equations and their variables were defined, as well as the numerical method used.

Methodology

Domain

The study domain consists of a PEM-type single fuel cell with a serpentine flow channel design. This geometry was chosen because of its ability to improve reagent distribution and water management.

The study domain includes several key regions. The gas flow channel is the region where gaseous reagents, such as oxygen and hydrogen, are transported. The gas diffusion layer (GDL) consists of a porous material that facilitates the transport of these reactants to the catalytic layers, as well as allowing the evacuation of water produced during the reaction. The catalytic layer is the area where the electrochemical reaction that converts chemical energy into electrical energy takes place, while the membrane is responsible for transporting the protons from the anode to the cathode. The dimensions of the cell are as follows: the channel is 1 mm wide and 1 mm high. The thickness of the GDL is 200 µm, the thickness of the catalytic layer is 10 µm, and the thickness of the membrane is 50 µm.

The domain was discretised using the Finite Volume Method (FVM) in OpenFOAM, due to its ability to solve complex fluid dynamics and heat transfer problems. The meshing was performed with a structured approach, paying special attention to the refinement at the interfaces between the catalytic layer, the membrane and the GDL, where the highest concentration and thermal gradients occur. The quality of the meshing was verified in a previous work (Ceballos et al., 2024) where a mesh independence study was performed.

Governing equations

The governing equations (Table 1) describe the fundamental physical and chemical phenomena occurring inside a PEMFC. These equations allow representing the flow of reactants, heat transfer and species transport inside the cell, key elements to understand and predict its behaviour. The correct implementation of these equations is essential to determine the dynamics of the system, from the distribution of reactants and products in the flow channels and porous media, to the impact of temperature on the electrochemical performance. In addition, these equations help to model water formation and management, which is critical to avoid problems such as excessive accumulation at the cathode and to ensure efficient operation. Together, the governing equations provide the basis for accurately simulating cell performance under different operating conditions, facilitating the analysis of key variables for optimisation.

Box 1

Table 1

Main governing equations

Ecuación	Number
Continuity $\nabla \cdot \left(\rho_g \vec{U}_g\right) = -S_l$	[1]
Moment $\nabla \cdot \left(\rho_g \vec{U}_g \vec{U}_g\right) = -\nabla p_g + \nabla \cdot \left(\mu_g \nabla \vec{U}_g\right) + S_M$	[2]
Chemical species $\nabla \cdot \left(\rho_g \vec{U}_g y_i\right) = \left(\nabla \cdot \rho_g D_g^{eff} \nabla y_i\right)$	[3]
Energy $\nabla \cdot \left(\rho_{mix} C_{p_{mix}} \vec{U}_g T\right) = \nabla \cdot \left(k_{mix} \nabla T\right) + S_E^{reac} + S_E^{PC}$	[4]
Liquid water transport $\nabla \cdot \left(\rho_l D_l \nabla S\right) - \nabla \cdot \left(\rho_g \vec{U}_g S\right) = S_l$	[5]

Source: Own elaboration

In equation 5, the effective diffusion coefficient is defined as

$$D_g^{eff} = D_i^{bulk} f(\varepsilon) f(S) \quad [6]$$

Where the overall diffusion coefficient through the flow channel is expressed as binary diffusion for each component of the gas mixture is obtained by

$$D_i^{bulk} = 10^{-4} \times \frac{10^{-3} \times T^{1.75} \left(\frac{1}{M_j} + \frac{1}{M_i}\right)^{0.5}}{p\left[\left(v_j\right)^{\frac{1}{3}} + \left(v_i\right)^{\frac{1}{3}}\right]^2} \quad [7]$$

where M_i, M_j the molar masses andv_i, v_j species diffusion volumes. $f(\varepsilon)$ and $f(S)$ are the normalised porosity and saturation functions, respectively. These functions account for the tortuosity due to porous media and the presence of liquid water.

$$f(\varepsilon) = \left(\frac{\varepsilon - 0.037}{1 - 0.037}\right)^{0.661} \quad [8]$$

$$f(S) = (1 - S)^{\tau} \quad [9]$$

The term represents the tortuosity due to the presence of water in the porous medium. In this study, it is analysed with values of 1.5 and 2.5, by varying the initial simulation temperatures of 323, 328 and 333 K, to observe the impact of this parameter on the overall performance of the cell.

