Proceedings of the 2023 International Conference on Functional Materials and Civil Engineering
DOI: 10.54254/2755-2721/23/20230624

Thermodynamic model of hydrogen-based fuel cell

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Abstract. The contemporary scholarly treatise expatiates on a lofty and refined mathematical schema of a Proton Exchange Membrane fuel cell seamlessly integrated into the Matlab Simulink milieu. The central aim of this model is to transcend the short descriptions of fuel cell functioning using parameters that denote certain physical connotations in an all-embracing manner. With minimal computational overhead, it could be extended to simulate an entire stack of fuel cells within the purview of an energetic system. The performance of each cell and its response to variations in pressure, temperature, humidity, and partial pressure of reactants are scrutinized with the utmost care, and the paramountcy of membrane hydration is exposed.

Keywords: Fuel cell, thermodynamic model, matlab simulink.

1. Introduction

Due to the fundamental premise of power generation using hydrogen fuel cells, hydrogen has earned the distinction of being a sustainable energy source, as it constitutes the reverse reaction of water electrolysis. It effectively mitigates greenhouse gas emissions vis-à-vis conventional means of energy generation, specifically those anchored in combustion-based power plants and engines. It also facilitates the direct, high-efficiency conversion of hydrogen energy into electricity with a remarkable reduction of power losses. Consequently, such features, which include reduced carbon footprint and superior energy performance, compound and, as such, accentuate the activeness of hydrogen as a preferred fuel option in both the domains of transportation and power generation [1].

In contemporary times, many methods can be employed to fabricate hydrogen fuel, such as natural gas reforming, which happens to be a thermal procedure, electrolysis that is prevalently adopted today, solar-driven mechanisms, and biological strategies. The fundamental mechanism undergirding the electrolytic reaction involves the disintegration of hydrogen gases located on the anode of the battery, under the enzymatic influence, into protons and electrons, with the positively charged protons subsequently navigating through the interstitial channel via the membrane to reach the counterpart, the cathode. Meanwhile, the negatively charged electrons operate outside the battery as an external circuit to generate electrical energy. Ultimately, the oxygen ions on the cathode react with protons and electrons to synthesize water via enzymatic involvement.

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In point of fact, many studies spanning the past four decades have furnished pivotal information regarding a diverse array of fuel cell blueprints. Bykoglu [2], in particular, has proffered a synopsis regarding the gestation of models for proton-exchange membrane fuel cells. Recently, multidimensional models were posited by Djilali, Lu [3], and Costamagna [4], while 3D modeling methods of a more advanced nature have also surfaced. Notably, scholars across the academic landscape have extensively researched to understand various aspects of fuel cell operational parameters, employing intricate modeling methodologies. For instance, Carton and Olabi [5] successfully engineered a 3D computational fluid dynamics (CFD) model for the pore-filled cell foam material in a flow plate, revealing that the reactant gas was uniformly dispersed during transit. Similarly, Ferreira and Falc [6] ea have refined their scrutiny to examine the biphasic flow that transpires within the anode gas channel of the PEM fuel cell, implementing the volumetric liquid method (VOF), and discerned that water migrated in the guise of hydrophilic or hydrophobic channel walls, respectively. Carton and Lawlor [7] employed a computational fluid dynamics (CFD) and volume of fluid (VOF)-based simulation technique to scrutinize the kinematic behavior of droplets and the genesis of slugs within the minute conduits of proton exchange membrane (PEM) fuel cells.

Quantitative studies have dominated the discourse on fuel cell modeling. In pursuit of optimal fuel cell functioning, Liu and Li [8] employed a numerical model to determine the most appropriate flow channel dimension. The derived model illuminates the incorporation of physical parameters in identifying performance enrichment as a sensory reality. In an experimental grid, enhancing an open fuel cell's performance via a superior electrocatalyst is unrelated to the felicific upshot of its physical mooring since it ensues spontaneously. Notably, numerous studies on energy systems have been ruminative venturings.

Recent research has primarily centered on developing individual constituent models in fuel cells—however, Z. Abdin, C.J. Webb, and E.MacA [1]. Gray has taken a distinct approach in this regard in their subsequent work. Their investigation aims to merge all component models, forming a comprehensive system model, which subsequently allows for the functionality of the planned energy system to be verified. The said triumvirate effectively demonstrated the applicability of component models as a promising tool for research, focusing on predicting the potential influence of significant variables, such as design parameters, materials, and environmental conditions, on outcomes, by utilizing the notion of a deliberate energy system. This concrete embodiment of a paradigm additionally proffers a novel insight into operationalizing the pragmatic models toward ascertaining aberrations inherent in modeled constituents or schemes via parameter adjustments. Inarguably, a perceptive augmentation to methodology formulation.

