



Investigating Performance of Hydrogen Fuel Cells in Different Charge Transfer Coefficients and its Effect on Maximum PowerPoint

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ABSTRACT

The charge transfer coefficient is a dimensionless coefficient used in the kinetics of chemical reactions. In this paper, the effect of the charge transfer coefficient on hydrogen fuel cell characteristics such as polarization curve and power diagram in terms of current density and losses is investigated. The charge transfer coefficient affects the activation losses of the fuel cell and therefore affects the performance of the fuel cell. For this investigation, a basic sample is selected and the changes of charge transfer coefficient are studied on its characteristics. The obtained results show that with an increase in this factor, the activation loss decreases. In addition, increasing the charge transfer coefficient increases the maximum power point. The increase in the power of this point is more visible in lower values of the charge transfer coefficient and when this coefficient exceeds the value of 0.5, this effect becomes very small. Also, the appropriate value of this coefficient is determined to maintain the balance of the chemical reaction. The activity of the fuel cell is disrupted due to an excess amount of the coefficient.

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NOMENCLATURE

R	J.mol ⁻¹ .k ⁻¹	Ideal gas constant	ppH_2	atm	Partial pressure of hydrogen
F	C	Farad's constant	ppO_2	atm	Oxygen partial pressure
T	K	Temperature	P_{out}	W	Output power
P_{H_2}	atm	Hydrogen pressure	E_{ernst}	V	Reduction potential
P_{air}	atm	Air pressure	V_{act}	V	Activation voltage drop
A_{cell}	cm ²	Cell area	V_{ohmic}	V	Ohmic voltage drop
N_{cell}	-	Number of cells	V_{conc}	V	Mass transfer voltage drop
i_o	A.cm ⁻²	Alternating current density	V_{out}	V	Output voltage
i_l	A.cm ⁻²	Limit current density	n	-	Number of electrons
G_{fiiq}	J.mol ⁻¹	Gibbs function of the liquid state	V_{imes}	-	Number of stoichiometric steps
r	Ω	Ohmic resistance	Greek Symbols		
K	-	Mass transfer constant	α	-	Charge transfer coefficient
i	A.cm ⁻²	Current density	ω	-	Amplification factor
P_{H_2O}	atm	Water saturation pressure			

INTRODUCTION

Nowadays, diversifying the energy basket is one of the most important indicators of achieving sustainable

development. In this context, renewable energy plays an important role in sustainable energy security and the world is witnessing an increase in the use of renewable energy (1). Energy usually appears in three forms: heat

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supply, electrical energy and water (2). Among types of renewable energy, hydrogen energy is one of the most well-known types. Hydrogen can provide the required thermal energy from the heat caused by its combustion. In addition, through a device which is called fuel cell, hydrogen energy can be directly converted into electricity. Because of the growth of electrification, the development of fuel cells is recognized as an important issue in scientific fields. The technology of this device is developing and there is still potential for research, development, and improvement of its performance.

Achieving the appropriate voltage and high power and efficiency in fuel cells is important and nowadays large number of research studies are carried out in these field. Important parameters affect the performance of hydrogen fuel cells. One of these parameters is the charge transfer coefficient. The charge transfer coefficient shows a fraction of the surface potential between the electrode and the electrolyte, which helps to reduce the free energy barrier for the electrochemical reaction. This parameter is dimensionless and is defined to describe the kinetics of chemical reactions and is used in the Butler-Volmer equation (3). The butler-Volmer equation is one of the most important relationships in chemistry and electrochemistry. This relation determines the flow of electrons in the common surface between the electrode and the electrolyte due to the reaction of the electrode with excess potential. Charge transfer coefficient can be defined separately in two sections of the hydrogen fuel cell. The oxidation charge transfer coefficient is defined where the oxidation reaction takes place in the anode. The reduction reaction charge transfer coefficient is related to the cathode area.

