Numerical Analysis of the Effect of PTFE on Heat Transfer in the Gas Diffusion Layers of a PEM Fuel Cell

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Abstract. In this study, a numerical investigation is conducted to analyze the influence of Polytetrafluoroethylene (PTFE) loading used in the Gas Diffusion Layers (GDL) of a Proton Exchange Membrane Fuel Cell (PEMFC), on the cell's heat transfer. A two-dimensional model was developed using COMSOL Multiphysics to simulate heat transfer phenomena within the cell. The temperature profiles are simulated for two distinct cases in order to evaluate the influence of PTFE content within the gas diffusion layer. The first case considers a GDL incorporating 5% PTFE, while the second case involves a significantly higher PTFE loading of 30%. Comparing these two configurations allows for a better understanding of how PTFE concentration affects heat transfer behavior within the PEM fuel cell. The results show that the temperature distribution is higher when a high PTFE content (30%) is used in the GDL compared to a lower PTFE content (5%). This behavior is mainly attributed to the low thermal conductivity of PTFE, which reduces the overall thermal conductivity of the gas diffusion layer. As a consequence, heat dissipation becomes less efficient, leading to elevated temperature levels within the GDL.

Key words

Fuel cell, PEMFC, heat transfer, Gas diffusion layer, PTFE, numerical analysis

1 Introduction

Energy plays an important role in the national economy of each country, not only as a ladder of economic and social development but also as a basic humanitarian need. The continuous improvement of quality of life and living conditions is accompanied by major energy and

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environmental challenges. Energy demand is growing rapidly, putting the world on the edge of a global energy crisis. In addition, the intensive use of conventional energy sources causes environmental pollution and leads to global warming [1-2]. At a time when the demand for energy, based essentially on hydrocarbons, is increasing irremediably, and an environmental crisis is emerging that threatens to disrupt our habits and the global ecosystem, hydrogen is emerging as a viable energy vector for the future. Hydrogen is a high-potential, clean, sustainable energy solution that can store energy efficiently [3]. Combined with fuel cells, hydrogen can supply electrical and thermal energy without local greenhouse gas emissions. Fuel cells are clean energy converters (converting chemical energy into electrical energy), whose only reaction products are water and heat [4]. In terms of applications, PEMFC-type cells can be used as a means of propulsion in cars. PEMFCs operate at peak performance at temperatures of 70 to 90°C. The power range for these applications remains relatively wide, from 0.1 to 250 kW [5]. The PEMFC stacks are composed of multiple protons exchange membranes, gas diffusion layers, catalyst layers, gaskets, and bipolar plates [6].

The efficiency and performance of proton exchange membrane fuel cells (PEMFCs) depends heavily on the heat and associated water imbalances because of their low operating temperature, which is typically less than 100 °C [7-8]. One of the parameters that directly affects both heat and water management of a PEMFC, as well as durability and longevity of its components, is the temperature distribution inside the membrane electrode assembly (MEA) [9-10]. This temperature distribution is highly dependent on the thermal conductivity of fuel cell components, especially gas diffusion layer (GDL) [11].

This layer must have sufficient porosity to ensure a homogeneous flow of reactive gases for optimum use of the electrode's entire active surface. It must have good electrical and thermal conductivity to ensure electron transfer and evacuation of the heat produced. It must be able to evacuate the water produced without drying out the membrane, whose ionic conductivity is directly linked to its water load. The GDL must also be able to resist corrosion in its environment and mechanically maintain the membrane-catalyst layer assembly.

Hence, accurate prediction of the GDL thermal conductivity and investigating its dependency on salient parameters such as compression, micro-structured characteristics, additive materials of Polytetrafluoroethylene (PTFE) and micro porous layer (MPL) are vital for understanding and improving the performance and longevity of PEMFCs.

GDLs are usually treated with different loads of hydrophobic PTFE for the purpose of water management. However, the added PTFE can change the thermal resistance of GDLs and, hence, affects the fuel cell heat management as well. Few studies have been to date performed to measure and model the thermal conductivity of GDLs treated with PTFE. Khandelwal and Mench [12] and Burheim et al. [13-14] reported that the PTFE treatment leads to a reduction in the GDL thermal conductivity.

