

Original Research

Numerical Study to Understand the Conservation of Hydrogen Through a Dynamic Fuel Supply System in Proton Exchange Membrane Fuel Cells (PEMFCs)

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Abstract

Reducing and conserving fuel usage is pivotal for any engineering system for the development of a sustainable energy solution. Proton exchange membrane fuel cells (PEMFCs) are one of the promising renewable energy systems that consume hydrogen as their source of fuel to generate electricity. This paper investigate the necessity of the constant supply of fuel (hydrogen) in the PEMFC system to ensure stable operation. We propose that a dynamic supply of fuel could help achieve similar performance and reduce the amount of fuel used. The effect of the multiple dynamic fuel inlet rates (0.3 m/s, 0.2 m/s, and 0.1 m/s) was studied numerically using a validated CFD PEMFC model. A transient inlet condition was introduced to replicate the pulsating effect. It was observed that up to 66% of fuel could be conserved (compared to the constant fuel supply condition) while maintaining the stable performance of the PEMFC under conditions of a dynamic fuel profile. A drop of approximately 29% in PEMFC performance was observed under conditions



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of a low dynamic fuel profile. The results reveal that the concept of dynamic fuel supply can be exploited to sustain the performance of PEMFC and realize a threshold value of performance under conditions of reduced fuel input.

Keywords

PEMFC; CFD; hydrogen; fuel; dynamic fuel profile; current

1. Introduction

Polymer electrolyte membrane fuel cell (PEMFC) utilizes hydrogen as its source of fuel. The cells participate in the electrochemical process to convert chemical energy to electrical energy to produce power [1]. A thin polymeric membrane acts as the electrolyte to electrochemically segregate the hydrogen molecules into protons and electrons [2-4]. The electrolyte restricts the flow of electrons from the anodic to the cathodic region within the PEMFC. This enables the spatial segregation of the two electrochemical half-reactions.

The inlet flow rate controls the flow of hydrogen. Entry of excess fuel can result in water accumulation within the PEMFC system. This can eventually result in flooding. Under these conditions, the pores of the electrodes in the gas diffusion layer are obstructed [5]. It is difficult to maintain the humidity level inside the system and conserve the material integrity of the membrane in PEMFCs. Hence, mismanagement of fuel supply can inadvertently result in the degradation of PEMFCs [5-7]. A low fuel supply, on the other hand, would result in starvation. Under these conditions, the number of reactants required for the stable operation of PEMFC is insufficient. Hence the generation of electricity cannot be sustained, resulting in the deteriorating performance of PEMFCs [5]. Proper control over fuel should be gained to ensure the steady operation of PEMFC. Even though carrying fuel in excess is recommended, an excess of fuel can potentially limit the applications in compact systems such as Unmanned air vehicles (UAVs). With more than 90% of the hydrogen separation techniques utilizing traditional energy resources such as natural gas, fossil fuels, and oil, fuel conservation becomes a crucial element in PEMFC application [8]. This can potentially reduce the load of the hydrogen storage tanks used and limit the excess usage of fuel. The polarization curve reflects the operation of PEMFCs over a range of voltage against the corresponding current density [1, 5, 7, 8]. The curves can be analyzed to evaluate the performance of the cells. The range of voltage demonstrates that the PEMFCs operate below the desired (ideal) thermodynamic voltage, and this is attributable to three types of regions associated with irreversible losses: activation region, ohmic region, and concentration (or mass transport) region. The extent of losses at the activation region is dictated by the amount of energy required to initiate the electrochemical process. The voltage losses observed in the ohmic region help increase the internal resistance associated with the fuel cells. The voltage drop observed at the concentration region is attributable to the increased transportation of the reactants entering the cathode channel from the anode [1, 5, 7, 8]. Efforts are being made to limit the extent of losses realized within the PEMFCs to prevent the fuel cell from deteriorating and lift the cells to the status of a potential

reliable energy source. The impact of dynamic loading on the PEMFCs was studied to understand the practical applications of the cells and study the fuel cell performance.

The impact of transient loads on PEMFC has been thoroughly examined experimentally to ascertain the transport and mobile applications [9-11]. An in-depth understanding of the dynamics of the changes in current, voltage, and power in PEMFCs is required as PEMFCs are attracting immense attention. Pei and Chen examined the primary causes that affect the lifetime of PEMFCs that are used in vehicles. The steady and transient performances of PEMFCs were considered [11]. Factors such as loading range, loading speed, stoichiometric ratio, humidity, and gas starvation were identified as the primary factors that affected the life of the PEMFCs with dynamic applications [9-11]. An in-house experimental investigation of PEMFC was conducted, and Woo and Benziger [12] regulated the fuel feed (hydrogen) to monitor the performance of the fuel cell by observing the current output. Pure hydrogen was used as the fuel with minimal impurities. Results revealed that the regulation of current by controlling the fuel supply improved the efficiency of the system and simplified the control system as the need for additional infrastructure to recycle excess fuel was eradicated. However, the practicality of replicating such an experimental setup to realize real-life applications should be investigated further. Huang et al. [13] examined the voltage response of the PEMFCs to the changes in the current densities and witnessed that different dynamic loading conditions affected the performance of PEMFCs. This could be attributed to the necessity of maintaining an appropriate hydration level within the fuel cell system. Dynamic operating conditions were also used for PEMFC systems to develop carbon corrosion mitigation strategies [14, 15].

Choi et al. [16] studied the process of reducing the fuel consumption in PEMFCs. They conducted experiments to reduce the purging frequency of water vapor (at the cathode channel) to address the difficulties faced during water management in a cathodic dead-end mode PEMFC to control flooding. A pulsating profile was applied to the pressure at the cathode outlet through a pressure regulator. Choi et al. [17] developed a way of reducing the purging frequency of water vapor using a pulsating hydrogen profile in an anodic dead-end fuel cell. A significant reduction in the purging frequency could be realized, and this indicated that fuel efficiency could be achieved using a pulsating fuel profile. The experimental results revealed that good fuel cell performance could be achieved, and this could be attributed to the enhanced diffusivity observed within the fuel cell membrane. The increase in diffusivity could be attributed to the oscillating fuel profile. Peng et al. [18] analyzed the effects of various parameters of a dead-end anode PEMFC. They studied the inlet pressure of anode gas and investigated the effects of a gas purging mechanism on the performance of the fuel cell. It was found that the dip in current could be correlated to the reduced hydrogen content, and a periodic purging mechanism improved the overall performance of the PEMFCs. Fan et al. [19] reported the effects of the pressure-based gas purging mechanism and evaluated its effect on the current density. It was found that the voltage of the fuel cell dropped significantly under conditions of high current density, and the dynamic purging process helped recover a significant amount of voltage loss. The positive effect of the purging mechanism was prominent at lower purge intervals. The effects helped maintain the fuel cell performance. Tuning the design of the recirculation ejector helped improve the performance of the PEMFCs by reducing the extent of voltage drop realized during the purging process. This helped reduce water flooding within the fuel cell system [20]. Further studies on the dynamic nature of pressure

associated with the purging process and its impact on PEMFC performance were also thoroughly investigated [21-23]. However, the effects on hydrogen conservation were not studied.

Wang and Wang [24] developed a three-dimensional single-channel PEMFC transient numerical model to study the transient dynamics of the fuel cells under conditions of varying current densities. The results were recorded under conditions of a step-change in the operating conditions. Shimpalee et al. [25, 26] and Dutta et al. [27] used the commercially available CFD solver to solve the governing equations. They presented the governing equations required for the modeling of PEMFC. The mandatory source terms for species transportation across the membrane were accounted for in the governing equations by developing subroutines in ANSYS Fluent [27-30]. Um et al. [28] constructed a transient, multi-dimensional fuel cell model to investigate the reactant flow, current distribution, and multi-component transport in a realistic fuel cell using the CFD approach. Similar analyses were also carried out to investigate several other CFD models [31-33]. A good approximation of the actual PEMFC performance was observed.