The conventionally employed fuel cell articulated in this essay has been dissected into four additional components for modeling: the anode, cathode, membrane, and voltage. The molar balance of reactant species and their partial pressures have been espoused in the anode and cathode. The membrane component vividly demonstrates the water transport mechanism and its uptake. The voltage component systematically depicts the overpotential. The author has instituted several simplifying presumptions in the mathematical model, which comprise a one-dimensional model and a uniformly-distributed current. Moreover, the hydrated reactant gases are envisaged as being in equilibrium with liquid water.

2. Method development

In this literary piece, we employ the conventional fuel cell, as depicted in Figure 1, partitioned into four subsidiary components for modeling. These subsidiary components are identified as the anode, cathode, membrane, and voltage. The anode and cathode ancillaries simulate the molar balance of reactant species and their partial pressures. The ancillary membrane models the water transport mechanism and water uptake into the membrane. The overpotential is modeled in the voltage ancillary.

The saturated hydrogen is conveyed to the anode and subsequently oxidized on the anode as per the guidelines presented in equation (1) [1].

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Similarly, humidified oxygen/air is conveyed to the cathode, where it is reduced on the cathode as per the regulations in equation (2) [1],

with resultant formation of water and release of heat:

Anode: $H_2 \rightarrow 2H^+ + 2e^-$ (1)

Cathode: $1/2O_2 + 2H^+ + 2e^- \rightarrow H_2O$ (2)

The conduction of protons amid the anode and the cathode occurs via the electrolyte membrane, while the transport of electrons toward the cathode transpires via an external circuit. Furthermore, the establishment of a mathematical model is predicated on certain simplifications that do not compromise the cell's efficacy, particularly:

a)The model is restricted to a one-dimensional framework with uniform electrical distribution, a premise that accords gas homogeneity at constant pressure;

b)The reactant gases, namely the anodic hydrogen and cathodic oxygen, remain in equilibrium with liquid water; and

c)The water activity of the membrane remains uniform and in equilibrium with its cathodic and anodic catalyst counterparts.

d)The presence of water in the form of vapor at the interface of the membrane electrode is an indisputable fact. This phenomenon corresponds to the constraint of capping the relative humidity at 100 percent. Consequently, it is impracticable to quantitatively gauge the impact of cathodic displacement when the partial pressure of water goes beyond the saturation vapor threshold. Yet, there is empirical evidence to support this assumption. In particular, fuel cells that operate at moderately elevated temperatures, above approximately 40°C, tend to exhibit this behavior. This trend is more pronounced in most practical settings, where the cell temperature is higher than the coolant temperature, which, in turn, is greater than the ambient temperature. Although water vapor may become condensed in the cathodic channel, its effectiveness remains unhindered.

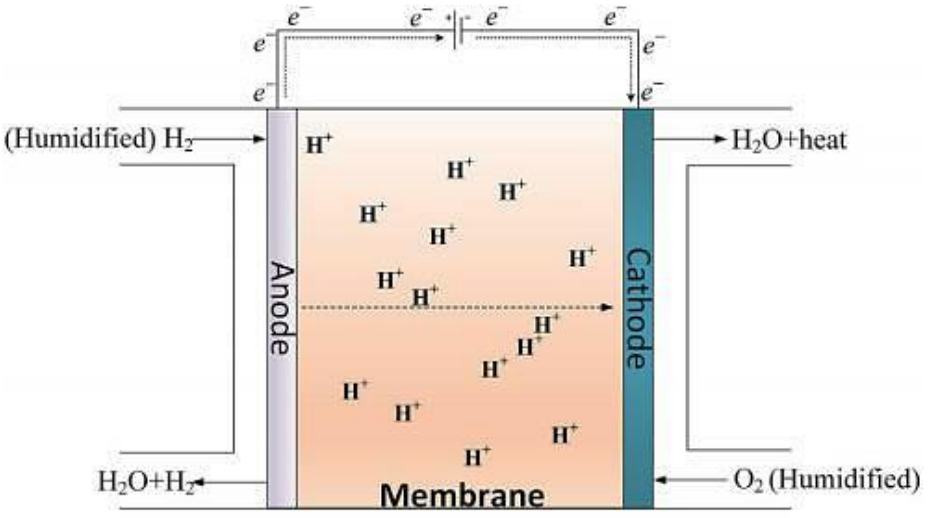

Figure 1. The conventional fuel cell [1].

2.1. Anode ancillary

According to Faraday's law, we can use the molar flow rate of hydrogen at the anode inlet and the molar flow rate of water at the anode inlet to calculate the molar fraction of hydrogen and water at the anode. The pressure of the anode can be defined.

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2.2. Cathode ancillary

Calculating the mole fraction of hydrogen and water at the cathode can be accomplished analogously to the anode by utilizing the molar flow values of hydrogen and moisture present in the inlet of the cathodic region.