A numerical study is carried out to investigate the effect of PTFE content within the Gas Diffusion Layers on the overall heat transfer of the PEM fuel cell. Two operating cases are considered: the first corresponds to a GDL containing 5% PTFE, while the second involves a higher PTFE loading of 30%. A two-dimensional model is developed in COMSOL Multiphysics to simulate the temperature distribution across the GDL and the other cell components. This approach enables a detailed assessment of how PTFE concentration influences thermal behavior within the cell. Since PTFE presents a low thermal conductivity, its proportion in the GDL is expected to significantly modify the effective thermal properties of the porous medium. By comparing both configurations, the study provides insight into the impact of PTFE loading on heat dissipation mechanisms and the resulting temperature gradients inside the PEMFC.

2 Materials and Methods

2.1 Model description

In this study, a bi-dimensional finite element model is applied to a fuel cell element comprising the membrane, electrode, and Gas Diffusion Layer (GDL) (Fig. 1).

The GDL, specifically Toray Carbon Paper 090 (TGP-H-090), is a carbon fiber composite paper that comes with a minimum of 5% weight wet proofing. The incorporation of PTFE (Teflon) in the GDL imparts hydrophobic properties to the carbon material, enhancing its performance as an electrode backing layer. This hydrophobicity helps in controlling water transport within the cell, preventing flooding while maintaining sufficient moisture to ensure proper membrane hydration. Additionally, the GDL ensures uniform distribution of reactant gases to the catalyst layer, facilitates the removal of water vapor, and aids in thermal management by dissipating heat generated during the electrochemical reaction.

In our numerical study, we analyze the temperature distribution in the fuel cell element, comparing two cases: one using 5% PTFE in the GDL and the other using 30% PTFE. The finite element method allows the complex geometry of the fuel cell section to be discretized into simpler elements, where heat transfer equations can be solved approximately, enabling a detailed investigation of the influence of PTFE content on the thermal behavior of the cell.

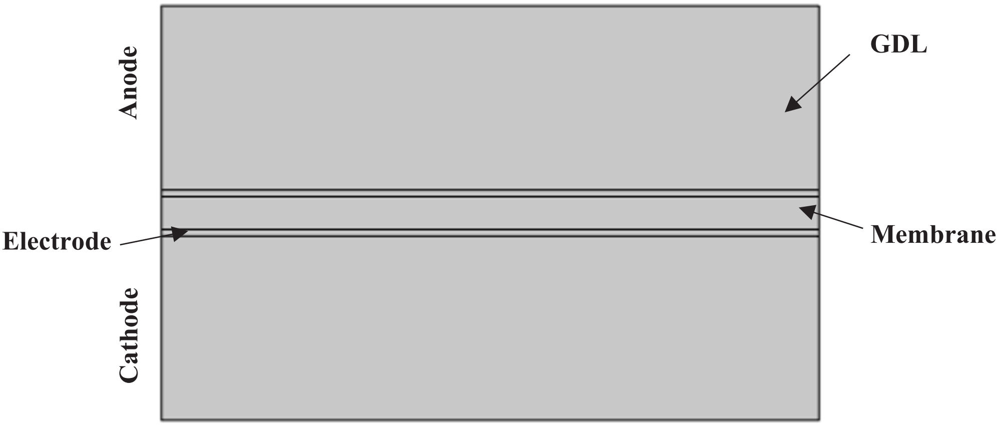

Fig. 1. Studied Element of the PEMFC Cell Geometry.

Table 1 presents the dimensions of the studied element

Table 1. Geometric dimensions of the studied Fuel Cell element.

Parameter	Dimension (µm)
GDL thickness	280
Membrane thickness	50
Electrode thickness	10
PEMFC section width	1000

In this study, we used a single GDL reference, the Toray Paper 090 (TGP-H-090), a carbon fiber composite paper.

Two cases are considered: the first with TGP-H-090 containing 5% PTFE, and the second with TGP-H-090 containing 30% PTFE.

The thermo-physical properties for each case are estimated based on the intrinsic properties of the H-090 GDL, taking into account the PTFE content. Since PTFE has a low thermal conductivity, its inclusion in the GDL reduces the overall thermal conductivity of the material. Consequently, the effective thermal conductivity is lower in the 30% PTFE case compared to the 5% PTFE case.

