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RESEARCH ARTICLE

Scattering of Free Electrons with Hydrogen Atoms in Proton Exchange Membrane Fuel Cell System

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ABSTRACT

The objective of this work is to study the Klein-Nishina (KN) cross section during the collision of free electrons and atoms (H-atom and Pt-atom) near the cathode of Proton Exchange Membrane Fuel Cell **(**PEMFCs). The developed KN cross section was computed using MATLAB shows KN cross section decrease with an increase with the temperature. The maximum KN cross section recorded for single scattering is about $-70.2\mathrm{m}^2$ and $-66\mathrm{m}^2$ in natural log terms during the collision of free electrons with H-atom and Pt-atom, respectively. The maximum KN cross section recorded for 1ml flow of hydrogen is about $-26.6\mathrm{m}^2$ and $-22.25\mathrm{m}^2$in natural log term during the collision of free electrons with H-atom and Pt-atom, respectively.

Keywords: Klein-Nishina cross section, Proton exchange membrane fuel cell, Efficiency

1 Introduction

Fuel cells have the potential to be used in a variety of applications, including major electrical plants, stationary electricity generation, portable power, and vehicle propulsion. The classification of fuel cells depends on a variety of factors, including operational circumstances (pressure, humidity, and temperature), fuel cell structure (application system and size), and the color of the polymer electrolyte used in fuel cells [1]. The type of electrolyte used to make fuel cells is often used to categorize them. Proton Exchange Membrane (PEM), Alkaline Fuel Cell (AFC), Phosphoric Acid Fuel Cell (PAFC), Solid Oxide Fuel Cells (SOFC), and Molten Carbonate Fuel Cell are examples of common fuel cell electrolytes (MCFC).

The polymer electrolyte membrane, which makes up the key part of the electrochemical device in a conventional PEMFC, is in charge of the proton conductivity that enables the transfer of protons from the anode to cathode. Due to high conductivity and favourable chemical and mechanical qualities, perfluorosulfonic acid polymer-based membranes, such as Nafion®, are among the many different types of fuel cells that are successfully used in low-temperature, high-relative-humidity environments. DuPont created Nafion® in the late 1960s, and it is still the most advanced low-temperature PEM available today [2], [3].

The catalyst is inserted between two electrodes between which the Polymer Electrolyte Membrane (PEM) is sandwiched. The PEM serves as an electrical barrier between the electrodes. The anode and cathode are made up of these two electrodes, respectively. The PEM is typically a proton permeable electrical insulating barrier made of fluoropolymer (PFSA). It is anticipated that hydrocarbon alternatives will replace fluoropolymers. This barrier makes it possible for protons to get from the anode to the cathode through membrane, but it compels electrons to take a circuitous route there instead. The Nafion XL, 112, 115, 117, and 1110 Nafion PEMs are the most frequently utilized types [4]. Typically, a carbon support, Pt particles, Nafion ionomer, and/or Teflon binder make up an electrode. The Teflon binder boosts the

electrode's hydrophobicity to reduce potential flooding, the Pt particles serve as reaction sites, the ionomer creates pathways for proton conduction, and the carbon support acts as an electrical conductor. Nearly 95 percent of new investments in power generation facilities globally are expected to be made in renewable energy-based facilities by 2026, according to the International Energy Agency (IEA). Hydrogen offers the lowest conversion losses of all chemical energy carriers and is produced in electrolysis procedures with efficiencies of between 70% and 80%. Compared to using green power directly, using green hydrogen in the transportation sector provides key benefits.

A hydrogen tank system has a volumetric energy density that is roughly 2.4 times higher than a lithium-ion arrangement with a got curious [5]. The second benefit of hydrogen is how quickly it can be used to fuel a vehicle. This is especially important for commercial vehicles since, like with machine tools, the operator's perception of breakeven depends on the usage rate for these vehicles [6]. Additionally, switching to regenerative energy sources in the transportation industry has a big impact on how much electricity is produced. The International Energy Agency (IEA) predicts that 197 TWh of power will be needed for electromobility in one scenario of sustainable development. Energy production and demand can be spatially and temporally separated if hydrogen can provide some of this requirement. According to market research firm Frost & Sullivan, green hydrogen production will reach 5.7 Mt, or 190 TWh of energy, by 2030 [6].

