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Proton exchange membrane fuel cells modeling: A review of the last ten years results of the Fuel Cell Research Center-IEEF

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Abstract
Fuel cell technology is expected to play an important role in meeting the growing demand for distributed power generation. In an ongoing effort to meet increasing energy demand and to preserve the global environment, the development of energy systems with readily available fuels, high efficiency and minimal environmental impact is urgently required. A fuel cell system is expected to meet such demands because it is a chemical power generation device, which converts the chemical energy of a renewable clean fuel (e.g. Hydrogen) directly into electrical energy. Still a maturing technology, fuel cell technology has already indicated its advantages, such as its high-energy conversion efficiency, modular design and very low environmental intrusion, over conventional power generation equipment. Among all kinds of fuel cells, proton exchange membrane (PEM) fuel cells have many superior advantages. These advantages have sparked development efforts in various quarters of industry to open up new field of applications for PEM fuel cells. Three key issues limiting the widespread commercialization of the PEM fuel cells technology which are better performance, lower cost, and long cell life. The strategy of the Fuel Cell Research Center at the International Energy and Environment Foundation (IEEF) is to develop the PEM fuel cells to improve their lifetime with a much higher power density and lower cost. An overview of innovations in this field is presented using the published results of the center over the last decade. These innovative improvements will show a new scenario for the future fuel cell market of the next years.

Keywords: PEM fuel cell; CFD; Modeling; Performance; Mechanical stress; Hygro-thermal stresses; Durability; Ambient air-breathing; Micro fuel cell; Novel design; Stack; Hydrogen.

1. Introduction

Proton Exchange membrane (PEM) fuel cells are still undergoing intense development, and the combination of new and optimized materials, improved product development, novel architectures, more efficient transport processes, and design optimization and integration are expected to lead to major gains in performance, efficiency, durability, reliability, manufacturability and cost-effectiveness [1].
The PEM fuel cell consists of a current collector (including gas channels), gas diffusion layer (GDL), and catalyst layer (CL) on the anode and cathode sides as well as an ion conducting polymer membrane.

Figure 1 shows the processes take place inside the PEM fuel cell. Obviously, the design of the components and properties of materials must accommodate this processes with minimum obstruction and losses. Because in some of the components more than one process takes place, very often with conflicting requirements, the properties and the design must be optimized. For example, the gas diffusion layer must be optimized so that the reactant gas may easily diffuse, yet at the same time that water, which travels in the opposite direction, does not accumulate in the pores. On top of that, the diffusion layer (or current collector layer as it is sometimes called) must be both electrically and thermally conductive. Similar requirements may be established for almost every fuel cell component. Although a fuel cell seems to be a very simple device, numerous processes take place simultaneously. It is therefore important to understand those processes, their mutual interdependence, and their dependence on components design and materials properties.

The performance of PEM fuel cells is known to be influenced by many parameters, such as operating temperature, pressure, stoichiometric flow ratio, gas channels width, GDL thickness, membrane thickness, GDL porosity, material properties, clamping pressure, and GDL thermal conductivity, etc. In order to improve fuel cell performances, it is essential to understand these parametric effects on fuel cell operations. Changing the cell operating parameters can have either a beneficial or a detrimental impact on fuel cell performance [2].

Durability is one of the most critical remaining issues impeding successful commercialization of broad PEM fuel cell transportation energy applications, and the durability of fuel cell stack components remains, in most cases, insufficiently understood. Lengthy required testing times, lack of understanding of most degradation mechanisms, and the difficulty of performing in-situ, non-destructive structural evaluation of key components makes the topic a difficult one. The need for improved lifetime of PEM fuel cells necessitates that the failure mechanisms be clearly understood and life prediction models be developed, so that new designs can be introduced to improve long-term performance [3].