Table 2 presents the thermo-physical properties of the two PTFE-treated GDL cases, as well as those of the other components of the studied element.

Table 2. Thermo-physical properties of the numerical simulation of the proposed model

Materials	Cp [J.Kg-1.K-1]	Thermal conductivity [W.m-1K -1]	Density [Kg.m-3]
Membrane N112	1050	0.259	2000
GDL (Carbon paper Toray H-90) (5% PTFE)	700.8	1.7	440
GDL (Carbon paper Toray H-90) (30 % PTFE)	779.5	0.9	480
Electrode (Platinum)	133	71.6	21450

2.2 Model equations

The transient heat transfer in solids is governed by the energy conservation equation, which in 2D includes a thickness scaling factor dz. The general form of the equation is described by:

$$d_z \rho C_p \frac{\partial T}{\partial t} + d_z \rho C_p u . \nabla T + \nabla . q = d_z Q + q_0 + d_z Q_{ted} \tag{1}$$

In the case of heat transfer in solids only, the velocity field u is zero, and no thermoelastic coupling is considered, which removes the advection term and the thermoelastic heat source Qted. The heat flux q is described by Fourier's law,

$$q = -d_z k . \nabla T \tag{2}$$

Where k is the thermal conductivity of the material. Substituting this relation into the energy equation leads to the classical transient heat conduction equation.

Thus, for solid materials without mechanical or fluid coupling, the preceding relationship becomes:

$$d_z \rho C_p \frac{\partial T}{\partial t} = \nabla.(d_z k \nabla T) + d_z Q \tag{3}$$

(+ imposed flows at borders: q0).

With Q representing any applied volumetric heat source and q0 corresponding to boundary heat fluxes. This formulation accounts for heat storage, conduction, and external heat inputs, providing an accurate representation of the time-dependent thermal behavior of the studied solid domain.

To model conductive heat transfer within the fuel cell components, the selected configuration consists of a representative element of the cell containing five distinct media, simulated using COMSOL Multiphysics.

Heat transfer within this domain is described using the two-dimensional heat conduction equation applied separately to each medium. In the membrane, heat generation arises primarily from the Joule effect, which acts as a uniform volumetric source. Because the membrane is isotropic and its thermal conductivity is assumed constant, the governing heat equation in this region simplifies to:

$$d_z \rho C_p \frac{\partial T}{\partial t} + \nabla.(-d_z k \nabla T) = d_z Q_{Joule} \tag{4}$$

Where QJoule represents the ohmic heating associated with proton transport through the membrane. This source term is expressed as:

$$Q_{Joule} = (R_{H^+}) i^2 \, (\frac{w}{m^3}) \tag{5}$$

With R_{H+} being the protonic resistance of the membrane and i the local current density. This formulation allows the Joule heating contribution to be accurately incorporated into the thermal analysis of the fuel cell element.

Continuity of heat flow at the membrane/electrode anodic interface

$$-nu.\nabla(-ku\nabla Tu) - nd.\nabla(-kd\nabla Td) = 0 \tag{6}$$

Heat transfer at the membrane/electrode cathodic interface with reversible and irreversible heat sources:

$$-n.q = q_{rev+irrev} \tag{7}$$

Thermal insulation is imposed on the external boundaries of the studied element:

$$-\mathrm{n}.q = 0 \tag{8}$$

2.3 Modeling and quantifying the various heat sources in the fuel cell

2.3.1 Joule heat QJ

The modeling and quantification of heat sources within the fuel cell require particular attention to the Joule heating generated in the membrane. This heat source, denoted QJ, originates from the resistance encountered by protons as they migrate through the polymer electrolyte. As a result, it appears as a uniform volumetric heat source distributed across the membrane thickness. The Joule heat generation is expressed as:

$$Q = (R_{H^+}) i^2 (\frac{w}{m^3}) \tag{9}$$

Where i is the local current density and R_{H+} is the protonic resistance of the membrane. This resistance is obtained from:

$$R_{H^+} = \int_0^{Lm} \frac{dx}{\sigma(x)} \tag{10}$$

With Lm is the membrane thickness and σ is the proton conductivity of the membrane. The latter depends strongly on temperature and membrane hydration. According to the correlation proposed by T. E. Springer et al. (1991), the proton conductivity is given by:

$$\sigma(\frac{S}{m}) = (0.005138\lambda - 0.00326) e^{1267(\frac{1}{303} - \frac{1}{T})} \tag{11}$$

Where λ represents the membrane water content and T the cell temperature in Kelvin. This formulation enables the Joule heating contribution to be accurately quantified as a function of both thermal and hydration conditions within the membrane.