Experimental and numerical studies were conducted to investigate the effects of reactant activity on the performance of PEMFCs. Dynamic loading and gas purging processes were used for analysis. The experiments were not explicitly directed toward characterizing the transient performance of fuel cells as a function of the fuel supply rate. The necessity of a continuous and constant fuel supply to ensure the performance stability of PEMFC is an area that is not widely investigated. We adopted a numerical approach to explore the effect of different transient fuel supply rates on the PEMFC performance. We also studied the modes of fuel conservation. An unsteady inlet profile was imposed on the fuel (hydrogen) supply rate of PEMFCs to identify the possible reduction in the fuel usage in PEMFCs. This had minimal impact on the performance of the cells. This study seeks to find ways of reducing hydrogen consumption without compromising the performance of the PEMFC.

2. Numerical Methodology associated with the PEMFC CFD Model

The transient numerical model developed by us is an extension of the works of Cheng et al. [34], where fuel cell performance was analyzed under steady-state operating conditions. The following key assumptions were considered during the modeling of the PEMFC model:

- 1) Laminar flow of reactants
- 2) Ideal gas law obeyed by all fluids
- 3) GDL and MEA (Membrane Electrode Assembly) were considered to be homogenous, isotropic, and porous
- 4) Single-phase analysis, i.e., water was assumed to exist only in the vapor phase
- 5) The dynamic fuel profile was implemented only after a stable PEMFC operation was established (PEMFC in steady-state condition)

2.1 Governing Equations of PEMFC

A specific add-on PEMFC module available for ANSYS Fluent was utilized to study the physical and electrochemical reactions of the model [35]. The following equations were derived from the principles that govern the physical and electrochemical models of PEMFC associated with CFD. These equations

were discretized based on the finite volume technique and numerically solved in ANSYS Fluent [35]. The equations were used to develop the PEMFC model to capture all physical and chemical phenomena in the various regions.

The equation for the conservation of mass can be expressed as follows:

$$\frac{\delta \rho_i}{\delta t} + \nabla \cdot (\rho_i u_i) = 0 \quad (1)$$

The equation for the conservation of momentum can be expressed as follows:

$$\frac{\delta(\rho_i u_i)}{\delta t} + \nabla \cdot (\rho_i u_i u_i) = -\nabla p_i + \nabla \cdot \tau_i + F_i \quad (2)$$

Equation (1) and Equation (2) were adapted from Wang et al. [31] and Um et al. [23]. These equations account for the momentum and mass balances that determine the fluid motion of a species i at a specific phase. The equations stated above were based on the assumption that a single domain approach was adopted for the fuel cell module, i.e., no interfacial conditions were considered to describe the existing internal boundaries between the various regions. The symbol ρ presents the density of the species at each phase, u is the velocity vector of the species at each phase, p is the pressure, τ is the shear stress tensor, and F represents the body forces of the species at each phase.

The equations for the conservation of charge can be expressed as follows:

$$\nabla \cdot (\sigma_{sol} \nabla \phi_{sol}) + R_{sol} = 0 \quad (3)$$

$$\nabla \cdot (\sigma_{mem} \nabla \phi_{mem}) + R_{mem} = 0 \quad (4)$$

The conservation of charge introduces several terms that determine the flow of electric current at various regions of the fuel cell. The symbols σ and ϕ refer to the electrical conductivity and electric potential of the solid region (CC) and membrane of the fuel cell, respectively. The source term, R , presents the volumetric transfer current associated with the solid and membrane phase. The solid and membrane phase terms are represented by sol and mem subscripts, respectively. These terms are the only non-zero terms at the catalyst layers of the fuel as these are the only two regions that facilitate the separation (anode catalyst layer) and combination (cathode catalyst layers) of hydrogen electrons.

The equation for the conservation of species can be expressed as follows:

$$\frac{\delta(\epsilon X_i)}{\delta t} + \nabla \cdot (\epsilon u X_i) = \nabla \cdot (D_i^{eff} \nabla X_i) + S_i \quad (5)$$

The equation for species balancing associated with PEMFC includes a diffusion term to account for the diffusivity of species at the gas phase in ANSYS Fluent [30]. The symbol X_i refers to an arbitrary species concentration, D_i^{eff} refers to the effective diffusivity of a species, and S_i signifies the source terms for each species. To account for the leakage in current occurring during species cross-over (from the anodic to the cathodic electrode (GDL)) via the membrane, terms accounting for specific leakage current (A/m^3) are also included in the PEMFC model in addition to the source terms.

2.2 PEMFC – Geometry and Mesh Methodology

A single three-dimensional fuel cell module of the complete fuel cell was considered for this study to replicate the entire cell. The module accounted for the symmetrical nature of the system. The PEMFC consisted of a parallel flow design, and the dimensions of the fuel cell model were adapted from the works of Cheng et al. [34]. The components constituting the fuel cell module consisted of layers of current collectors (CC), gas channels (GC), and gas diffusion layers (GDL) on the anode and cathode sides. The MEA was sandwiched between the GDL (Figure 1a and Figure 1b).

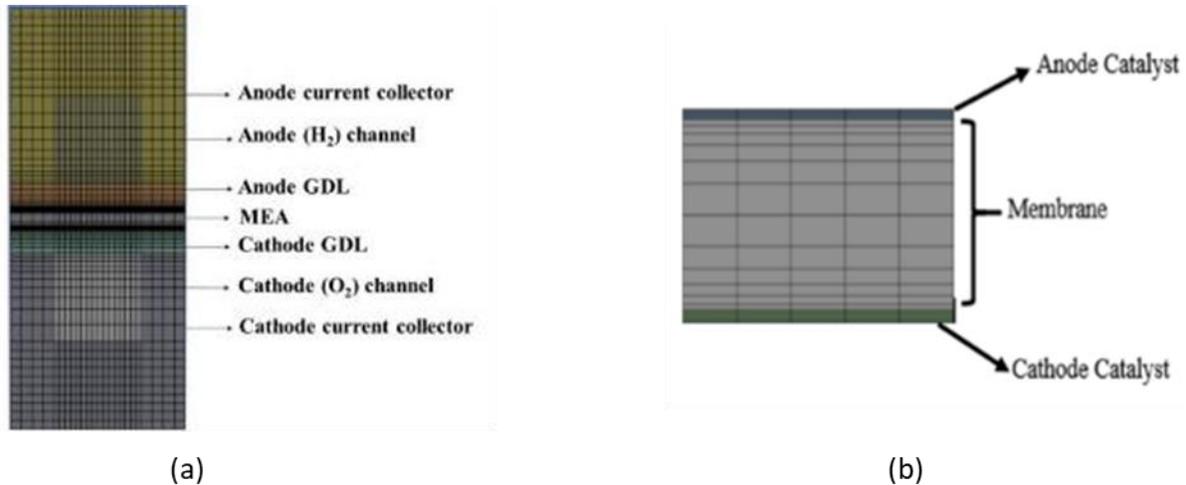


Figure 1 (a) Grid arrangement corresponding to the PEMFC CFD model and (b) enlarged view of the membrane electrode assembly (MEA).

A hexahedral meshing scheme was used to develop the fuel cell module. The model was subdivided into multiple blocks based on the different components of the PEMFC to identify the mesh settings. The maximum emphasis (lowest grid spacing) was given to the study of MEA as this region accounted for the occurrence of physical and chemical phenomena, including the electrochemical process, electro-osmotic drag, and diffusion of reactants. It is important to understand the principles of physics governing the flow of reactants in this region to obtain a reliable and accurate solution using the ANSYS Fluent CFD solver. The grid independence test was conducted to understand the mesh redundancy of the CFD model. The spacing between the grids within the MEA defined the variations observed in the cases of the coarse, medium, and fine mesh arrangements. The polarization curve was analyzed to study the mesh independence of the PEMFC model (Figure 2). The results revealed that a medium-mesh arrangement produced a computationally efficient mesh model, which consisted of 211200 grids and 224724 nodes.