The presence of microelectromechanical system (MEMS) technology makes it possible to manufacture the miniaturized fuel cell systems for application in portable electronic devices. The majority of research on micro-scale fuel cells is aimed at micro-power applications. There are many new miniaturized applications which can only be realized if a higher energy density power source is available compared to button cells and other small batteries. In small-scale applications, the fuel cell should be exceptionally small and have highest energy density. A key advantage of fuel cells for such applications is the much longer continuous operation and almost instantaneous refueling (as opposed to the recharging time required by batteries). The viability of PEM fuel cells as battery replacements requires that PEM fuel cells undergo significant miniaturization while achieving higher power densities. One way to achieve these requirements is to reduce the thickness of the cell (compacted-design) for increasing the volumetric power density of a fuel cell power supply. This presents challenges for small scale and micro-fuel cells in terms of design, materials, effective transport of reactants, and heat management [4].

The stacking design and cell assembly parameters significantly affect the lifetime and performance of fuel cells. Adequate contact pressure is needed to hold together the fuel cell stack components to prevent leaking of the reactants, and minimize the contact resistance between layers. Every stacking design has a unique assembly pressure due to differences in fuel cell materials and stack design. The required clamping force is equal to the force required to compress the fuel cell layers adequately while not impeding flow. The assembly pressure affects the characteristics of the contact interfaces between components. If inadequate or non-uniform assembly pressure is used, there will be stack-sealing problems, such as fuel leakage, internal combustion, and unacceptable contact resistance. Too much pressure may impede flow through the GDL, or damage the MEA, resulting in a broken porous structure and a blockage of the gas diffusion passage. In both cases, the clamping pressure can decrease the cell performance and lifetime. Due to thin dimensions and the low mechanical strength of the electrodes and electrolyte layer versus the gaskets, bipolar plates, and end plates, the most important goal in the stack design and assembly is to achieve a proper and uniform pressure distribution [1].

This paper has been focused on ten specific topics, that are considered the most interesting and promising, and structured consequently in: innovative designs, innovative algorithm, maximum power and long cell life, air breathing PEM fuel cells, micro PEM fuel cells, micro air breathing PEM fuel cells, mechanical and hygro-thermal stresses in the PEM fuel cells, natural vibration of the PEM fuel cell stacks, and integrated PEM fuel cells. The objective of this paper is to give to the scientific community a review of the actual and possible trend in the research of the Fuel Cell Research Center at the International Energy and Environment Foundation in the field of PEM fuel cells.