2.3.2 Entropic heat of reactions QRev

Reversible source of heat from half-reactions responsible for creating entropy related to the overall reaction. Entropic reversible heat is the difference between the total chemical energy of the reactants and the maximum usable work.

An increase in the entropy ΔS (KJ/mol) of the system is responsible for heat release at a fixed temperature, which can be written as follows:

$$Q_{reac} = -T\Delta S . N_{H2} = -T\Delta S \ \frac{i}{2F} \tag{12}$$

Since,

$$\Delta S_{(H_2 + \frac{1}{2}O_2 \rightarrow H_2O_{liquid})} = -163 \frac{KJ}{mol(H2)/K} \tag{13}$$

at 25°C

N_{H2} (mol/m^2.s) being the hydrogen flow

i (A/m^2) is the current density

F (Coulomb/mol), Faraday constant

We deduce the heat release from the reaction:

$$Q_{\left(H_2 + \frac{1}{2}O_2 \rightarrow H_2O_{liquid}\right)reac} = -48{,}7 \ \frac{i}{2F} \ (\frac{KW}{m^2}) \tag{14}$$

at 25°C

Given the rapidity of the half-reaction kinetics on the anode side, we assume that the oxidation of hydrogen does not give off heat, and that the reduction of oxygen is solely responsible for the entropy created by the overall reaction.

$$Q_{anode\ reac} = 0 \tag{15}$$

2.3.3 Irreversible heat of electrochemical reactions QIrrev

The energy supplied to the system via the enthalpies of the reactants is not entirely converted into electricity. Some of this energy is dissipated as heat, reflecting variations in the system's entropy. These variations reflect the irreversibility of the transformation. This is a source of irreversible heat associated with overvoltage at the electrodes: activation overvoltage (ηactiv) and concentration overvoltage (ηconc).

Total activation and concentration overvoltages are negligible on the anode side:

$$Q_{anode\ irr} = Q_{active\ irr} + Q_{conc\ irr} \approx 0 \tag{16}$$

Thus:

$$Q_{Total\ irre} = Q_{Cathode\ irre} = i\left[\frac{RT}{nF\ln\left(\frac{i_l}{i_l - i}\right)} + \frac{RT}{nF\alpha\ln\left(\frac{i}{i_{0c}}\right)}\right] \tag{17}$$

3 Results and discussion

3.1 2D/1D Temperature profiles in the cell using 5% PTFE-treated GDL

For the case using a TGP-H-90 GDL with 5% PTFE, the simulation results indicate that the fuel cell achieves an optimal temperature distribution. With the 5% PTFE-treated GDL, the results show that the temperature reaches a maximum of 88.85 °C and a minimum of 83.85 °C, which remains within an efficient operating range for the fuel cell (Fig. 2 & 3).

The relatively low PTFE content has only a minor impact on reducing the effective thermal conductivity of the GDL, allowing heat to be dissipated efficiently across the layer. As a result, thermal transfer remains effective, preventing excessive temperature rise and promoting stable operating conditions within the PEMFC. This demonstrates that a 5% PTFE-treated GDL offers a good balance between hydrophobicity and thermal performance, contributing positively to fuel cell operation.