One of the biggest concerns facing the present and the future is climate change. Because the current technology has a problem with carbon emission, a lot of research is being done on battery and fuel cells to prevent climate change. However, whereas fuel cell and battery technology emit nearly no carbon, PEMFCs have an efficiency issue, meaning their efficiency is only about 50%. Numerous studies are being conducted to improve the remaining 50 percent of efficiency, but the main obstacle is collision, which causes temperature to rise near the fuel cell electrode.

2 Literature Review

The topic of fuel cells is not new, and origins can be found in 1839, when Welsh scientist William Grove created it for the first time but during the oil crisis in 1970s fuel cell vehicles first came to the attention of the world. The first commercially available fuel cell vehicle was released by Toyota in 2014, capping years of research and development work. As a result, the public began to view fuel cell cars as a significant component of the future of transportation rather than as an experimental technology. Countries including China, the US, Japan, and a number of European nations concentrated their efforts on advancing this technology over the following five years (till present) [7]. When hydrogen and oxygen interact chemically, they generate heat and energy. Because hydrogen has a vast storage capacity, it stands out as an alternative energy source beyond the capabilities of other ecologically benign energies. Beyond technological advancement and innovation, the switch from fossil fuels to hydrogen energy will alter the industrial paradigm and become a key determinant of future national competitiveness [8].

The International Energy Agency (IEA) estimates that in 2019, worldwide transportation-related emissions increased by less than 0.5%. Despite their slowing growth, transportation-related CO_2 emissions account for 24% of the total, with road vehicles (cars, lorries, buses, and two- and three-wheelers) making up 75% of this total. Additionally, emissions from shipping and the aircraft industry are rising. Commercial cars powered by hydrogen are also becoming more popular. In 2000, Ford Moto unveiled a two-wheel-drive car with a fuel cell stack and battery as its power source [9]. Starting with this, Toyota Motor Company and Hyundai Motor Company currently control the majority of the passenger-car market for hydrogen. Fuel cell vehicles cost 40 percent more to manufacture because of important parts like stacks. The growth of hydrogen fuel cell vehicles will be significantly aided by decreasing stack costs [10]. Recently, many attempts have been made to conduct research on technological analysis and prediction in the area of hydrogen fuel cell-based transportation. Patent study for hydrogen vehicle technology was able to identify significant technological choices while also confirming the potential of high-pressure storage technology. It allowed technology prediction using patent analysis in addition to identifying potential innovations [11]. Production, storage, and conversion of hydrogen energy were found to be core technologies, and the

conversion and application of hydrogen technology was validated as a mainstream technology [12]. Research to quantify the confluence of science and technology has been attempted as this field of study has grown over time.

Fuel cell technology is employed in a wide range of vehicle types, in part due to its simplicity. The PEMFCs Hamiltonian and output are studied by Saddam et al. [13] and the established model predicts that the Hamiltonian is directly related to current and cell voltage at constant response time (Nano-second). The Hamiltonian of the PEMFC grows with current density at activation overpotential 90mV smoothly, but at activation overpotential 1mV, a bump is seen at 0.47mAcm^{-2}. In addition, Hamiltonian of PEMFC at low temperature is greater than that at high temperature. The efficiency of the PEMFC can be boosted by reducing heat by looking at the Hamiltonian with temperature and its link to an output of PEMFCs because the temperature decreases the efficiency of PEMFCs which is one of the major challenges in PEMFCs technology [13]. PEMFCs have an electrical efficiency range of 40% to 60%. The operating efficiency of PEMFC can be increased to about 60% when high-purity H_2 is used as fuel. The electrical efficiency is down to about 40% due to the relatively low hydrogen level. PEMFC's low operating temperature helps it sustain over 50% of rated power even at a cold start. It also has infinite thermal cycling, quick startup or shutdown, excellent load tracking, and a straightforward BOP [14]. The comparable air flow of hydrogen is same, the total efficiency of mixture gas is 47%, while the highest efficiency of pure hydrogen is 52%, according to the fuel efficiency curve determined from the experimental data by Zhao et al. [15]. The maximum efficiency of mixture gas is also reduced by about 10% compared to the total efficiency of pure hydrogen [15].