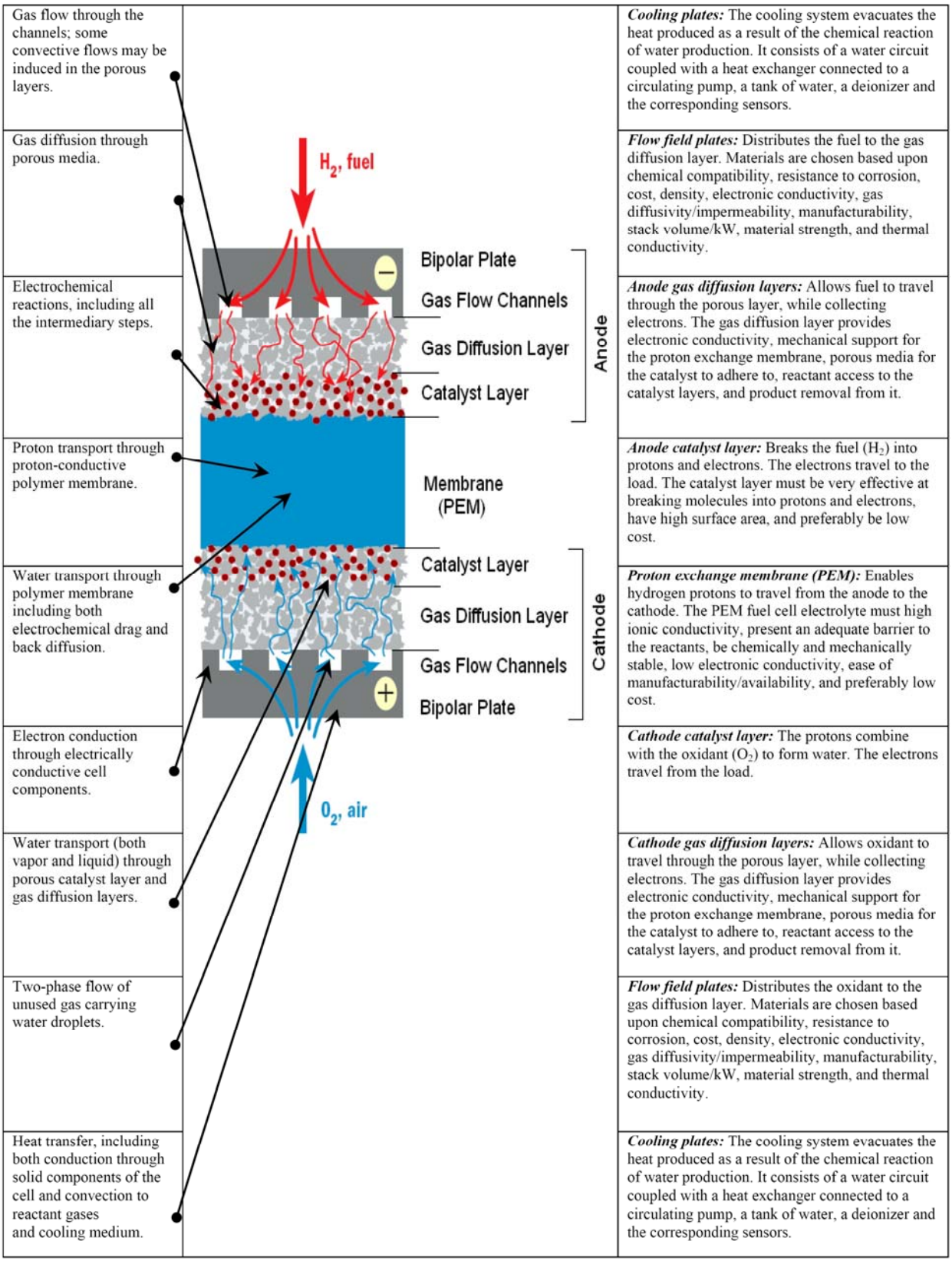


Figure 1. Main PEM fuel cell components and processes.

2. Performance modeling of PEM fuel cell

Fuel cell modeling has received much attention over the past 10 years in an attempt to better understand the phenomena occurring within the fuel cell. Parametric models allow engineers and designers to predict the performance of the fuel cell given geometric parameters, material properties and operating conditions. Such models are advantageous because experimentation is costly and time consuming. Furthermore, experimentation is limited to designs, which already exist, thus does not facilitate innovative design. Given the highly reactive environment within the fuel cell, it is often impossible to measure critical parameters, such as temperature, pressure and potential gradients, or species concentration within the cell. Thus, detailed transport models, which accurately predict the flux and concentration of multiple species, are required. Such information is very useful to develop the fuel cells [5].

A fuel cell model may fall into one of three categories: analytical, semi-empirical, and mechanistic (theoretical). Analytical models are only approximate and do not give an accurate picture of transport processes occurring within the cell. They are limited to predicting voltage losses and water management requirements for simple designs. They may be useful if quick calculations are required for simple systems. The processes occurring within a PEM fuel cell include mass, momentum, species, and energy transports in the various layers of fuel cells. All these processes can be described, mathematically, by fundamental conservation laws. However, it is impossible to provide analytical solutions of these processes without simplifying the fundamental equations (see some examples in reference [5]).

Semi-empirical modeling combines theoretically derived differential and algebraic equations with empirically determined relationships. Empirical relationships are employed when the physical phenomena are difficult to be modeled or the theory governing the phenomena is not well understood [6]. Semi-empirical models are, however, limited to a narrow corridor of operating conditions. They cannot accurately predict performance outside of that range. They are very useful for making quick predictions for designs that already exists. They cannot be used to predict the performance of innovative designs, or the response of the fuel cell to parameter changes outside of the conditions under which the empirical relationships were developed. Empirical relationships also do not provide an adequate physical understanding of the phenomena inside the cell. They only correlate output with input. Semi-empirical models are very useful for estimating the performance of PEM fuel cell stacks and optimization of fuel cell system integration and operation [7].