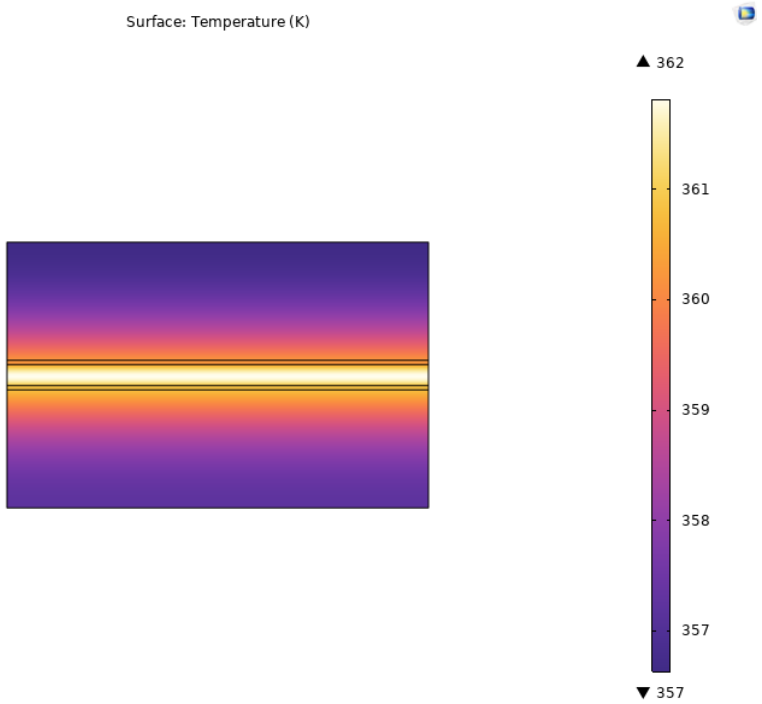

Fig. 2. 2D temperature profile in the cell using 5% PTFE-treated GDL

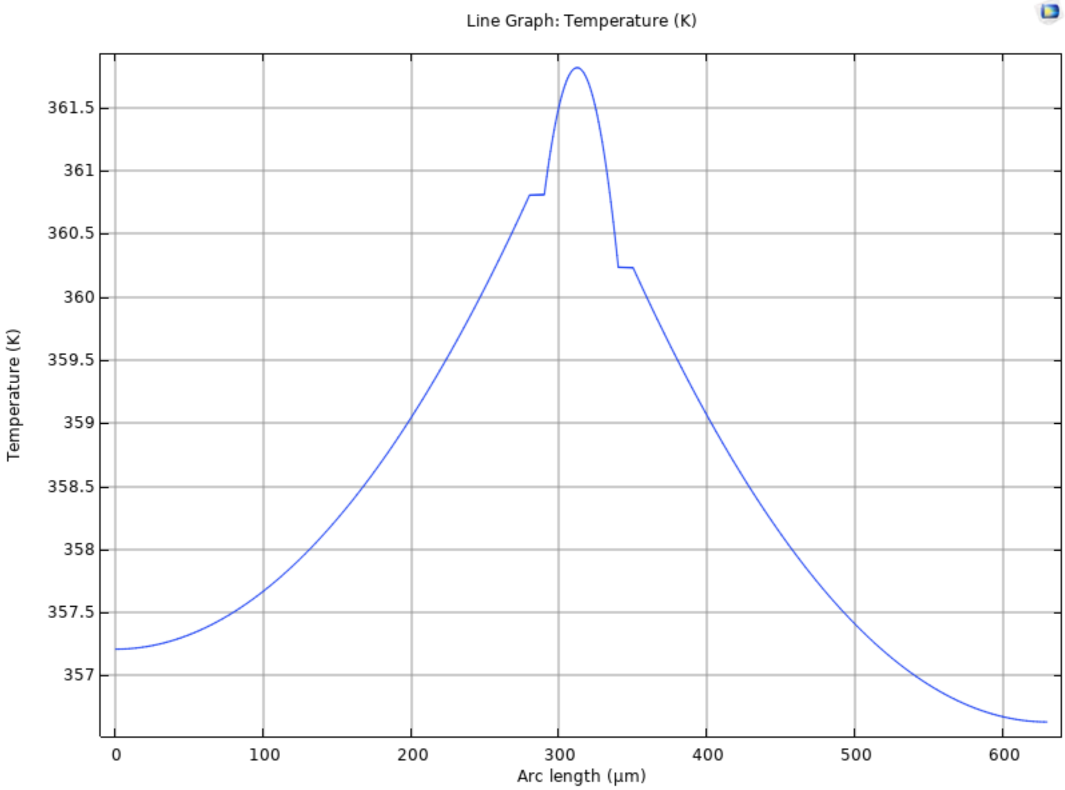

Fig. 3. 1D temperature profile in the cell using 5% PTFE-treated GDL

3.2 2D/1D Temperature profiles in the cell using 30% PTFE-treated GDL

For the case using a TGP-H-90 GDL treated with a higher PTFE content of 30%, the simulation results show a significantly elevated temperature range compared to the 5% PTFE case.