Numerical method.

OpenFOAM is used, solves the incompressible laminar Navier-Stokes equations using the Pressure Implicit with Splitting of Operator (PISO) algorithm and discretises the equations based on the finite volume method. The Preconditioned Bi-Conjugate Gradient Gradient (PBiCG) method was used to find convergence in the energy equation, and the Preconditioned Bi-Conjugate Gradient Stabilised Gradient (PBiCGStab) for other variables (continuity, momentum, species transport, energy and liquid water transport). For all variables, the convergence criterion was a residual of $^{1x10^{-9}}$.

Results

Data validation.

The validation of the simulation data was carried out in the previous study (Ceballos et al., 2024) where the independence of results was verified with the mesh and the construction of the polarisation curve of the coil-type geometry. The study was performed from 12,159 to 96,141 hexahedral elements analysing the values of maximum current densities, reaching mesh independence with 45,170 elements.

Impact of tortuosity on the maximum temperatures on the cathode side.

Figure 1 presents the initial operating temperatures of the cell, corresponding to 323 K, 328 K and 333 K; and the maximum temperatures reached at the cathode during operation. The two sets of data correspond to tortuosities of 1.5 and 2.5.

The results show that as the initial temperature increases, so does the maximum temperature at the cathode, reflecting an expected trend due to heat accumulation inside the cell during the electrochemical reaction. However, the tortuosity is observed to have a significant impact on the magnitude of the maximum temperature reached.

For a tortuosity of 1.5, the maximum cathode temperatures are lower compared to the values obtained for a tortuosity of 2.5. This can be explained by the fact that a higher tortuosity value increases the resistance to gas flow in the porous medium, which can lead to higher heat accumulation due to the difficulty in evacuating water and reaction products. In turn, the reduced efficiency of heat transfer to the surrounding regions contributes to a higher temperature rise at the cathode.

It is noticeable that the difference in the maximum temperatures between the two tortuosities widens as the initial temperature increases. For example, at 323 K, the difference between the maximum temperatures for tortuosities of 1.5 and 2.5 is relatively small; however, at 333 K, the difference is considerably larger. This suggests that the effect of tortuosity becomes more relevant as extreme thermal conditions increase within the cell, exacerbating the effects of thermal and water mismanagement in more tortuous media.

Impact of tortuosity on peak current density on the cathode side.

Figure 2 shows the relationship between the initial operating temperature of the cell and the maximum current density obtained at the cathode, with two data sets representing tortuosities of 1.5 and 2.5. The analysis reveals that, as the initial cell temperature increases, the maximum current density also increases, which is consistent with the general trend that higher temperatures favour electrochemical reactions by increasing the mobility of protons in the membrane and enhancing catalytic activity.

However, the tortuosity of the porous medium has a noticeable impact on the magnitude of the current density achieved. For the tortuosity of 1.5, it is observed that the cell achieves higher peak current densities compared to the tortuosity of 2.5. This is because a lower tortuosity favours the transport of reagents towards the catalytic layer, reducing the resistance to oxygen flow and improving the access of the reagents to the active site where the oxygen reduction reaction occurs at the cathode.

On the other hand, when the tortuosity is 2.5, a significant decrease in the peak current density is observed, which can be attributed to the fact that a more tortuous porous medium generates a higher resistance to the transport of reactants and products, limiting the efficiency of the electrochemical reaction. In addition, the accumulation of water in more tortuous media can clog porosity and gas channels, further affecting the availability of oxygen for the reaction.