Using semi-empirical equations for modeling a proton exchange membrane fuel cell is proposed for providing a tool for the design and analysis of fuel cell total systems. A semi-empirical model of a PEM fuel cell has been developed and the effect of operation conditions on the cell performance has been investigated [6-9]. The objective was to develop a semi-empirical model that would simulate the performance of fuel cells without extensive calculations. The model take into account not only the current density but also the process variations, such as the gas pressure, temperature, humidity, and utilization to cover operating processes, which are important factors in determining the real performance of fuel cell. The model can be used to investigate the influence of process variables for design optimization of fuel cells, stacks, and complete fuel cell power system. This can be demonstrated by some examples in Figure 2. At the moment, to the author's knowledge, only few such approaches, especially in literature studies, have been published.

Mechanistic modeling has received the most attention in the literature [10-13]. In mechanistic modeling, differential and algebraic equations are derived based on the physical and electro-chemical principals governing the phenomena internal to the cell. These equations are solved using some sort of computational method. The development of physically representative models that allow a reliable simulation of the processes under realistic conditions is essential to the development and optimization of fuel cells, improve long-term performance and lifetime, the introduction of cheaper materials and fabrication techniques, and the design and development of novel architectures. The difficult experimental environment of fuel cell systems has stimulated efforts to develop models that could simulate and predict multi-dimensional coupled transport of reactants, heat and charged species using computational fluid dynamic (CFD) methods. The strength of the CFD numerical approach is in providing detailed insight into the various transport mechanisms and their interaction, and in the possibility of performing parameters sensitivity analyses [14]. These models allow engineers and designers to predict the performance of the fuel cell given design parameters, material properties and operating conditions.

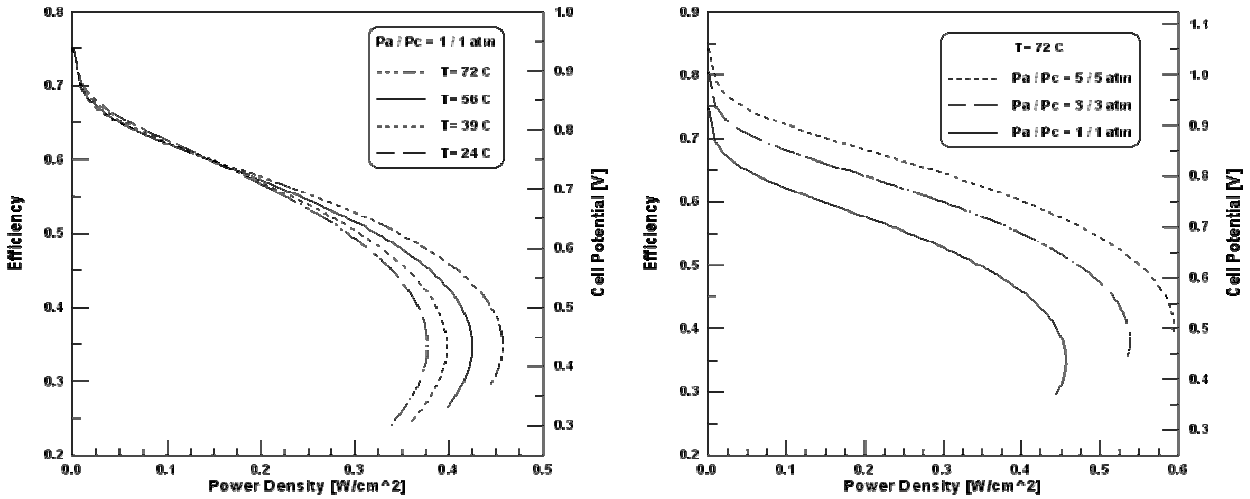
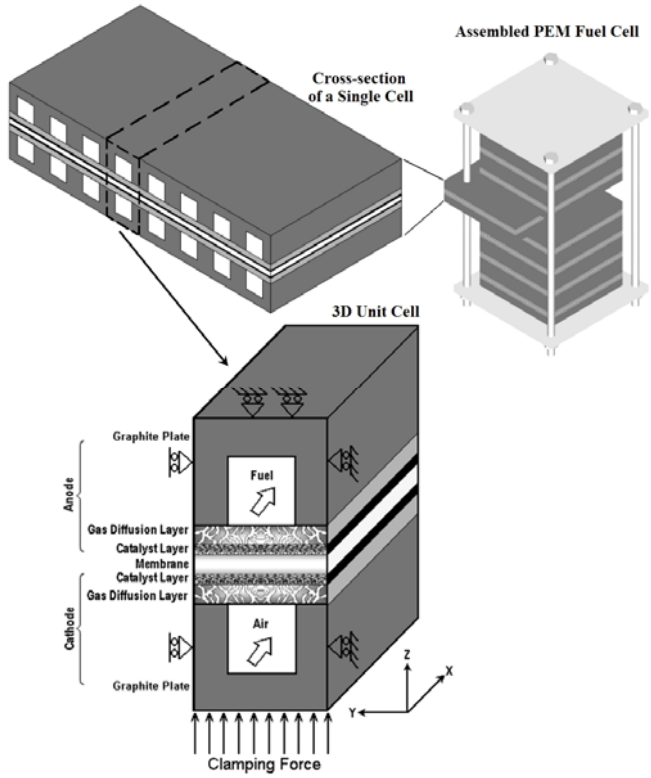