In previous studies, the results of measuring the charge transfer coefficient in the reaction of oxygen on a composite electrode have been presented (4). This measurement was performed using the potentiostatic technique. This method allows relatively fast measurement of the value of the charge transfer coefficient (4). More measurements proved that the capacity of the double-layer electrodes depends on the amount of adsorbed hydrogen and can be changed. It was also found that the charge transfer coefficient also varies in the range of 0.5 to 1 according to the absorbed hydrogen content (5). Three types of transfer coefficients are defined in reactions, which are heat transfer, mass transfer and charge transfer coefficients. Given this matter, models have been proposed in which, through the combination of independent heat and mass transfer modeling in the cell, the charge transfer coefficient is obtained, and an example of these has been constructed with porous electrodes (6). With the expansion of research, novel methods have been developed to estimate the coefficients of cathodic and anodic charge transfer from the voltage-current curves of solid oxide fuel cells. One of the studies includes charge transfer coefficients based on the characteristics of the fuel cell polarization

curve (7). An investigation has recently been conducted on the effect of charge transfer coefficient on fuel cells, as well as its impact on hydrogen electrolyzers. In this regard, a systematic model has been introduced and studied. The improvement in performance through charge transfer coefficient and current density to the polarity and performance characteristics of proton exchange membrane electrolyzers has been expressed in literature (8). In one of the most recent studies, an experimental investigation on two parameters of current density and charge transfer coefficient has been carried out in a standard hydrogen fuel cell model (9).

The performance of fuel cells is dependent on many parameters. In this paper, a subset of parameters related to the flow field is examined. Flow field parameters are divided into three main categories: those inspired by nature, conventional parameters and parameters related to losses. This paper has been focused on the loss-related subset which is illustrated in Figure 1 (10).

Group one is related to temperature and this group is further divided into temperature and stack temperature (11–13). Geometric factors are divided into two categories: mechanical and thermal-electric (14, 15).

The effect of the charge transfer factor on the polarization curve, maximum power point and fuel cell losses are investigated in this paper. Most of the studies on the effect of charge transfer has been done in the form of measurements and experimental tests. In this research, the method of investigating the effects of this coefficient is numerical simulation. However, the simulation of hydrogen fuel cells is usually performed with the help of software that ignores the charge transfer coefficient. The purpose of this paper is to further investigate the effect of changes in this coefficient in the mentioned cases, which is done with MATLAB software. In this paper, the reason behind assuming a value of 0.5 for the charge transfer coefficient in some cases has been investigated. Considering this case that the charge transfer coefficient always deviates from the value of 0.5 due to the non-ideality of the charge transfer coefficient, the effect of this difference on the performance of the investigated system and its characteristics is calculated and expressed in the results.

The organization of the paper is as follows: First, the importance and process of simulation to achieve the results are introduced along with the symbols. Then the important and effective conditions and factors in the simulation section were examined. In this section, the relations governing the system are also introduced. These relations are used in the simulation process in MATLAB software. An authentic sample along with its working conditions and other physical details have been selected as the base sample and in the studied system section, the obtained results of this paper have been compared with the published results of the base sample. For this purpose, power diagrams in terms of current density were compared with each other. In the losses section, the types

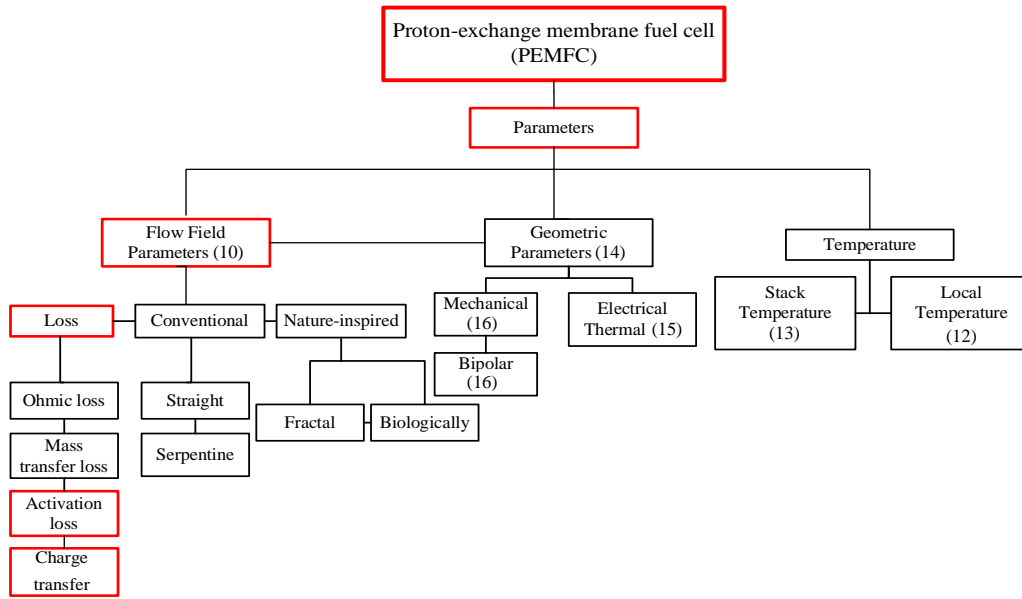


Figure 1. Parameters of proton-exchange membrane fuel cell (PEMFC)

of losses in fuel cells are introduced and categorized along with the voltage drop relations of each of them. The maximum power point section introduces the maximum power point in fuel-cell systems. Fuel cells will have the highest output power by working at the voltage and current of this point. In this section, one of the most practical algorithms that have a suitable performance in these systems is introduced under the title of disturbance and observation with the explanation and drawing of the algorithm. This algorithm helps the fuel cell to find the maximum power point and work at that point when the working conditions changed.