Importantly, the effect of tortuosity is amplified at higher temperatures. At 333 K, the difference in peak current density between the 1.5 and 2.5 tortuosities is much more pronounced than at 323 K. This suggests that, at higher temperatures, the tortuosity effect is amplified. This suggests that, at higher temperatures, the transport capacity of the reagents becomes even more critical for electrochemical performance, highlighting the importance of optimising the structure of the porous medium to ensure efficient transport of oxygen and water within the cell

Box 2

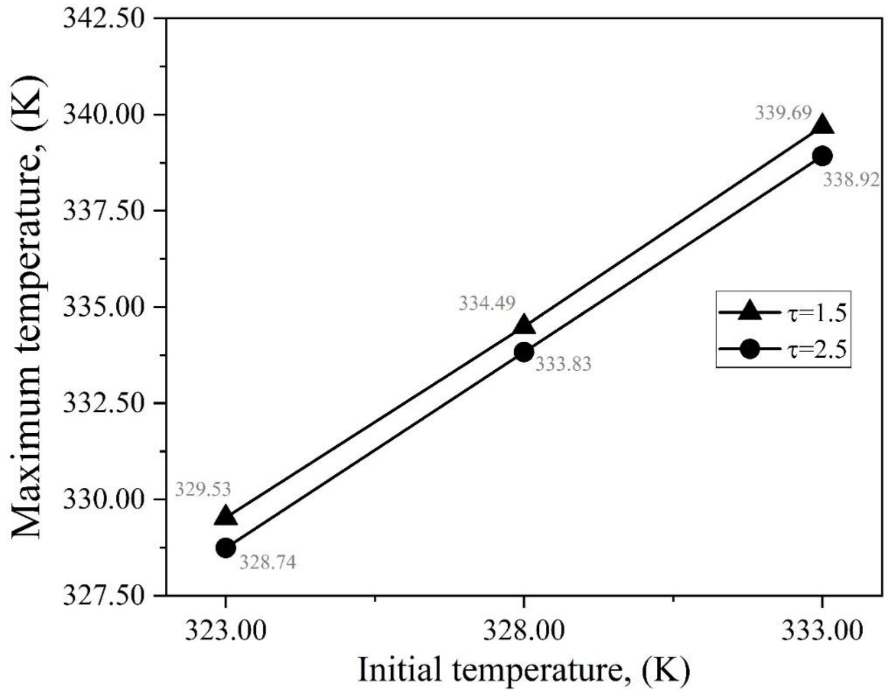


Figure 1
Effect of tortuosity on the maximum temperature gradients on the cathode side

Source: *Own elaboration*

Impact of saturation on cathode side peak current density

The water saturation contours for the 1.5 and 2.5 tortuosities show how the water accumulation within the cell varies as both the operating temperature and the structure of the porous medium changes. As the temperature increases, a significant increase in saturation values is observed for both tortuosities, although this increase is more pronounced in the 2.5 tortuosity cell.

For the 1.5 tortuosity, the saturation values go from 0.34 at 323 K, to 0.38 at 328 K, and finally reach 0.71 at 333 K. This indicates that, although there is an increase in water accumulation at higher temperatures, the porous medium with lower tortuosity still allows a relatively efficient evacuation of the water generated during the electrochemical reaction.

On the other hand, the cell with a tortuosity of 2.5 shows slightly higher saturation values than the 1.5 tortuosity at all temperatures tested. At 323 K, the saturation is 0.36, increasing to 0.40 at 328 K and reaching a remarkable value of 0.79 at 333 K. This steeper increase in saturation as temperature increases highlights the limitations of a more tortuous porous medium to handle water transport. A tortuosity of 2.5 imposes greater resistance to water flow, leading to greater accumulation at the cathode, especially at elevated temperatures.