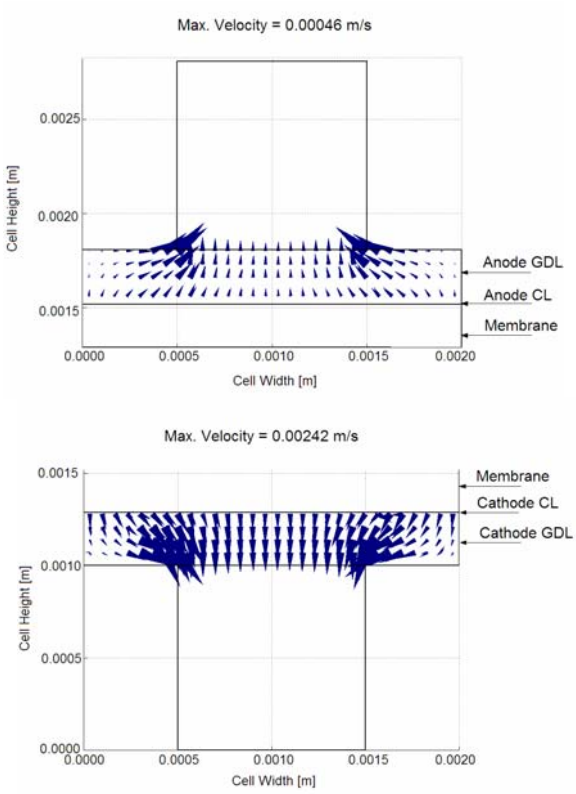
Figure 2. Relationship between fuel cell efficiency and power output for different values of cell temperatures and pressures [6].

A comprehensive three–dimensional, multi–phase, non-isothermal, CFD model of a PEM fuel cell that incorporates the significant physical processes and the key parameters affecting fuel cell performance has been developed [10-13]. The model was developed to improve fundamental understanding of transport phenomena in PEM fuel cells and to investigate the impact of various operation parameters on performance. The model accounts for both gas and liquid phase in the same computational domain, and thus allows for the implementation of phase change inside the gas diffusion layers. The model includes the transport of gaseous species, liquid water, protons, energy, and water dissolved in the ion-conducting polymer. Water is assumed to be exchanged among three phases; liquid, vapor, and dissolved, and equilibrium among these phases is assumed. Water transport inside the porous gas diffusion layer and catalyst layer is described by two physical mechanisms: viscous drag and capillary pressure forces, and is described by advection within the gas channels. Water transport across the membrane is also described by two physical mechanisms: electro-osmotic drag and diffusion. The physics of phase change are included in this model by prescribing the local evaporation term as a function of the amount of liquid water present and the level of undersaturation, whereas the condensation has been a function of the level of oversaturation. The new feature of the algorithm developed in this model is its capability for accurate calculation of the local activation overpotentials, which in turn results in improved prediction of the local current density distribution. This model also takes into account convection and diffusion of different species in the channels as well as in the porous gas diffusion layer, heat transfer in the solids as well as in the gases, and electrochemical reactions. The model reflects the influence of numerous parameters on fuel cell performance including geometry, materials, operating and others. The model is shown to be able to: understand the many interacting, complex electrochemical and transport phenomena that cannot be studied experimentally; identify limiting steps and components; and provide a computer-aided tool for design and optimization of future fuel cell with much higher power density and lower cost [15]. In addition, the results show that the model is capable of identifying important parameters for the wetting behavior of the gas diffusion layers and can be used to identify conditions that might lead to the onset of pore plugging, which has a detrimental effect of the fuel cell performance, especially in the mass transport limited region. This can be demonstrated by some examples in Figure 3.