STUDIED SYSTEM

In Table 1, the symbols of each of the parameters and constant coefficients used in the simulation are introduced.

The studied system is adopted from one of the simulations available in literature (7). The solution information can be adopted as described in Table 1. This example is a hydrogen fuel-cell stack with 90 cells.

The simulation results of the power diagram in terms of current density for validation can be seen in Figure 2.

The comparison of these two graphs shows an extremely small amount of simulation error, which is due to receiving the information of the validation sample graph with Plot Digitizer software.

Waste investigation

One of the issues investigated in this paper is the effect of the charge transfer coefficient on fuel cell losses. The simulation of this paper has been done with the help of

Table 1. Simulation information of the validation sample (2)

Parameters	Value	Unit
T	353.15	K
P _{H2}	3	atm
P _{air}	3	atm
P _{H2O}	0.4669	atm
A _{cell}	100	cm ²
N _{cell}	90	-
r	0.19	Ω
α	0.5	-
ω	0.085	-
i _o	10 ^{-6.912}	A/cm ²
i _l	1.4	A/cm ²
Gf _{liq}	-228170	J/mol
k	1.1	-

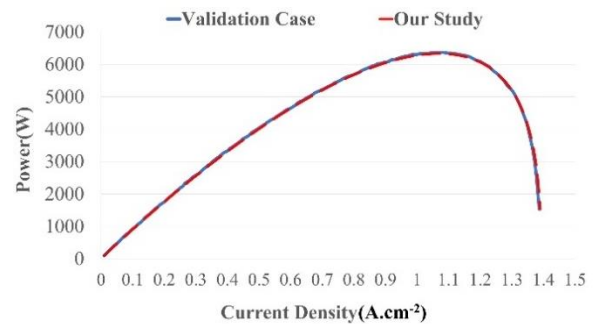


Figure 2. Comparison of the power diagram according to the current density of the base sample and the simulation sample

MATLAB software. Initially, it is necessary to specify the current density as an input. For this purpose, after defining and valuing the parameters according to Table 1, a loop is defined in MATLAB software to determine the current density from 0 to 1.5 A.cm² with the number of 150 iterations. The relations required for simulation are relations 1 to 6. The partial pressure of hydrogen and oxygen is calculated with the use of the thermodynamic relations of real gases. It is also investigated that fuel cells have practical limitations in performance that cause losses and reduce the efficiency.

The three general categories of losses are:

- Activation losses
- Ohmic losses
- Mass transfer losses

To calculate the activation loss voltage, Tofel's equation is used according to Equation 1 (2):

$$V_{act} = -b \log \left(\frac{i}{i_0} \right) \quad [1]$$

where b is the TOEFL ratio coefficient and can be calculated from Equation 2:

$$b = R \frac{T}{2 \alpha F} \quad [2]$$

To calculate ohmic losses from Ohm's law, calculations are made according to Equation 3 (2):

$$V_{ohmic} = -i r \quad [3]$$

Mass transfer losses can be calculated through Equation 4 (7):

$$V_{conc} = \omega i^k \log \left(1 - \frac{i}{i_l} \right) \quad [4]$$

To calculate the mass transfer loss voltage, it should be considered that if the ratio of current density to the limit current density becomes negative, the value of mass transfer loss voltage should be considered zero.