3 Method and Materials

3.1 Principle of PEMFCs with formation of current generating species

Hydrogen and oxygen are injected into a fuel cell independently, with oxygen being provided to one electrode and hydrogen to the other of PEMFCs. The electrolyte, which functions as a filter to prevent the cell reactants from mixing directly with each other and to regulate how the charged ions formed during the complete cell reactions are permitted to reach each other, separates the two electrodes. As a result of the hydrogen molecules' reaction with the catalyst atop the anode, which also releases electrons, a positively charge ion is created. The second electrode is where these ions traverse the electrolyte and come into contact with the oxygen. However, the electrolyte prevents the electrons from passing. Instead, they enter a circuit that produces electricity, which powers the fuel cell device. The only consequence of the process is water vapor, which is formed at the cathode when hydrogen ions and electrons bind with oxygen from the air. Free electron, proton, and leftover hydrogen are created when hydrogen comes into touch with the electrodes' catalyst. When the formation electron collides with the hydrogen atom, a great deal of collisions occurs in the system, which causes heat to be produced. However, in this instance, we take into account the collision of a hydrogen atom and a free electron. PEMFCs have a serious issue with fuel cell efficiency because of the heat produced during collisions.

3.2 Klein-Nishina cross section for PEMFCs

Our main goal is to understand the differential cross section (Klein-Nishina) that results from the collision of an electron and a hydrogen atom. The classical Thomson scattering can be described using the generalized Klein-Nishina differential formula for Compton scattering with a finite train of pulses. $d\Omega$ is a solid angle, and the number of scattering photons produced into it equals

$$\frac{dN_{scat}}{d\Omega} = \int_{-\infty}^{\infty} \frac{\epsilon_0 c|E_x(\omega)|^2}{2\pi\hbar|\omega|} \frac{d\sigma}{d\Omega} d\omega \tag{1}$$

And because the scattered photon has energy $\hbar\omega'$, the total scattered energy is:

$$\frac{dU_r}{d\Omega} = \int_{\infty}^{\infty} \frac{\epsilon_0 c|E_x(\omega)|^2}{2\pi} \frac{\omega'}{\omega} \frac{d\sigma}{d\Omega} d\omega \tag{2}$$

The input gamma ray impacts an atomic electron, causing atomic ionization, and this is the primary scattering process for 511 Kev photons. The KIein-Nishina differential cross section equation will determine the angle at which the incident photon will scatter,

$$\left(\frac{d\sigma}{d\Omega}\right)_a = \frac{Zr_e^2}{2}\left(\frac{1}{1+\alpha(1-cos\theta)}\right)^2\left((1+\cos^2\theta)+\frac{\alpha^2(1-cos\theta)^2}{[1+\alpha(1-cos\theta)]}\right) \quad (3)$$

A nonlinear atomic cross - section area solution for K-N can be found here. Additionally, the total atomic K-N cross section can be expressed by Knoll in 1989,

$$\sigma_a = 2\pi\int_0^{\pi}\left(\frac{d\sigma}{d\Omega}\right)_a sin\theta d\theta \quad (4)$$