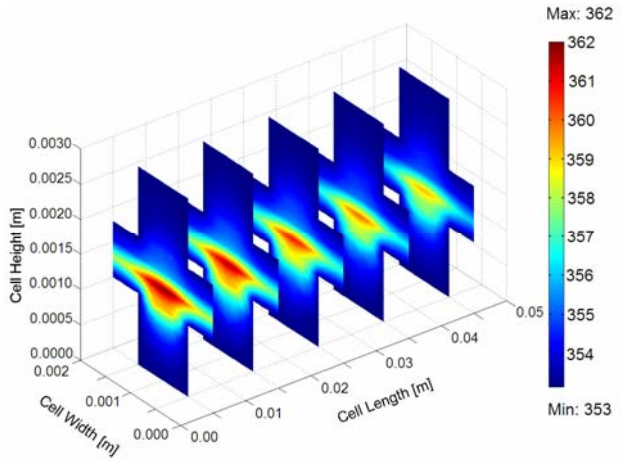
A parametric study using three-dimensional, multi–phase, nonisothermal CFD model of a PEM fuel cell has been performed. A detailed analysis of the fuel cell performance under various operating conditions has been conducted and the effects of operating, design, and material parameters have been examined [16-19]. The analysis helped identifying critical parameters and shed insight into the physical mechanisms leading to a fuel cell performance under various conditions. Optimization study of a PEM fuel cell performance has been performed. The study quantifies and analyses the impact of operating, design, and material parameters on fuel cell performance and get an optimal conditions for PEM fuel cells to generate maximum power. To the author's knowledge, this has not been specifically studied before. Results with deferent conditions for the cell operates at nominal current density of 1.2 A/cm^2 are presented in Figure 4.



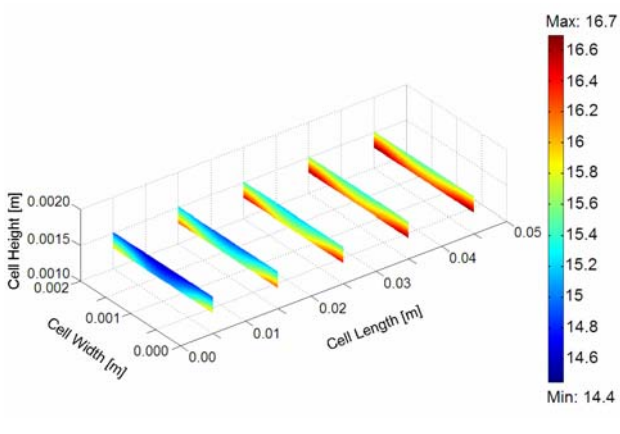
Three-dimensional computational domain



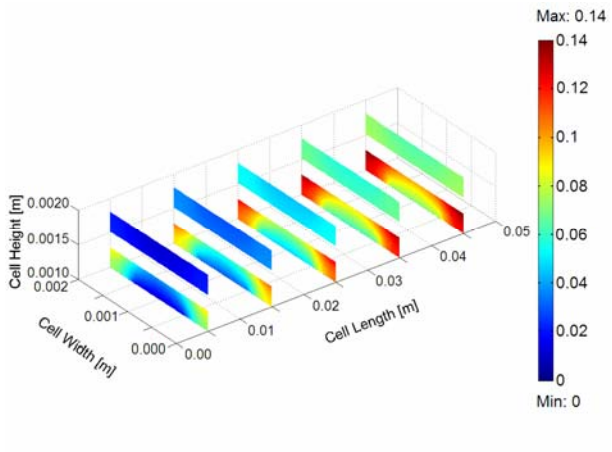
Liquid water velocity vectors inside GDLs