The output voltage of the fuel cell, which is important for the consumer, is the result of the difference in the collection of all three types of losses from the reduction potential of the battery. This reduction potential can be calculated through the Nernst equation according to Equation 5 (7).

$$E_{nernst} = -\frac{Gf_{liq}}{2F} - \frac{RT}{2F} \ln \frac{P_{H2O}}{pp_{H2} pp_{O2}^{0.5}} \quad [5]$$

Finally, the output voltage of a fuel cell is calculated from Equation 6 (7):

$$V_{out} = E_{nernst} + V_{ohmic} + V_{act} + V_{conc} \quad [6]$$

The charge transfer coefficient can be considered as a measure of the symmetry of the energy barrier. This can be shown by considering the intersection of energy curves. If the geometry of the curves is symmetrical, it means that the performance of the fuel cell is in equilibrium and if the reaction is not in equilibrium, this value for the charge transfer coefficient is between zero and 0.5 or between 0.5 and 1. Equation 7 expresses the

difference between the charge transfer coefficient in the two oxidation and reduction reactions:

$$\Delta\alpha = \frac{n}{V_{times}} \quad [7]$$

Maximum power point

In recent decades, due to the increase in pollution and global warming, scientists are trying to optimize and increase the performance and production of renewable energy units. Hydrogen fuel cells, which provide safe, efficient and clean electrical energy, have their own special importance (16). The maximum power point is the point where a fuel cell produces the highest power in its working voltage and current. Different algorithms are used to track this point. One of the most popular of which is the perturbation and observation or P&O algorithm in fuel cells (10). Figure 3 shows this algorithm (9).

Due to the direct use of voltage and current, this algorithm is a suitable option among other algorithms for tracking the maximum power point.

This method is based on trial and error in finding and tracking the maximum power point and it oscillates around the maximum power point by creating disturbance in specific time intervals.

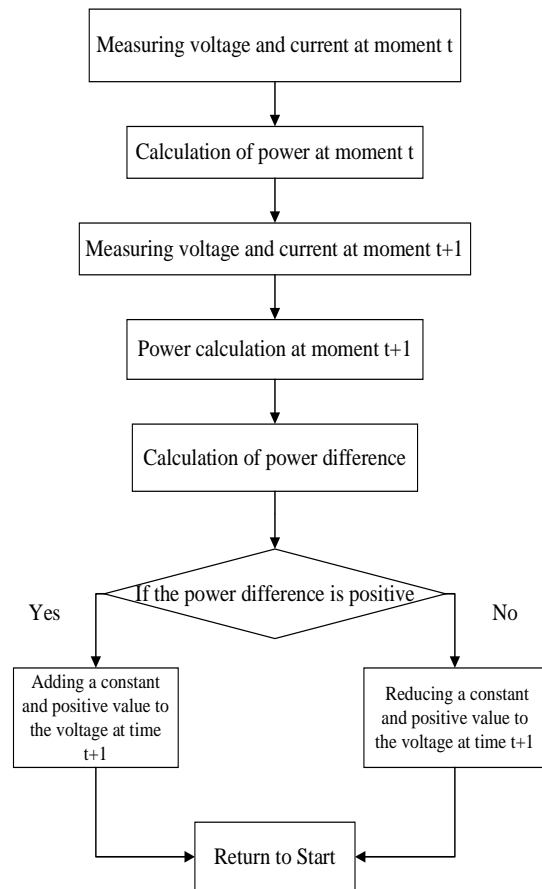


Figure 3. Perturbation and observation algorithm

SIMULATION RESULTS

Changes in the charge transfer coefficient have a direct effect on the simulation loss voltage, so in the results section, a comparison of three different values for this coefficient and its effect on the share of the activation loss voltage among the total loss voltages has been made. In this work, it has been assumed that the fuel cell function takes place at the maximum power point. Therefore, the maximum power points are first obtained by the perturbation and observation algorithm; then, calculations are performed to examine the effect of the charge transfer coefficient on various variables.

In Figure 4, samples one, two and three are for charge transfer coefficients of 0.3, 0.5 and 0.7, respectively. The results are summarized in Table 2.

By increasing the charge transfer coefficient, the activation voltage loss decreases. But ohmic losses and mass transfer losses increase with increasing charge transfer coefficient.

In the simulation, the effect of changing the charge transfer coefficient from 0.1 to 1 during ten steps on the diagrams of polarity, power in terms of current density and also the maximum power points are analyzed. For ten specific values of the charge transfer coefficient, the maximum power value is shown in Figure 5.

The changes of the maximum power points in the second half of the studied interval have smaller values than another half of the studied interval. In other words, with the increase of the charge transfer coefficient, the value of the maximum power point changes are negligible. In Figure 6, these changes were compared.