Where θ is scattering angle overall photons. Now from (3) and (4), we get:

$$\sigma_a = 2\pi\int_0^{\pi}\frac{Zr_e^2}{2}\left(\frac{1}{1+\alpha(1-cos\theta)}\right)^2\left((1+\cos^2\theta)+\frac{\alpha^2(1-cos\theta)^2}{[1+\alpha(1-cos\theta)]}\right)sin\theta d\theta \quad (5)$$

On solving the total KN cross section per atom is obtained as:

$$\sigma_a = Z2\pi r_e^2\left\{\frac{1+\alpha}{\alpha^2}\left[\frac{2(1+\alpha)}{1+2\alpha}-\frac{\ln(1+2\alpha)}{\alpha}\right]+\frac{\ln(1+2\alpha)}{2\alpha}-\frac{1+3\alpha}{(1+2\alpha)^2}\right\} \quad (6)$$

Since electronic cross-sections are multiplied by each element's charge number Z to get Klein-Nishina atomic cross-sections, equation (5) states that the electronic cross-sectional area for KN with the help of $\sigma_a = Z.\sigma_e$ is:

$$\sigma_e = 2\pi r_e^2\left\{\frac{1+\alpha}{\alpha^2}\left[\frac{2(1+\alpha)}{1+2\alpha}-\frac{\ln(1+2\alpha)}{\alpha}\right]+\frac{\ln(1+2\alpha)}{2\alpha}-\frac{1+3\alpha}{(1+2\alpha)^2}\right\} \quad (7)$$

where Z is the target molecule's nuclear charge, $r_e = 2.818\,fm$ is the classical electron radius, and $\alpha = \frac{E}{m_e c^2} = \frac{hf}{0.511MeV}$ reported by Knoll in 1989. As a result, this equation provides the mass attenuation coefficient, also known as the Compton mass attenuation coefficient, in terms of KN parameters. Where Z is the atomic number, A is the material's atomic mass, and N A is the Avogadro's number (6.02×10^{23} $atom/\,mol$) [16]. $E = \sigma T^4$ is the equation when the heat flux is replaced by the thermal radiation produced by the impact, where $\sigma = 5.6693 \times 10^{-8}\mathrm{W/(m^2.K^4)}$ then rewrite equations (6) and (7) as,

$$\sigma_{aT} = Z2\pi r_e^2\left\{\frac{1+\alpha_T}{\alpha_T^2}\left[\frac{2(1+\alpha_T)}{1+2\alpha_T}-\frac{\ln(1+2\alpha_T)}{\alpha_T}\right]+\frac{\ln(1+2\alpha_T)}{2\alpha_T}-\frac{1+3\alpha_T}{(1+2\alpha_T)^2}\right\} \quad (8)$$

$$\sigma_{eT} = 2\pi r_e^2\left\{\frac{1+\alpha_T}{\alpha_T^2}\left[\frac{2(1+\alpha_T)}{1+2\alpha_T}-\frac{\ln(1+2\alpha_T)}{\alpha_T}\right]+\frac{\ln(1+2\alpha_T)}{2\alpha_T}-\frac{1+3\alpha_T}{(1+2\alpha_T)^2}\right\} \quad (9)$$

Where $\alpha_T = \frac{\sigma T^4}{0.511MeV} = \frac{5.6693\times10^{-8}T^4}{0.511MeV}$, the given equation (8) and (9) determine the atomic and electronic cross section near electrode of fuel cell because the crosse section determine the reaction region where hydrogen atom and free electron get collision.

4 Results and Discussion

4.1 Scattering cross section due electron and residual hydrogen atom near PEMFCs electrode.

When hydrogen get contact with catalyst (platinum) coated electrode, the free electrons formed due to ionization of hydrogen atom. The free electron gets collide with residual hydrogen atom and platinum

atom of electrode (other collision like electron-proton, electron is the limitation of this study, that we don't take on consideration of study), the KN differential cross section per atom of hydrogen atom for single reaction shown in figure 1 and flow of 1ml hydrogen towards cathode electrode shown in figure 2 of PEMFCs. The single cross section per atom of figure 1 and 1ml flow of hydrogen of figure 2 is taken in nature log. The nature of KN cross section shows linear decrease with increasing in temperature. Since we assume that the collision taken place near electros due to which temperature increase. The impact of temperature causes the deviation on the current of PEMFCs. The maximum KN cross section was recorded for single scattering is about $-70.2\mathrm{m}^2$ in natural log term.