Box 3

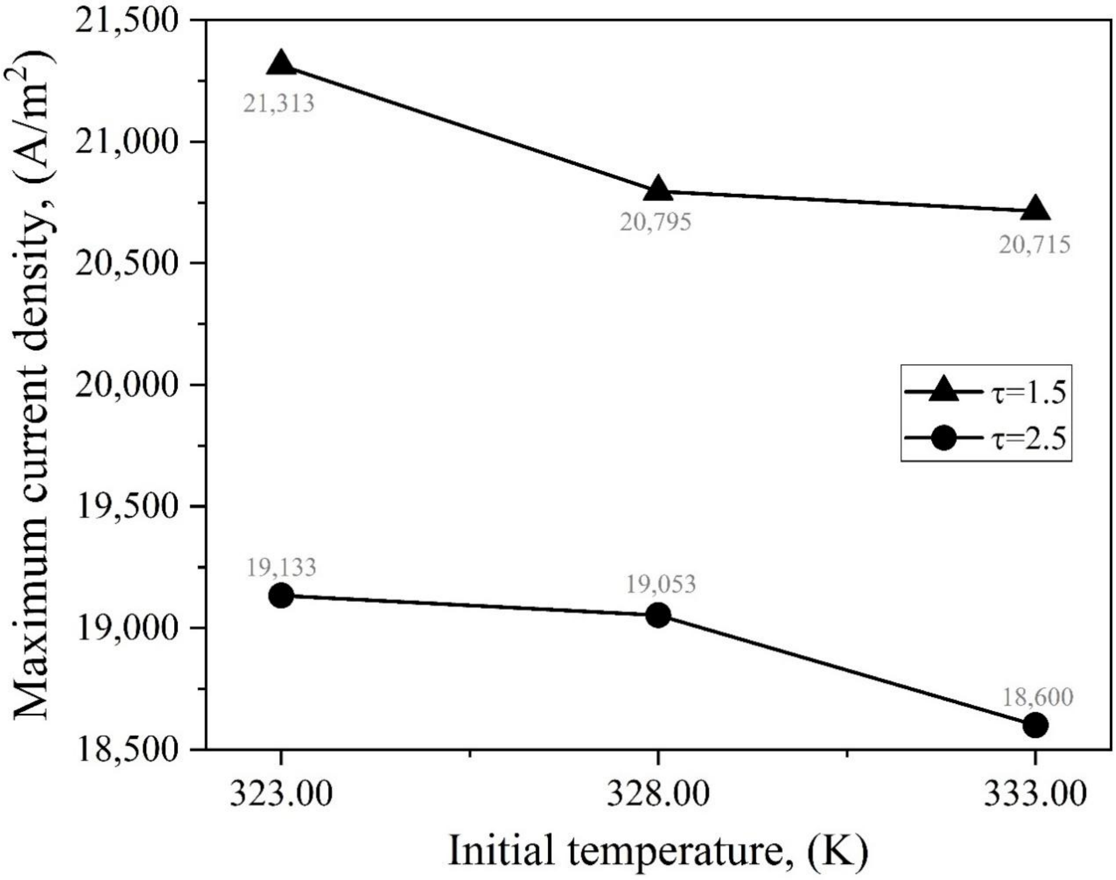


Figure 2
Effect of tortuosity on the values of peak current densities on the cathode side

Source: *Own elaboration*

On the other hand, the cell with a tortuosity of 2.5 shows slightly higher saturation values than the 1.5 tortuosity at all temperatures analysed. At 323 K, the saturation is 0.36, increasing to 0.40 at 328 K and reaching a remarkable value of 0.79 at 333 K. This steeper increase in saturation as temperature increases highlights the limitations of a more tortuous porous medium to handle water transport. A tortuosity of 2.5 imposes greater resistance to water flow, leading to greater accumulation at the cathode, especially at elevated temperatures.

Comparative analysis between the two tortuosities reveals that, although the difference in saturation is minimal at low temperatures (with differences of 0.02 at 323 K and 328 K), the disparity is amplified considerably at 333 K, where the 2.5 tortuosity has a saturation value 0.08 points higher than the 1.5 tortuosity. This suggests that, as thermal conditions become more severe, the ability of the porous medium to evacuate water is more compromised in cells with higher tortuosities, which could negatively affect cell performance due to pore clogging and reduced reagent transpor.