2.3. Membrane ancillary

The customary solid electrolyte employed in the Proton Exchange Membrane fuel cell primarily constitutes a perfluorinated ionomer, wherein an inactive yet chemically robust polymer backbone with no ionic conduciveness induces stability and durability to the system. The spine, in essence, is furnished with the affixation of sulfonic acid-based lateral chains that are receptive to ionic transport. Notably, the SO_3 chains are widely diffused across the membrane as distinguishable, sporadic agglomerates.

2.4. Voltage ancillary

The voltage, being bestowed as a consequence of the fuel cell operations, is disclosed as $E=E_{oc}+E_{ovp}$. Establishing its constituents, we would consider E_{oc} as the battery's open circuit voltage. In contrast, E_{ovp} would account for the voltage loss or overpotential led by electron shipment in the electrocatalyst layer, bipolar plate, electrode backing side, and protonic dissemination in the PEM. Studying the temperature range, attained from 23-120°C, the open-circuit voltage of the PEM fuel cell revealed discernible temperature dependency, characterizing values that are invariably lesser than the anticipated theoretical values. To this day, a real explanatory cause behind such open-circuit voltage conduct has not been presented empirically. Larminie and Dicks have advanced contributions that attribute this behavior to the effects of H_2 crossover and internal current.

During the physical operation of a fuel cell, an assortment of voltage losses emanating from within the cell gives rise to the manifestation of an actual cell voltage inferior to the open circuit cell voltage. Pertinent to this cause is the cumulative effects of cell voltage losses, also known as overpotentials, stemming from the activation overpotential (E_{act}), a result of electric catalyst layers, concentration overpotential (E_{con}), caused by the mass transfer constraints when confronted with higher levels of current densities, and ohmic overpotential (E_{ohm}), exemplified by electron migration in the bipolar plates and electrode backing and proton migration in the PEM. The formulaic representation of these facts is typically embodied by Eq, which is nothing other than $E= E_{oc}-E_{act}-E_{con}-E_{ohm.}$

Notwithstanding, the scrutiny of inquiry methods necessitates the recognition of certain restraints. The formulation of experimental protocols constitutes a substantial expenditure of material and fiscal resources. Moreover, the acquisition of specific parameters that elude direct measurement involves the adjustment of the model to experimental observations, subject to normal circumstances, encompassing a temperature of 25°C, humidification transpiring at 25°C, and the atmospheric pressure of 1 a.t.m. Among these parameters are the distortion factor, charge transfer coefficients, and interstitial solutes' density in the reference state. These characteristics were subsequently solidified to enable a comparative evaluation of the model under different circumstances with experimental data while exploring the ramification of moisture content temperature and humidification ratio. The potency of the interstitial solvents is intrinsically dependent upon the variable temperature and the ruggedness of the electrode surface, which is gauged by the effective electrode area in proportion to its geometric counterpart.

3. Conclusion

The conclusion is drawn by positing a persistent, committed, and one-dimensional framework rooted in physical parameters for proton exchange membrane (PEM) fuel cells. Such a paradigm offers vast flexibility about the scale of fuel cells while the computational demands remain suitably moderate to model the whole system. Moreover, the prescience of the model can serve the advancement of superior electrodes that mitigate supra-normal activation overpotential by characterizing PEM fuel cell efficacy

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at basic tiers. Corroborating the effectiveness of the numerical model is achieved via two distinct approaches.

Initially, it should be noted that the mathematical framework aligns with the experimentally derived depictions of cellular polarization that have been published. Further, it facilitates the integration of physically significant parameters whose incremental acquisition constitutes a formidable undertaking. The precise calibration of the parameter evaluations attests to their inherent faithfulness to anticipated boundaries. Subsequently, a comprehensive comparison of the model vis-à-vis its three distinct counterparts with varying degrees of intricacy evinced an effective performance parity among the contemporaneous appraisals.

The verification of the method's feasibility utilizing the simplified one-dimensional approach has accordingly been ascertained. The input parameters of the atmosphere, that is to say, the temperature, pressure, and humidity of the reactive gas, are manipulated during the parametric analysis, and the aspects of the proton exchange membrane fuel cell are examined, thereby exhibiting the model's aptitude to replicate the rudimentary characteristics. Specifically, it is inferred that when the water vapor content of the constituent gas is diminished, the dehydration of the membrane ensues, inducing higher resistance locally. Therefore, one of the chief difficulties is conceptualizing models grounded in physical principles to gauge the membrane's water absorption capability, the initial feed's humidity, and the cell's temperature.

Acknowledgements

Yiqu Zhou, Wenxuan Wu, and Qiyue Wang contributed equally to this work and should be considered co-first authors.

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