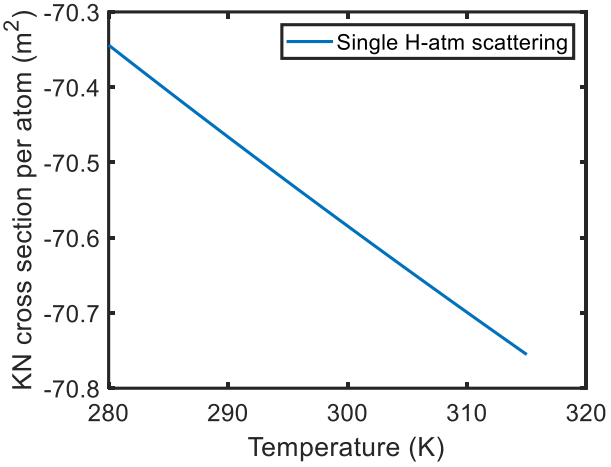

Figure 1: *KN differential cross section of single hydrogen atom and electrons*

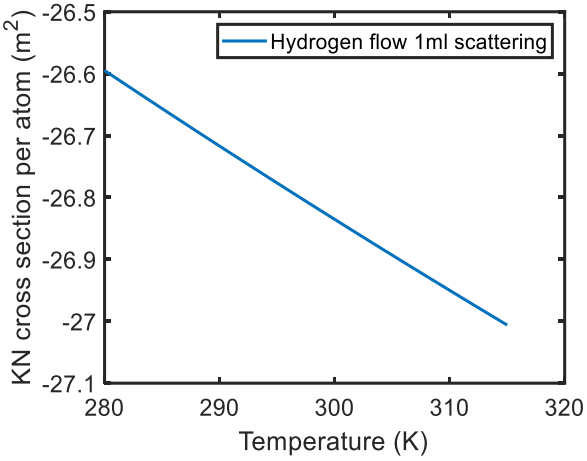

Figure 2: *KN differential cross section with flow of 1ml hydrogen and electrons*

Comparing figure 1 and figure 2, shows that the KN differential cross section goes decrease with increase but the KN differential cross shows with increasing the flow of hydrogen. The KN differential cross section with flows of 1ml of hydrogen (10^{19} hydrogen atoms) per section great than single flow atom or lower number of hydrogen input in PEMFCs at cathode side. The greater the flow of hydrogen per second cause the lower differential cross section and lower differential cross section cause higher electron density. The higher electron density has probabilities to cause more collision which generate more heat radiation and this heat radiation cause the damage of internal mechanism of PEMFCs. In addition, the temperature also cause decrease in efficiency of PEMFCS. Therefore, we are searching the best flow rate of hydrogen and suitable cross section area of hydrogen atom which is beginning through this work. The maximum KN cross section was recorded for 1ml flow of hydrogen is about $-26.6\mathrm{m}^2$ in natural log term.

4.2 Scattering cross section due electron and Pt-atom PEMFCs electrode.

When free get collied with catalyst (platinum) coated electrode, the interaction between free electron and Pt-atoms takes places. The interaction take place in the region is defined by KN differential cross section, this interaction also produce heat whose impact is observed in output current and voltage of PEMFCs. As in literature it was found that the temperature is the major cause of reduced in efficiency of PEMFCs, therefore from figure 3 and figure 4 it was observed that the impact of temperature to KN differential cross section is linear. The single cross section per atom of figure 3 and 1ml flow of hydrogen of figure 4 is taken in nature log. Since we assume that the collision taken place near electros due to which temperature increase. The impact of temperature causes the deviation on the current of PEMFCs. The maximum KN cross section was recorded for single scattering is about $-66\mathrm{m}^2$ in natural log term.