The maximum temperature reaches 94.85 °C, while the minimum is 91.85 °C, indicating a higher overall thermal level within the PEMFC (Fig. 4 & 5).

This increase is mainly due to the substantial reduction in the effective thermal conductivity of the GDL caused by the high PTFE loading.

As the thermal conductivity decreases, heat transfer through the GDL becomes less efficient, leading to reduced heat dissipation and consequently higher operating temperatures.

Therefore, while higher PTFE content improves hydrophobicity and water management, it negatively affects thermal regulation.

To achieve a balanced performance between heat management and water removal in the fuel cell, using a lower PTFE concentration in the GDL remains the more suitable and efficient choice.

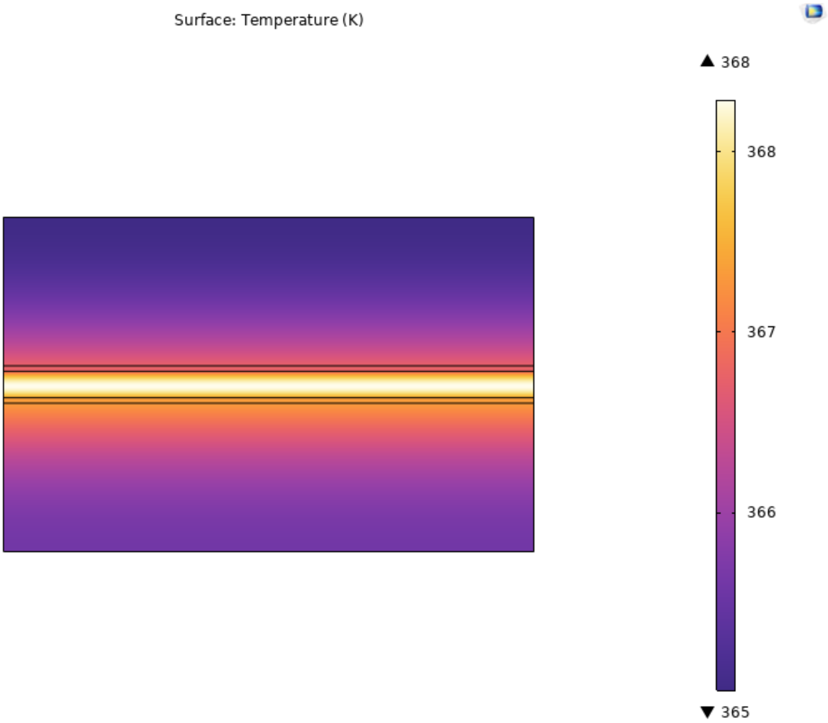

Fig. 4. 2D Temperature profile in the cell using 30% PTFE-treated GDL

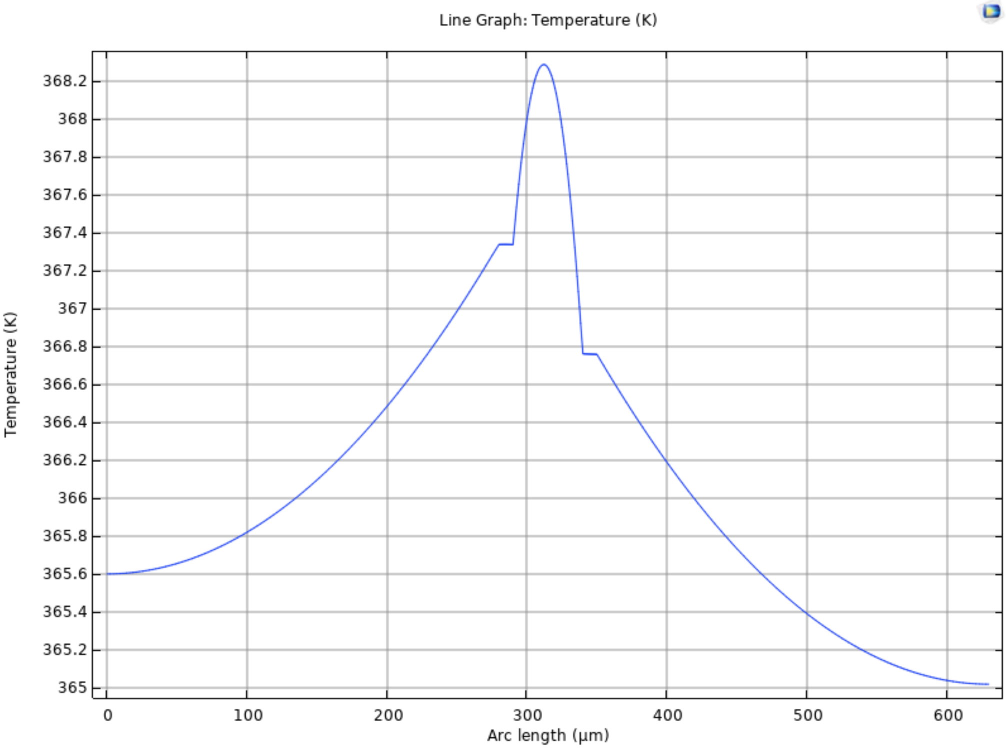

Fig. 5. 1D Temperature profile in the cell using 30% PTFE-treated GDL

The numerical results obtained in this study are validated by comparison with experimental trends and reference data reported in the literature for PTFE-treated gas diffusion layers (GDLs) [15]. The model predicts a consistent decrease in the through-plane thermal conductivity with increasing PTFE loading for all investigated GDL configurations. This behavior is physically justified by the low intrinsic thermal conductivity of PTFE, which increases the overall thermal resistance of the GDL structure. The predicted trends are in qualitative agreement with previously published experimental and numerical studies, notably those reported by Khandelwal and Mench [12] and Burheim et al. [13-14], which also showed a reduction in GDL thermal conductivity as a result of PTFE treatment. This consistency with established literature confirms the reliability of the proposed numerical model in capturing the influence of PTFE loading on the thermal transport properties of GDLs.