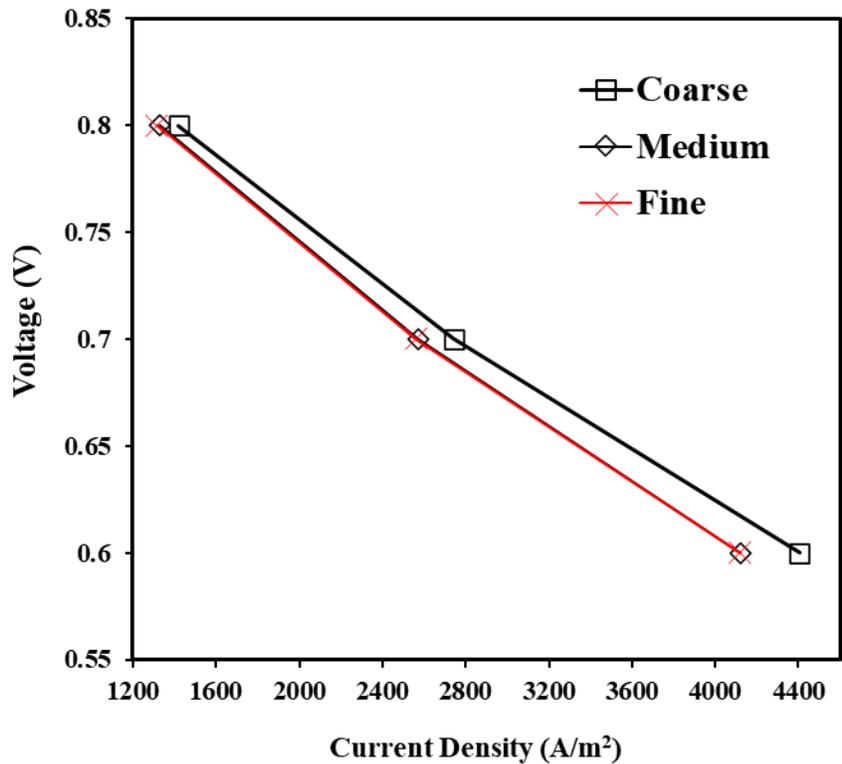


Figure 2 Results from grid independence test.

2.2.1 Boundary Conditions

The boundary conditions for the PEMFC numerical model were adopted from the experimental works of Cheng et al. [34]. The flow of the reactants was specified under a fixed inlet velocity condition. The inlet velocities of hydrogen and oxygen were 0.3 m/s and 0.5 m/s, respectively, and a pressure outlet condition was specified for the outlet of the anode and cathode channels. A constant electric potential (cell voltage) was maintained to attain the corresponding current density. A User Defined Scalar (UDS) was used for the same. The top and bottom surfaces of the CC were defined as the anode and cathode terminals, where the electric potential of the anode CC was assigned as 0 V (ground voltage), and the cathodic CC was varied from 0.8 to 0.6 V to plot the polarization curve. The exteriors of the MEA, GDL, and other components were considered stationary walls under the no-slip condition. The operating pressure and temperature were assumed to be 1 bar and 343 K, respectively. These boundary conditions reflected the fuel cell operation conditions under steady-state conditions. The transient boundary condition will be detailed further in the following sections.

2.2.2 Inlet Treatment for Fuel Supply

It was postulated that the flow rate of the fuel supplied at the anode could vary as a function of time. It was assumed that the variation in the flow rate could help reduce the extent of fuel consumption. Under this condition, the fuel supply would fluctuate between a maximum and minimum

flow rate to ensure the availability of fuel at regular intervals. Hence, a transient boundary condition at the inlet of the anode channel would facilitate the variation in the fuel feed rate. It must be noted that the transient boundary condition should be applied to the PEMFC once a stable condition is achieved, i.e., under steady-state operation conditions of PEMFC. We aimed to identify whether a fluctuating fuel flow rate could help maintain stable PEMFC operation and eventually help conserve fuel. A novel dynamic fuel supply profile has been introduced in Equation (6) to address the problems associated with fuel supply fluctuation by adopting the Fourier series method. The equation can be expressed as follows:

$$f(t) = \frac{H^2}{2} + \frac{2H^2}{\pi} \left(\frac{\sin((2n - 1)(\pi t))}{(2n - 1)} \right), \tag{6}$$

where \dot{H}_2 indicates the flow rate of the hydrogen gas entering the PEMFC, and t refers to the simulation time step. This expression was defined as a User Defined Function (UDF) in ANSYS Fluent and assigned as the transient inlet condition at the entry of the anode gas channel. This fluctuating effect would constantly alternate every second, from $t = 0$ s to $t = 10$ s (Figure 3). The performance of PEMFC under this condition was compared with the performance recorded under the experimental and constant fuel supply conditions. The results were arrived at by analyzing the polarization curve.

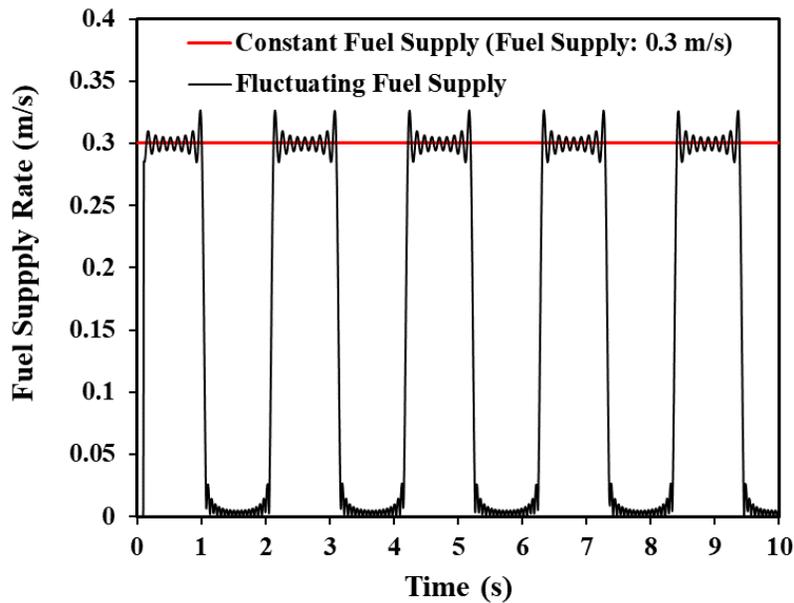


Figure 3 Steady-state and pulsating profiles of fuel flow rate.

2.3 Validation and Implementation of Dynamic Fuel Profile

The validity of the numerical model was determined based on the performance of the PEMFCs achieved under conditions of a constant fuel supply rate (Figure 4). This served as a baseline of comparison against the effect of the pulsating fuel supply on the PEMFC performance. A total of 10

simulation runs were performed for the current section of the analysis. The steady-state fuel cell performance was monitored at 5 different cell voltages: 0.8 V, 0.75 V, 0.7 V, 0.65 V, and 0.6 V. The numerical model was able to capture the behavior of the fuel cell at all cell voltages. A considerable variation between the numerical and experimental results was noticed at the higher voltage region (low current density) of 0.8 V. The discrepancy could be attributed to the slow reaction rate of the reactants. The discrepancy was noted during the initial phase of the electrochemical process. Under these conditions, sufficient energy was gained to overcome the surface overpotential. However, the current density attained using the numerical model at other cell potentials deviated within 5% of the accepted value. This established the high fidelity of the numerical model developed.