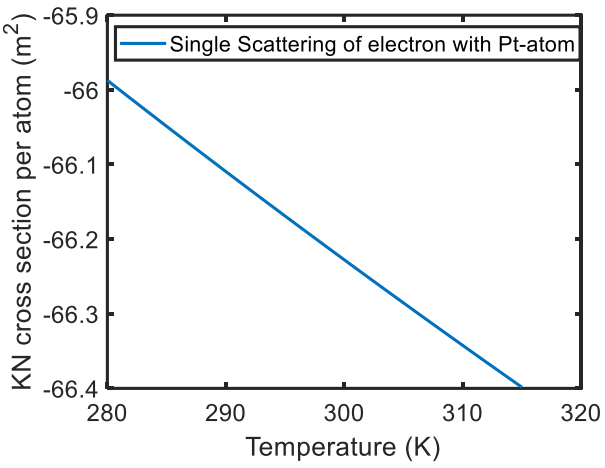

Figure 3: *KN differential cross section of single Pt-atom and electrons collision*

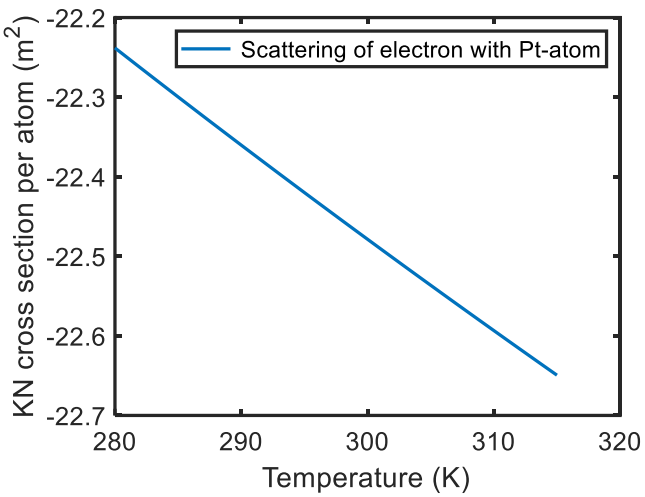

Figure 4: *KN differential cross section with flow of 1ml hydrogen, with Pt-atom and electrons collision*

Comparing figure 3 and figure 4, shows that the KN differential cross section goes decrease with increase but the KN differential cross shows with increasing the flow of hydrogen. The greater the flow of hydrogen per second cause the lower differential cross section and lower differential cross section cause higher electron density. The higher electron density has probabilities to cause more collision which generate more heat radiation and this heat radiation cause the damage of internal mechanism of PEMFCs. In addition, the temperature also cause decrease in efficiency of PEMFCS. Therefore, we are searching the best flow rate of hydrogen and suitable cross section area of hydrogen atom which is beginning through this work. The maximum KN cross section was recorded for 1ml flow of hydrogen is about $-22.25\mathrm{m}^2$ in natural log term.

5 Conclusion

KN differential cross section in this work is calculated for collision of free electron with hydrogen and platinum as target. The maximum KN cross section was recorded for single scattering is about $-70.2\mathrm{m}^2$ in natural log term and with 1ml flow of hydrogen was recorded about $-26.6\mathrm{m}^2$ in natural log term when collision take place between hydrogen atom and free electrons. The maximum KN cross section was recorded for single scattering is about $-66\mathrm{m}^2$ in natural log term and with 1ml flow of hydrogen was recorded about $-22.25\mathrm{m}^2$ in natural log term when collision take place between platinum atom and free electrons.

6 Declarations

6.1 Competing Interests

The authors declared that they have no conflict of interest related to this work.

6.2 Publisher's Note

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