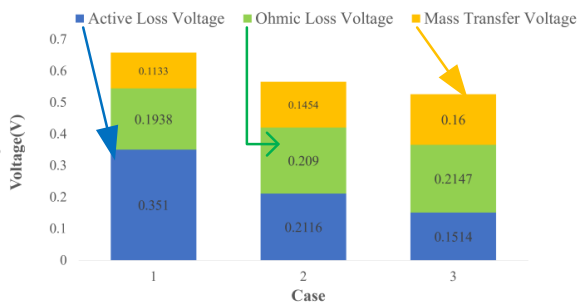


Figure 4. Comparison of different types of losses for charge transfer coefficient

Table 2. Comparison of voltage losses in three different charge transfer coefficient values in the working conditions of the maximum power point of the fuel cell

α	0.3	0.5	0.7
Seri	1	2	3
V_{act}	0.3510	0.2116	0.1514
V_{ohmic}	0.1938	0.2090	0.2147
V_{conc}	0.1133	0.1454	0.1600

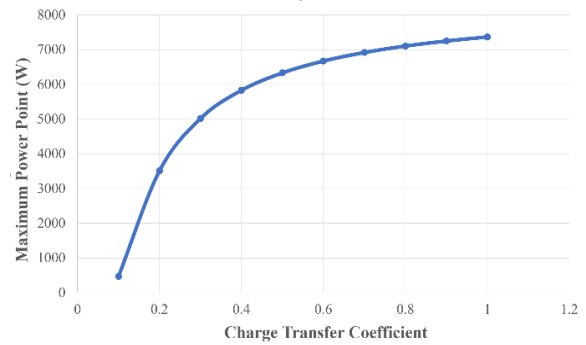


Figure 5. Waveform of maximum power points in different values of charge transfer coefficient

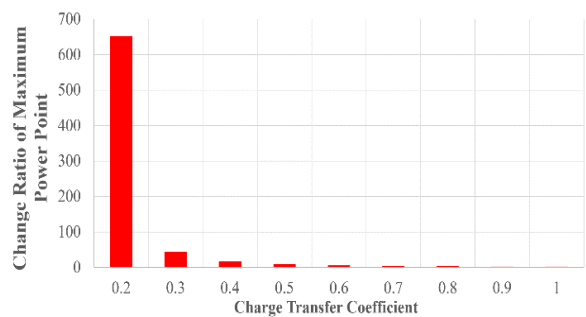


Figure 6. Ratio of power changes at the maximum point in each charge transfer coefficient

The ratio of maximum power point decreases as the number of steps, get increase. According to this figure, for the charge transfer coefficient of 0.5 and more, the changing ratio is very small.

In Figure 7, power changes are plotted in terms of charge transfer coefficient in four different values of current density. For the current density of 0.6 and 0.8, the power value has increased with increasing current density. But for the current density of 1 and 1.2, a small difference between the powers of each is observed. The reason for this is that the maximum power point is located between these two current density values.

Regardless of the issue of the balance of chemical reactions in a fuel cell, by increasing the charge transfer coefficient, the increase in voltage and power can be seen for the same current density. In Figure 7, the polarity curves of a fuel-cell stack are drawn for different values of the charge transfer coefficient.

In addition, this comparison is drawn in Figure 7 for the power curve in terms of current density.

In Figure 8, the polarity is drawn based on the base sample in ten different values of the charge transfer coefficient. According to this diagram, in a certain current density, the voltage increases with the increase of the charge transfer coefficient. Following the increase in voltage at a certain current density, the output power will also increase. The comparison of power values is shown in Figure 9.

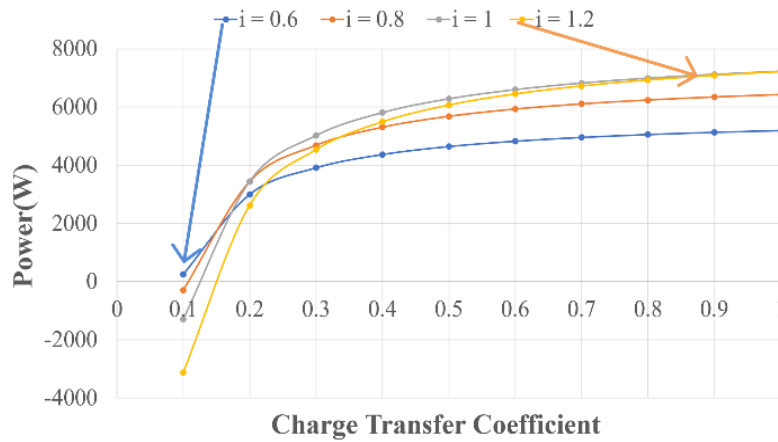


Figure 7. Comparison of power in terms of charge transfer coefficient in different current density