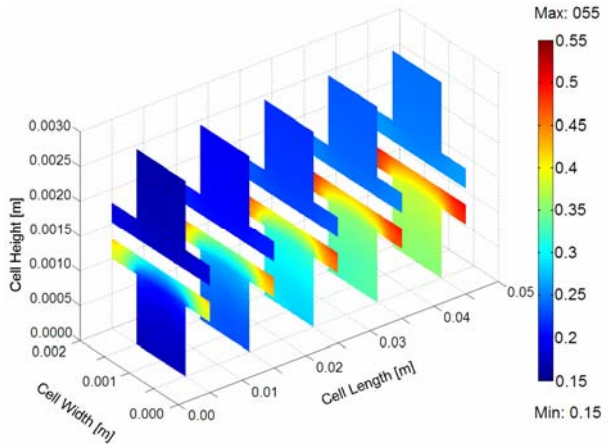
Temperature distribution inside the fuel cell



Water content profile through the membrane



Liquid water saturation inside the GDLs



Water vapor molar fraction distribution in the cell

Figure 3. Three Dimensional modeling results of a PEM fuel cell [10].

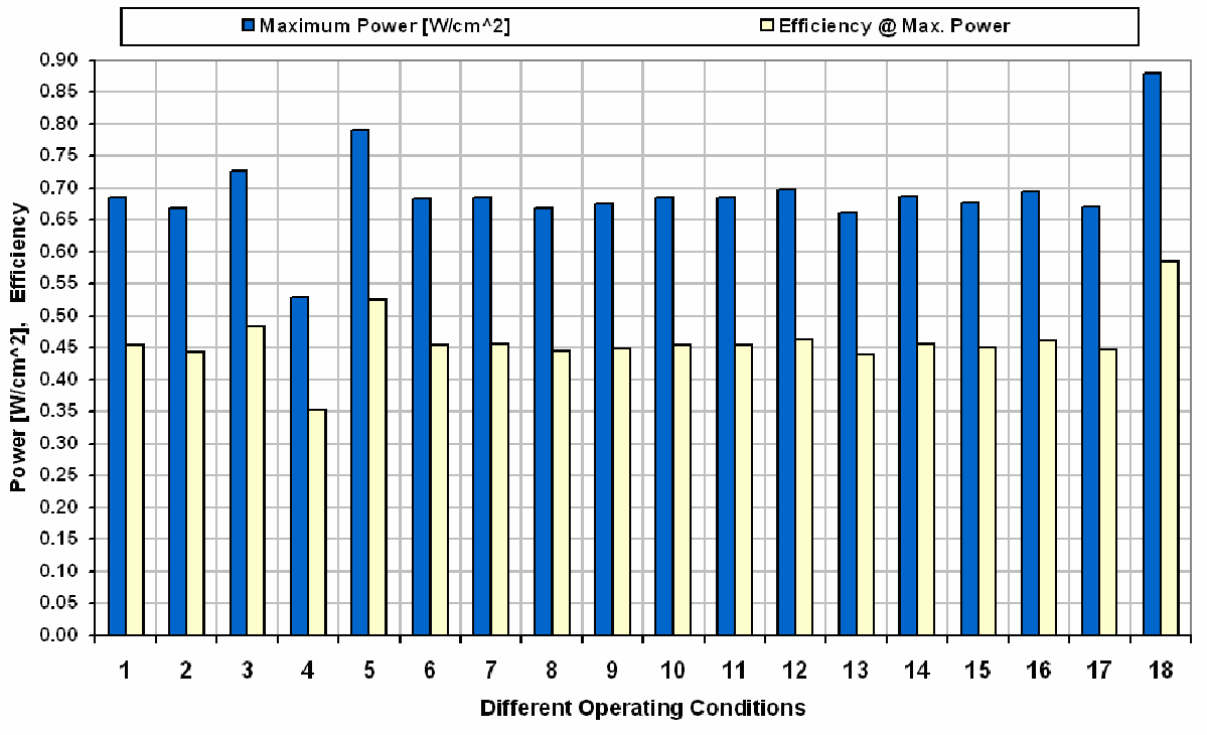


Figure 4. Cell power with corresponding efficiency for different operating conditions [17].