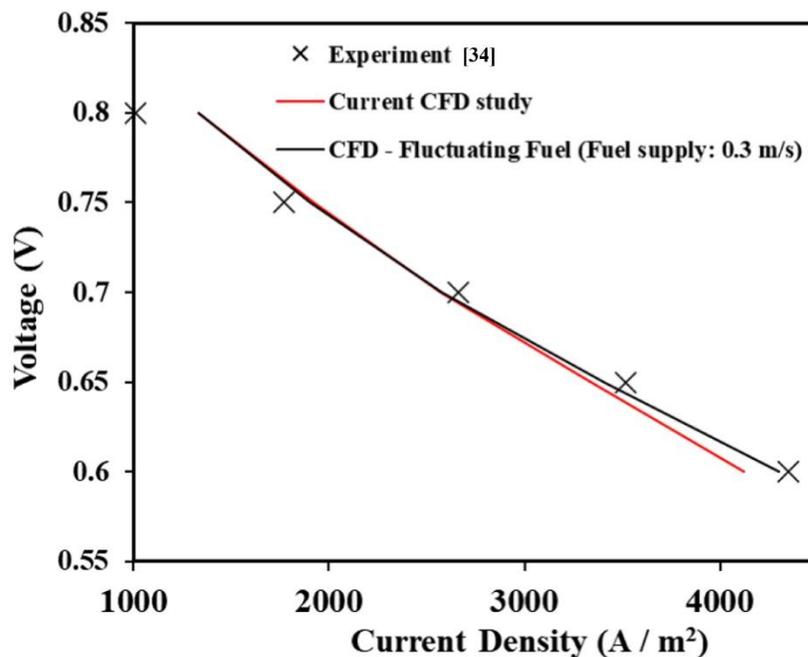


Figure 4 Comparison of the polarization curves.

The dynamic inlet condition for fuel supply was incorporated into the validated numerical model. An unsteady simulation was carried out at the cell voltages specified earlier to study the effect of the dynamic inlet profile on the PEMFC performance. The transient simulation results were plotted along with the steady-state simulation and experimental results (Figure 4). The results were highly encouraging as the PEMFC performance did not drop significantly under conditions of pulsating fuel profile. The current density achieved at all different cell potentials under conditions of the pulsating fuel supply did not vary significantly from the current density achieved under conditions of constant fuel supply.

Results from the initial simulation runs conducted on the dynamic inlet condition were analyzed to reduce fuel consumption. We assumed that the fuel supply rate was 0.3 m/s. This was similar to the rate reported by Cheng et al. [34]. Two low fuel flow rates were considered to study the effect of the oscillating fuel supply profile at different flow rates. Hereafter, we shall report the dynamic response

of the PEMFCs under conditions of three transient fuel inlet conditions. The PEMFC performance will also be characterized. Moving forward, the simulation cases will be performed over 10 s. The pulsating fuel supply profile would be termed as Case 1, Case 2, and Case 3 for the inlet fuel flow rates of 0.3 m/s, 0.2 m/s, and 0.1 m/s, respectively (Figure 5).

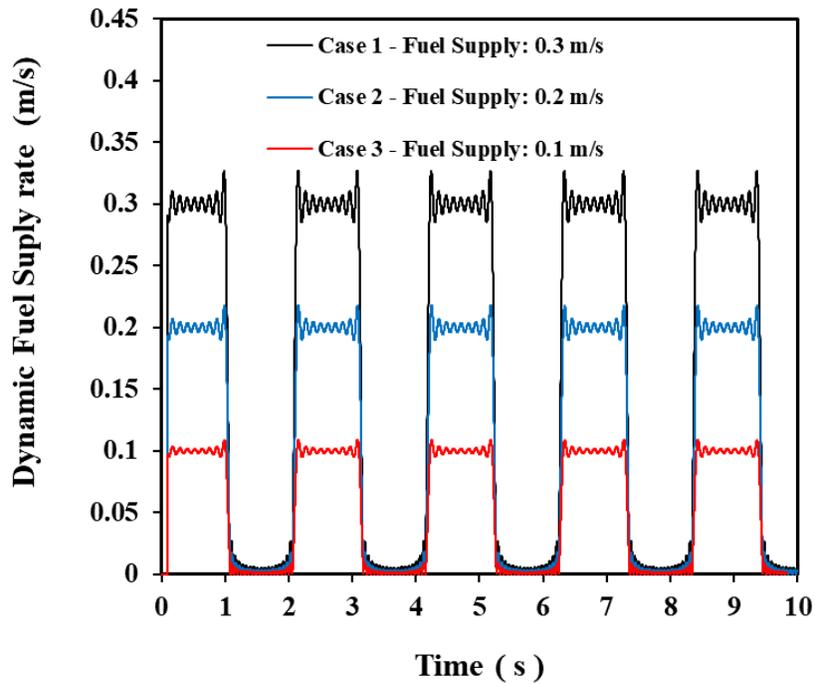


Figure 5 Variation of dynamic fuel supply profiles.

3. Results and Discussion

3.1 Transient PEM Fuel Cell Performance

Fuel cell voltages of 0.7 V and 0.6 V were used to represent the high electric potential regions (0.8 V, 0.75 V, and 0.7 V) and low electric potential regions (0.65 V and 0.6 V), respectively, as the CFD results were similar for all cases. The effect of the fluctuating hydrogen concentration was studied by analyzing the changes in the pattern of current generation observed in these regions. The ratio between dynamic current and the steady-state current ($\frac{\text{Dynamic Current}}{\text{Constant Current}}$) was plotted against hydrogen concentration to determine the relationship between the current generated under conditions of fluctuating fuel supply and the steady-state current (constant fuel supply). A sawtooth-like profile was noticed for the hydrogen concentration profiles in all cases (Figure 6 and Figure 7). The instantaneous increase and decrease in the hydrogen content at every second reflected the nature of the fluctuating fuel supply profile (Figure 5). At 0.7 V, an insignificant difference was observed between the overall current density achieved under conditions of constant fuel supply and current density achieved under conditions of dynamic fuel supply in Cases 1 and 2. The results were comparable (Figure 6). The concentration of hydrogen decreased slightly as the rate of fuel flow decreased in Cases 1, 2, and 3. However, the effect of the reduction in the hydrogen content on the PEMFC performance was insignificant as the ratio

between the current generated under conditions of fluctuating fuel profiles, and constant fuel supply was approximately 1 over the entire time cycle despite hydrogen fluctuation. These observations explain the minimal variations between the total current generated for Cases 1 and 2 and the current generated under steady-state conditions (Figure 3 and Figure 5). The reduced fuel supplied in Case 3 was sufficient to sustain the rate of electrochemical reaction within PEMFC (Figure 6). The results revealed that the current generated under conditions of reduced fuel supply was comparable to that generated under conditions of constant fuel supply. This helped in stable power generation (Figure 8).

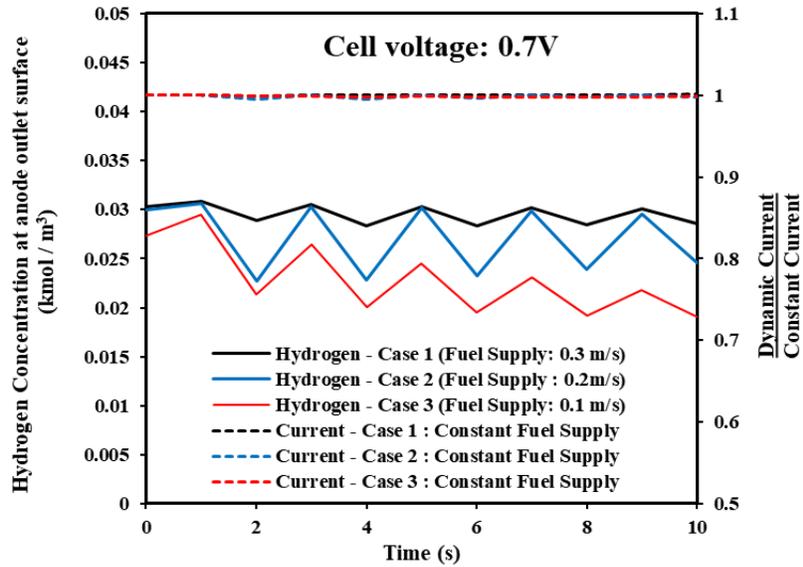


Figure 6 Current generated under different fluctuating fuel profiles at the cell voltage of 0.7 V.