4 Conclusion

In this study, a finite element method was employed to numerically simulate heat transfer within a PEM fuel cell components containing the membrane, gas diffusion layers GDL, and electrodes, using COMSOL Multiphysic's heat transfer model, with a particular focus on assessing the influence of PTFE content in the Toray TGP-H-90 gas diffusion layer (GDL). The results demonstrate that PTFE loading plays a critical role in governing thermal behavior inside the cell. For the case of a 5% PTFE-treated GDL, the temperature distribution remains within an optimal operating range, with a maximum temperature of 88.85 °C and a minimum of 83.85 °C. This favorable performance is attributed to the relatively low PTFE concentration, which only slightly reduces the effective thermal conductivity of the GDL, allowing heat to be dissipated efficiently. In contrast, increasing the PTFE content to 30% leads to a notable decrease in thermal conductivity [15], due to the intrinsically low conductivity of PTFE. As a result, the fuel cell exhibits higher operating temperatures, with values ranging from 91.85 °C to 94.85 °C, indicating reduced heat dissipation. Overall, the numerical findings highlight that moderate PTFE loading such as 5% offers a more balanced compromise between hydrophobicity and thermal management, ensuring more stable and efficient thermal performance within the PEM fuel cell.

Nomenclature

Cp : Calorific capacity (J/mol/K)
F : Faraday constant
k : Thermal conductivity ($W.m^{-1}.K^{-1}$)
i : Current density (A/m^2)

Greek symbols and abbreviations

λ : Water content in the membrane
α : Thermal expansion coefficient (K^{-1})
σ : Proton conductivity of the membrane (S/m)
ηactiv : Activation overvoltage (volt)
ηconc : Concentration overvoltage (volt)
ΔS : Reaction entropy (KJ/mol)
PEMFC : Proton-exchange membrane fuel cell
GDL : Gas diffusion layer
PTFE : Polytetrafluoroethylene

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