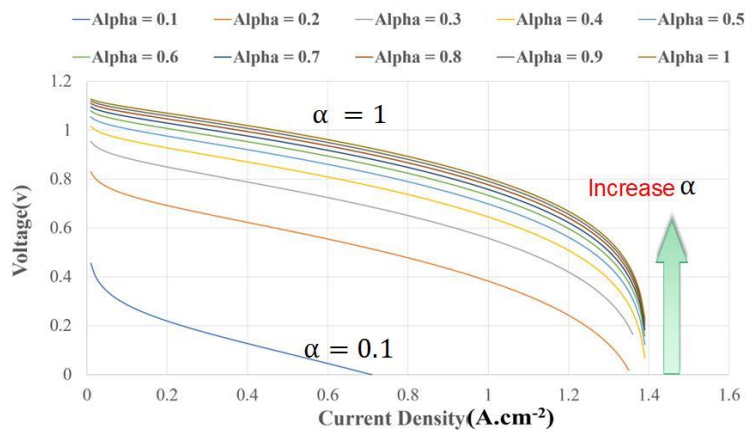


Figure 8. Variations of polarities in terms of current density under charge transfer coefficient change

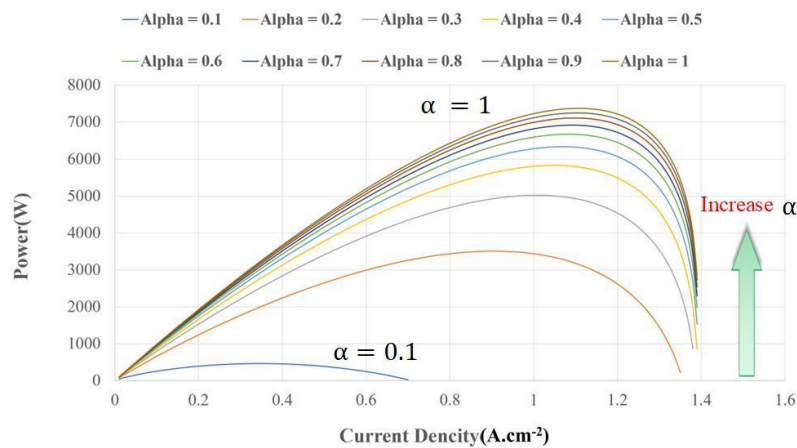


Figure 9. Power waveform in terms of current density under charge transfer coefficient change

Charge transfer coefficient affects the obtained value for the activation voltage because this factor has an inverse effect with coefficient b in Equation 1 (according

to Equation 2). Therefore, it affects the total voltage behavior and consequently the non-linear power effect, which is observable in Figure 9.

CONCLUSION

Increasing the charge transfer coefficient directly reduces the activation losses and total losses of the entire system. On one hand, this issue leads to an increase in voltage and power, but it should be noted that this increase in power is small for charge transfer coefficients greater than 0.5. On the other hand, the balance of chemical reactions is provided within the value range of 0.5 for charge transfer coefficient. As a result, increasing it up to a certain value can help improve the efficiency and stability of the system.

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Persian Abstract

چکیده

ضریب انتقال بار، یک ضریب بی‌بعد است که در سینتیک واکنش‌های شیمیایی به کار برده می‌شود. در این مقاله، اثر ضریب انتقال بار بر ویژگی‌های سلول سوختی هیدروژن مانند منحنی پلاریزاسیون، نمودار توان به ازای چگالی جریان و هدررفت‌ها مورد بررسی قرار می‌گیرد. ضریب انتقال بار بر هدررفت‌های فعال‌سازی سلول سوختی اثر داشته و بنابراین به عملکرد سلول سوختی اثر می‌گذارد. در این تحقیق، یک نمونه اساسی انتخاب شده و تغییرات ضریب انتقال بار بر ویژگی‌های آن مورد مطالعه قرار می‌گیرد. در نتایج به دست آمده، مشاهده می‌شود که با افزایش این عامل، هدررفت فعال‌سازی کاهش می‌یابد. همچنین، افزایش ضریب انتقال بار نقطه بیشینه توان را افزایش می‌دهد. افزایش توان این نقطه در مقادیر کمتر ضریب انتقال بار به طور واضح‌تر است، و زمانی که این ضریب مقدار ۰/۵ را تجاوز می‌کند، اثر این افزایش بسیار کوچک می‌شود. همچنین، مقدار مناسب این ضریب برای حفظ تعادل واکنش شیمیایی تعیین می‌شود. بیشتر از این مقدار، فعالیت سلول سوختی به خطر می‌افتد.