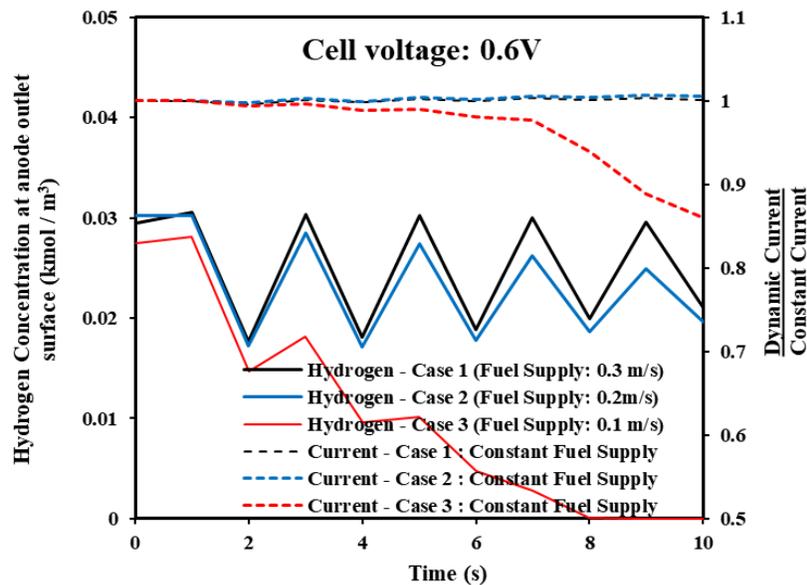


Figure 7 Current generated under different fluctuating fuel profiles at the cell voltage of 0.6 V.

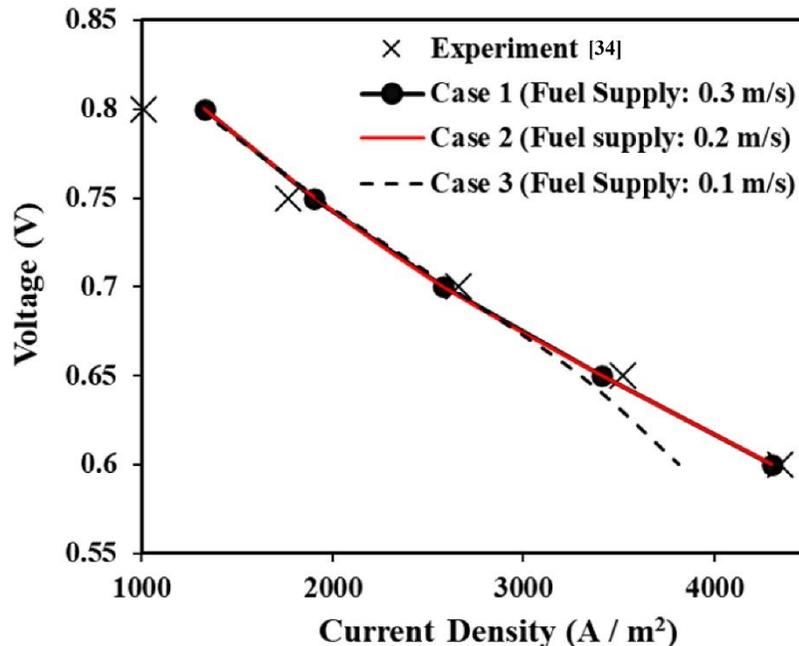


Figure 8 Polarization curves recorded under conditions of dynamic inlet fuel profiles.

At the operating cell voltage of 0.6 V, similar observations were noticed for Cases 1 and 2. The difference between the current generated under fluctuating fuel and constant fuel inlet conditions was minimal, even though a constant fluctuation in the hydrogen concentration was more noticed at low cell voltages (Figure 7). A significant drop in the hydrogen concentration was observed for Case 3 at 0.6 V. As the hydrogen was supplied at a low rate, the fuel available for Case 3 could have been in a lean state. Hence, the hydrogen content along the anode channel was significantly reduced, and this was evident from the complete deficiency of hydrogen at the outlet of the anode channel at the cell voltage of 0.6 V (Figure 7). On the contrary, no visible deterioration in the PEMFC performance was observed for Case 3 at 0.7 V (Figure 6). This proved that the amount of fuel supplied for Cases 1, 2, and 3 was sufficient for the PEMFC to sustain its performance at high cell potentials.

The PEMFC performance deteriorated at the low voltage region when fuel was supplied using the profile of Case 3 (Figure 7). Analysis of the polarization curves plotted under varying rates of fuel supply revealed the drop in the current density at 0.6 V for Case 3 (Figure 8). This was approximately 12% lower than that recorded for Case 1. The high extent of fuel-saving that Case 3 promises in comparison to Case 1 would be achieved at the expense of significantly compromised PEMFC performance. Such a reduction in the current density within a short operating period of 10 s can raise major concerns about the reliability of PEMFC as a sustainable and renewable energy source. Hence, it was evident that a threshold point should be identified to conserve fuel while sustaining the stable performance of PEMFC through the dynamic fuel profile. The data presented in the following section complements the current findings and focuses on the effect of different fuel conditions on the performance of PEMFC in the low cell voltage regions. The results obtained at the cell voltage of 0.6 V were taken as an example.

3.2 Effects of Dynamic Fuel Supply at Low Electric Potentials (0.6 V)

3.2.1 Constant Fuel Supply against Fluctuating Fuel Supply

To understand the impact of the fluctuating fuel supply on the PEMFC performance at low cell voltages, results from Cases 1, 2, and 3 were compared against the results obtained under the constant fuel feed rate. The maximum amount of fuel was detected at the inlet of the anode channel. The content decreased progressively, reflecting the consumption of fuel along the PEMFC module. This could be visualized by analyzing the reduction in the hydrogen content along the PEMFC module from the inlet to the outlet (Figure 9 and Figure 10). The trend in fuel consumption along the fuel cell module was similar for all cases (constant fuel supply, Case 1, 2, and Case 3). The fraction of hydrogen at the outlet of PEMFC was analyzed to study the possible fuel availability at the time step of $t = 10$ s. Fuel was not supplied at $t = 10$ s under the dynamic fuel profile conditions (Figure 11). The presence of unutilized hydrogen was observed at the anodic GDL for Cases 1 and 2 despite the fact that fuel was not supplied at $t = 10$ s. However, a complete absence of hydrogen was noticed for Case 3. It was perceived that hydrogen was completely consumed for Case 3 at $t = 10$ s over the entire length of the fuel cell module.

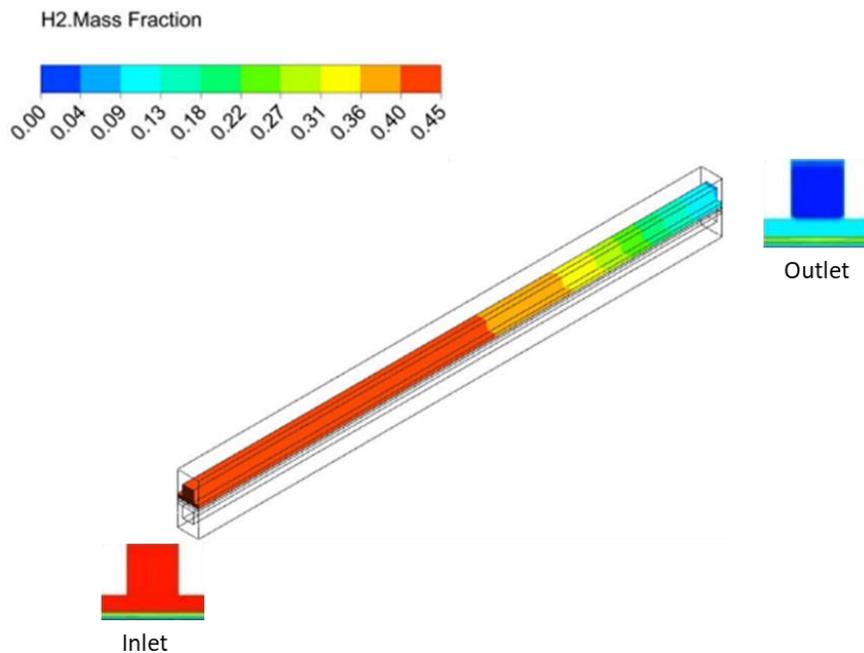


Figure 9 Hydrogen availability for Case 1 at $t = 10$ s.