Box 4

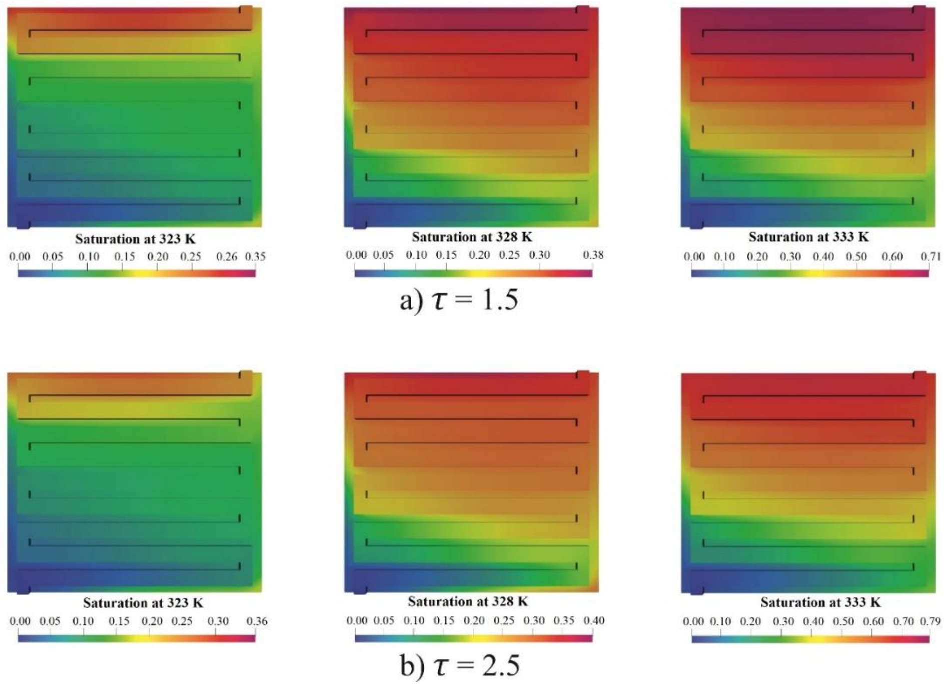


Figure 2
Saturation contours on the cathode side

Source: *Own elaboration*

Conclusions

From the results obtained, it is concluded that increasing the operating temperature of the PEM cell causes a significant increase in water saturation in both 1.5 and 2.5 tortuosity cells. At 333 K, saturation levels are considerably higher compared to 323 K and 328 K, highlighting the importance of proper thermal control to avoid excessive water accumulation at the cathode, which could negatively affect the electrochemical performance of the cell. Cells with a tortuosity of 1.5 present a more effective capacity to handle the generated water, showing relatively lower saturation values at all temperatures analysed.
This behaviour suggests that a porous medium with lower tortuosity facilitates water evacuation, which reduces the risk of flooding at the cathode and improves the overall performance of the cell. In contrast, cells with a tortuosity of 2.5 tend to accumulate more water, which could clog the gas channels and limit oxygen diffusion towards the catalytic layer. As the temperature increases, the difference in saturation between the 1.5 and 2.5 tortuosities becomes more noticeable. At 333 K, the saturation in the 2.5 tortuosity cell is considerably higher than in the 1.5 tortuosity cell, highlighting the limitations of a more complex porous structure for water transport at elevated thermal conditions. This behaviour highlights the importance of optimising tortuosity to avoid water blockages that impair electrochemical performance.

Statements

Conflict of interest

The authors declare that they have no conflicts of interest. They have no financial interests or personal relationships that could have influenced this book.

Authors' contribution

Ceballos-Pérez, José: Contributed to the project idea, research method and technique.

Ordóñez-López, Leadership in the planning and execution of the research activity.

Sierra-Grajeda, Juan: Development or design of methodology; creation of models.

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