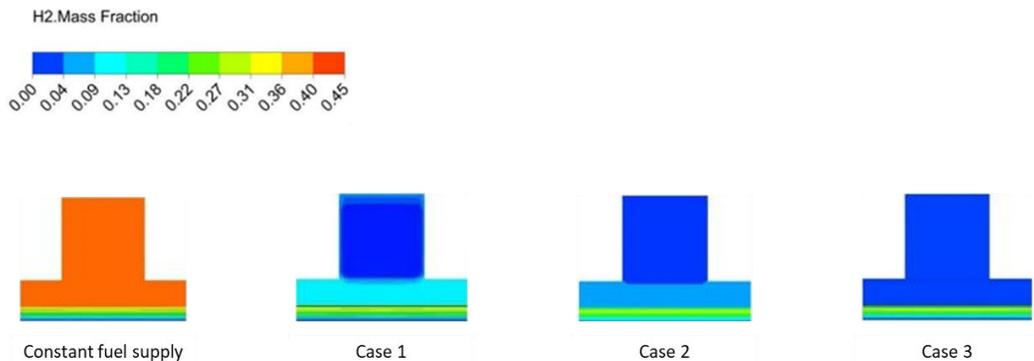


Figure 10 Hydrogen availability at the outlet of the PEMFC module at $t = 10$ s and 0.6 V.

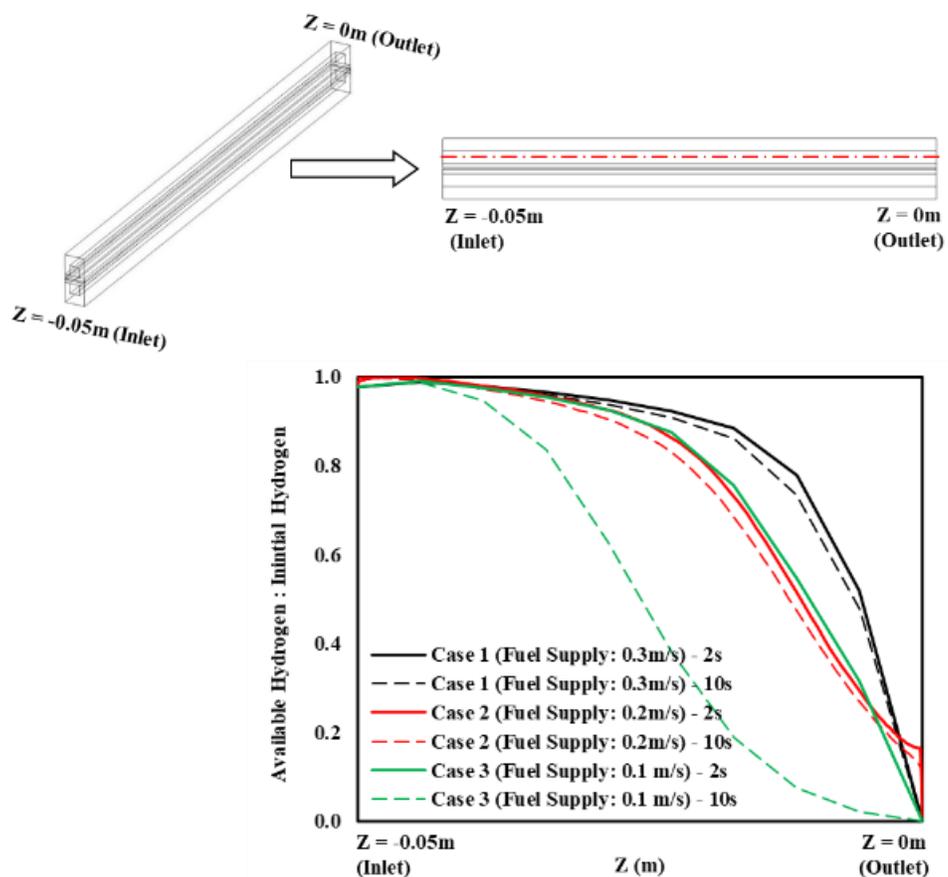


Figure 11 Fuel content along the horizontal length of the anode channel at 0.6 V.

To obtain a better understanding of the nature of fuel flow, the profile of fuel along the horizontal direction of the anode channel was analyzed at two different time steps: $t = 2$ s and $t = 10$ s, where the fuel supply rate was 0 m/s. Thus, the fuel availability at periods where no fuel was supplied can be observed. The results can help understand the effect of dynamic fuel supply on the PEMFC performance. Analysis of the profiles revealed that a large amount of fuel was required and maintained for Cases 1 and 2 over the entire period of 10 s. The amount of fuel available at each timestep was

compared to the initial amount of fuel present (at $t = 0$). This was equivalent to the amount of fuel available under conditions of a constant fuel supply. The gradients of the fuel profiles observed for Cases 1 and 2 were similar when a large amount of fuel was required to be maintained at the time steps where no fuel was supplied. This revealed the rich fuel content (Figure 11). The fuel content recorded for Case 2 was lower than that recorded for Case 1. However, a rich fuel content was recorded for Case 2 at $t = 10$ s. This could, hence, be a representation of the promising ability of both cases to produce a highly stable PEMFC performance (Figure 6). However, in the case of Case 3, a significant drop in fuel was observed over the period of 10 s. The fuel availability reduced significantly with every time step as the time period increased. At $t = 10$ s, the amount of fuel in the PEMFC at $z = -0.02$ m was approximately 30% for Case 2, in comparison to approximately 90% for Case 1 (Figure 11). The high amount of fuel deficiency could result in fuel starvation within the PEMFCs. This could eventually result in performance deterioration, as evidenced by simulation results reported previously herein (Figure 6).

3.2.2 Extended Duration of PEMFC Operation at Low Electric Potential (0.6 V)

Further investigation was conducted to study the trend in change in the PEMFC performance at an extended time duration of 20 s. The purpose of this investigation was to determine the possibility of producing a stable trend in hydrogen fluctuation during the continued application of PEMFC under conditions of pulsating fuel profiles. A new pulsating fuel supply profile, Case 4 that exhibited a dynamic fuel flow rate of 0.15 m/s, was introduced to investigate the possibility of improved fuel saving while maintaining a stable fuel cell performance, as an insignificant drop in the hydrogen content was observed for Case 3 (Figure 12). The localized effect of the fuel supplied through Cases 1 to 4 was analyzed by analyzing the thermal and current contours near the outlet region of the PEMFCs ($z = -0.005$ m) at $t = 2$ s and $t = 20$ s. They were compared against the PEMFC properties observed under conditions of a constant fuel supply to observe the possible variation in performances. Under the constant fuel supply condition, the center of the PEMFC (the MEA region) functioned as a highly active region. This was represented by the thermal behavior of the fuel cell (Figure 13). This could reflect the electrochemical reaction occurring within the PEMFCs. The reaction involved the separation of hydrogen protons and electrons and the transfer of the hydrogen protons from the anodic to cathodic region. The electrochemical reaction, thus, results in the generation of current (Figure 14). The rate of this reaction was sustained for Cases 1, 2, and 4 for the entire duration of the PEMFC operation. The minimal deviation was observed between the current generated under these conditions to the current generated under conditions of constant fuel supply.

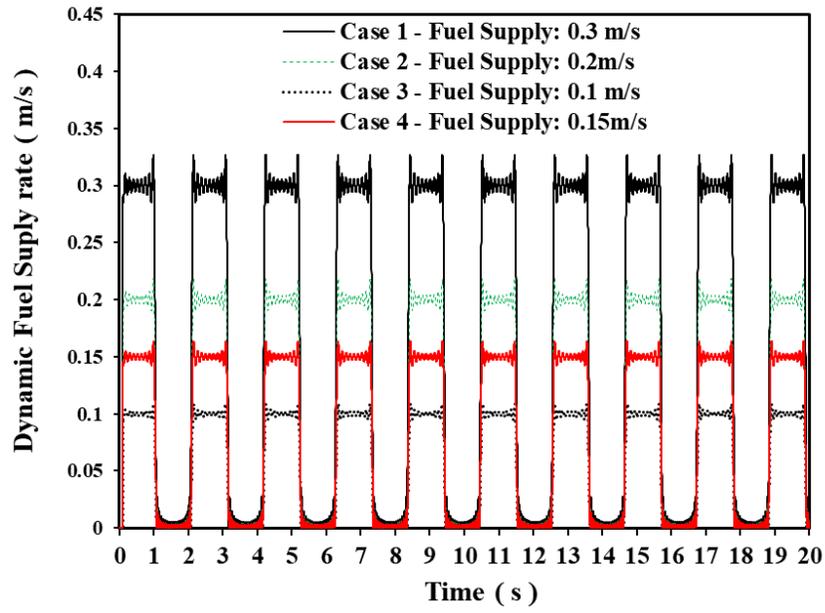


Figure 12 Fluctuating fuel profiles recorded over $t = 20$ s.

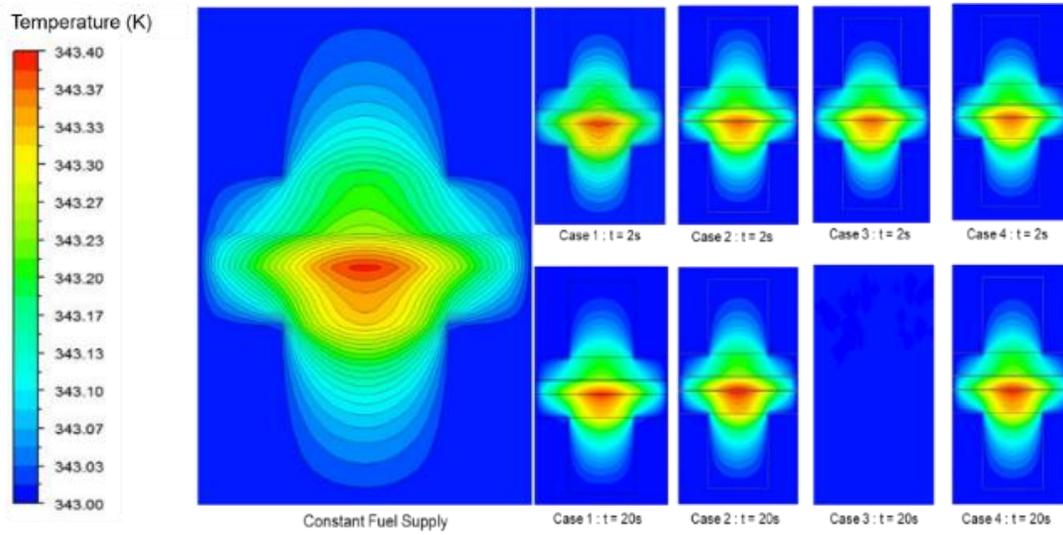


Figure 13 Thermal profiles recorded under the dynamic fuel conditions at $z = -0.005$ m.

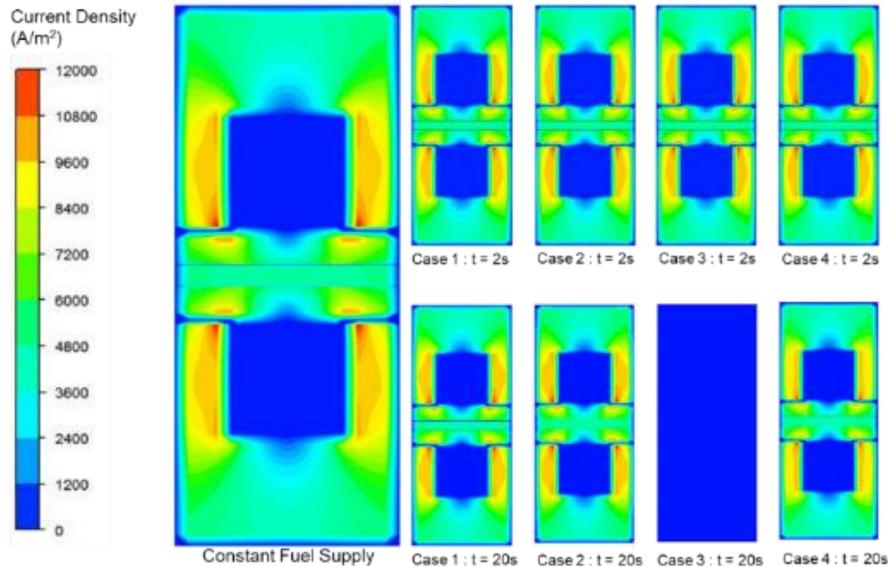


Figure 14 Current density profile recorded under the dynamic fuel conditions at $z = -0.005$ m.

Visible signs of local thermal variation and current generation near the outlet region of the PEMFC module were not observed for Case 3 (Figure 13 and Figure 14). The electrochemical reaction that results in the current generation (and hence power) cannot be sustained for the entirety of the PEMFC module, and this could be attributed to the low supply of hydrogen observed in Case 3. The rate maintained during the pulsating fuel flow in Case 3 was not sufficiently high to generate the required amount of fuel to realize a stable operation. However, a stable operation condition could be achieved through other dynamic flow profiles. The possible increase in the extent of reactant consumption at the low voltage regions could also have played a part in the deceleration of the electrochemical reaction observed in Case 3. This would explain the significant drop in PEMFC performance at $t = 20$ s for Case 3 (downstream; fuel cell module).

To observe the changes in the hydrogen concentration under conditions of varying rates of hydrogen supply, the changes in fuel concentration over the volume of the anode channel, GDL, and MEA, were studied for Cases 1 to 4. The hydrogen concentration was observed to be constant over 20 s for Cases 1 and 2 (Figure 15). A constant content was recorded for the entire operation cycle for Cases 1 and 2. This shows that the dynamic fuel profiles introduced in Cases 1 and 2 could help achieve a constant fuel supply that is sufficient to realize a stable PEMFC operation despite the increase in the fuel cell operation time. A stable fuel supply resulted in the generation of a current that was highly comparable to the current produced under conditions of a constant fuel supply (Figure 16). When the fuel supply rate was constant at the rate of 0.3 m/s, approximately 50% and 66% of the fuel could be conserved under conditions of the fluctuating fuel profile observed in Cases 1 and 2, respectively. This demonstrates the possible application of the fluctuating fuel profile as a reliable replacement for the constant fuel supply conditions to sustain the performance of the PEMFC systems. Fuel usage could be conserved simultaneously. The fuel profile corresponding to Case 4 produced a stable current during the 20 s of PEMFC operation. This helped in fuel-saving (approximately 75%). However, a decrease in

the hydrogen concentration was observed within 20 s (Figure 15). This reflected the fact that the PEMFC system might not exhibit a stable performance beyond 20 s, and the deterioration in the PEMFC performance was foreseen. Therefore, the operation of PEMFC under the dynamic fuel profile conditions was not recommended for the case of Case 4.

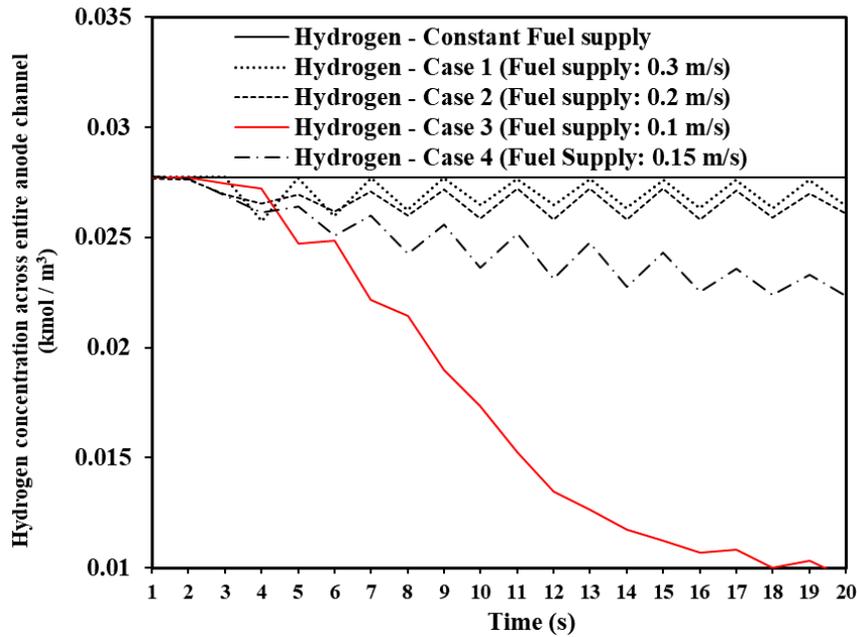


Figure 15 Changes in the hydrogen content over 20 s of PEMFC operation.

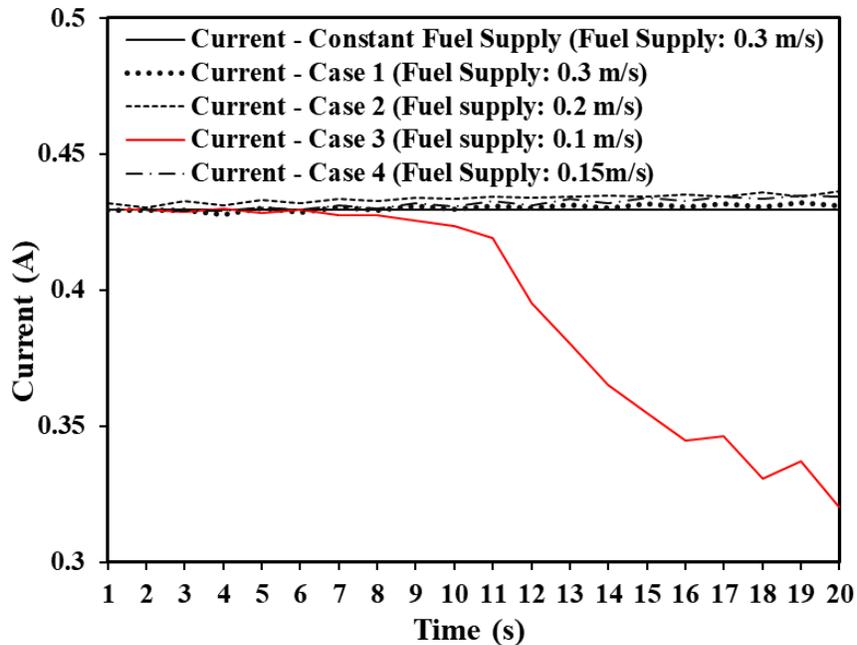


Figure 16 Changes in current generation over 20 s of PEMFC operation.

The hydrogen concentration and current generated in Case 3 reflect the fact that the rate of local electrochemical reaction was decelerated, and the extent of current generated was reduced. The lack of fuel supply results in fuel cell starvation (Figure 15). Under these conditions, the rate of current generation decreased progressively, resulting in a drop to approximately 29% of the current generated under the constant fuel supply conditions (Figure 16).

The absence of hydrogen might have severely limited the presence of electrons flowing through the external circuit to generate electric current. Analysis of the results obtained for Case 3 revealed that a threshold value for the rate of fuel flow into the PEMFC system resulted in sustainable PEMFC performance. Fuel was simultaneously conserved. This could indicate that a dynamic fuel supply rate (0.1 m/s) was highly undesirable. If the fuel supply rate at the inlet of the anode channel adopts the dynamic fuel profile represented by Cases 1 and 2, the sustainability of the PEMFC performance would not be compromised. Under these conditions, a significant reduction in fuel usage could be realized. The results revealed the promising effect of the dynamic inlet condition. Under these conditions, PEMFC performance could be sustained, and fuel could be conserved. The dynamic inlet conditions adopted for CFD simulation were comparable to the experimental conditions reported by Choi et al. [16, 17], who realized a sustainable PEMFC performance by imposing a pulsating fuel profile.

The results achieved through the current CFD simulation study pave the way to realize a stable PEMFC performance while simultaneously reducing the fuel content under conditions of the fluctuating fuel supply profile. The concept of implementing a dynamic fuel profile can be exploited by researchers and engineers to reduce the extent of fuel or energy consumption in an engineering system.

4. Conclusion

Studies on the transient fuel supply in PEMFCs have focused on purging mechanism and strategies and their effects on the performance of the PEMFC. The necessity of a continuous fuel supply to ensure the performance stability of PEMFC has not been widely investigated. We followed a numerical approach to explore the effect of different transient fuel supply rates on the PEMFC performance and studied the probability of achieving hydrogen conservation. The application of a dynamic inlet boundary condition that was developed using the Fourier Series technique enabled the recreation of a pulsating effect on the incoming fuel supply rate. CFD investigation was carried out to study the impact of the inlet conditions on PEMFC performance and to observe the possibility of fuel conservation. Three different dynamic inlet conditions were initially imposed on the system to validate the PEMFC CFD model. The simulation conditions assumed stable operating conditions at a steady state. The paper was separated into two major sections. The first section reported the effects of the three dynamic inlet conditions on the PEMFC performance operating at different operating voltages. The second portion of the paper presents an in-depth investigation of the PEMFC performance at the cell voltage of 0.6 V. The performance of the PEMFC system was evaluated based on the current generation value and the extent of fuel consumption realized under conditions of the dynamic fuel supply.

The following findings were obtained:

- Analysis of the polarization curve revealed that the performance of PEMFC under conditions of a constant fuel supply was similar to the performance recorded under conditions of a dynamic fuel profile.
- Promising results were obtained under conditions of dynamic fuel profiles at high supply rates (Case 1 and 2) at 0.7 V, and 0.6 V. Insignificant differences were observed between the current generated between these conditions and the steady-state PEMFC operation.
- A threshold in the application of the dynamic fuel profile potentially exists as a drop of approximately 29% was observed for the current during PEMFC operation in Case 3. The lack of fuel supply resulted in fuel cell starvation, which eventually resulted in the reduction in the ability of the system to generate stable power.
- Cases 1 and 2 can be analyzed to ensure stable PEMFC performance while conserving up to 66% of fuel savings. Fuel could be saved further in Case 4 at the expense of unstable PEMFC operation.
- The constant fuel supply observed in Cases 1 and 2 over the extended fuel cell operation duration reveals that the conditions of constant fuel supply can be replaced throughout the entire duration of PEMFC operation.

The adoption of dynamic fuel profiles paves the way for manipulating these profiles computationally to reduce the unnecessary consumption of fuel. The numerical methods were validated against the current experimental work. Future investigation should be conducted to replicate an experimental study based on the parameters specified herein. From a numerical point of view, the results reported herein can be extended to include various phases of water within PEMFC that would be encountered during the practical application of the fuel cells. Different profiles of fuel can also be developed using the Fourier Series technique to further study the possibility of hydrogen conservation in PEMFC applications.

Author Contributions

Jeggathishwaran Panisilvam: Methodology, Writing – original draft. **Wang Peng Cheng, Jeggathishwaran Panisilvam, Hui An:** Conceptualization, Writing – review & editing **Wang Peng Cheng, Jeggathishwaran Panisilvam, Hui An:** Data curation, Visualization. **Jeggathishwaran Panisilvam:** Validation, Formal analysis. **Wang Peng Cheng, Hui An:** Investigation, Supervision.

Competing Interests

The authors have declared that no competing interests exist.

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