Key:

1- Base case
2- Cell operating temperature = 60 C
3- Cell operating temperature = 90 C
4- Cell operating pressure = 1 atm
5- Cell operating pressure = 5 atm
6- Stoichiometric flow ratio = 1.5
7- Stoichiometric flow ratio = 3
8- GDL porosity = 0.3
9- GDL porosity = 0.5
10- GDL thermal conductivity = 0.5 W/m.K
11- GDL thermal conductivity = 2.9 W/m.K
12- Gas channel width = 0.8 mm
13- Gas channel width = 1.2 mm
14- GDL thickness = 0.2 mm
15- GDL thickness = 0.3 mm
16- Membrane thickness = 0.2 mm
17- Membrane thickness = 0.26 mm
18- Optimal design to generate maximum power

Small fuel cells have provided significant advantages in portable electronic applications over conventional battery systems. Competitive costs, instant recharge, and high energy density make fuel cells ideal for supplanting batteries in portable electronic devices. Micro fuel cells belong to the category of portable fuel cells, but are used in the miniaturized electronic devices with low power, such as micro sensors. The presence of microelectromechanical system (MEMS) technology makes it possible to manufacture the miniaturized fuel cell systems for application in portable electronic devices. There are many new miniaturized applications which can only be realized if a higher energy density power source is available compared to button cells and other small batteries. Micro-fuel cells are considered as promising electrochemical power sources in portable electronic devices. The majority of research on micro-scale fuel cells is aimed at micro-power applications.

The difficult experimental environment of fuel cell systems has stimulated efforts to develop models that could simulate and predict multi-dimensional coupled transport of reactants, heat and charged species using computational fluid dynamic (CFD) methods. Three-dimensional, non-isothermal CFD models for different designs of micro proton exchange membrane (PEM) fuel cells have been developed and used to investigate the cell performance [20-22]. The models are shown to be able to: understand the many interacting, complex electrochemical and transport phenomena that cannot be studied experimentally; identify limiting steps and components; and provide a computer-aided tool for the design and optimization of future micro fuel cells to improve their lifetime with a much higher power density and lower cost. This can be demonstrated by some examples in Figures 5-7.

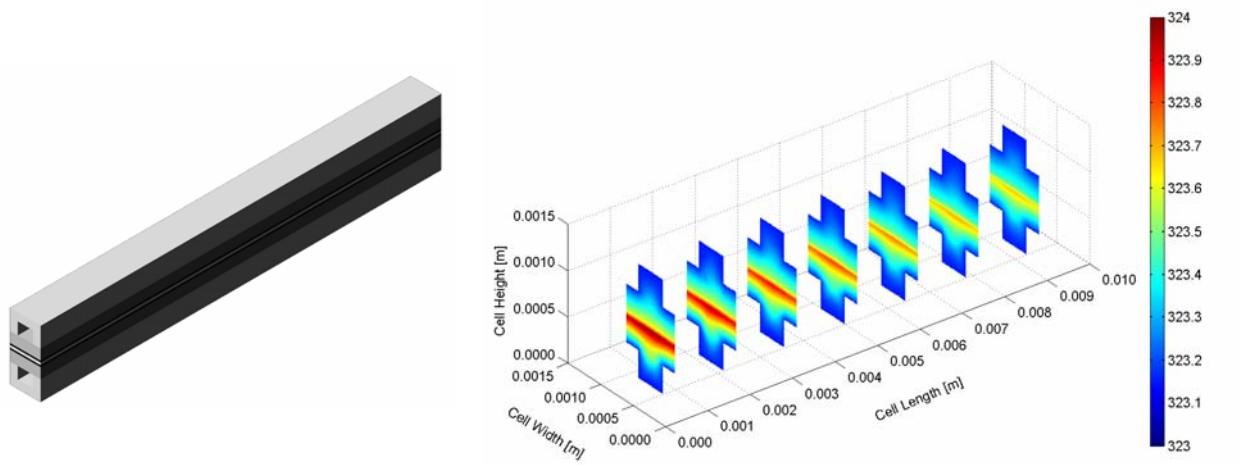


Figure 5. Three-dimensional computational domain and temperature distribution inside micro PEM fuel cell with straight gas flow channels [20].

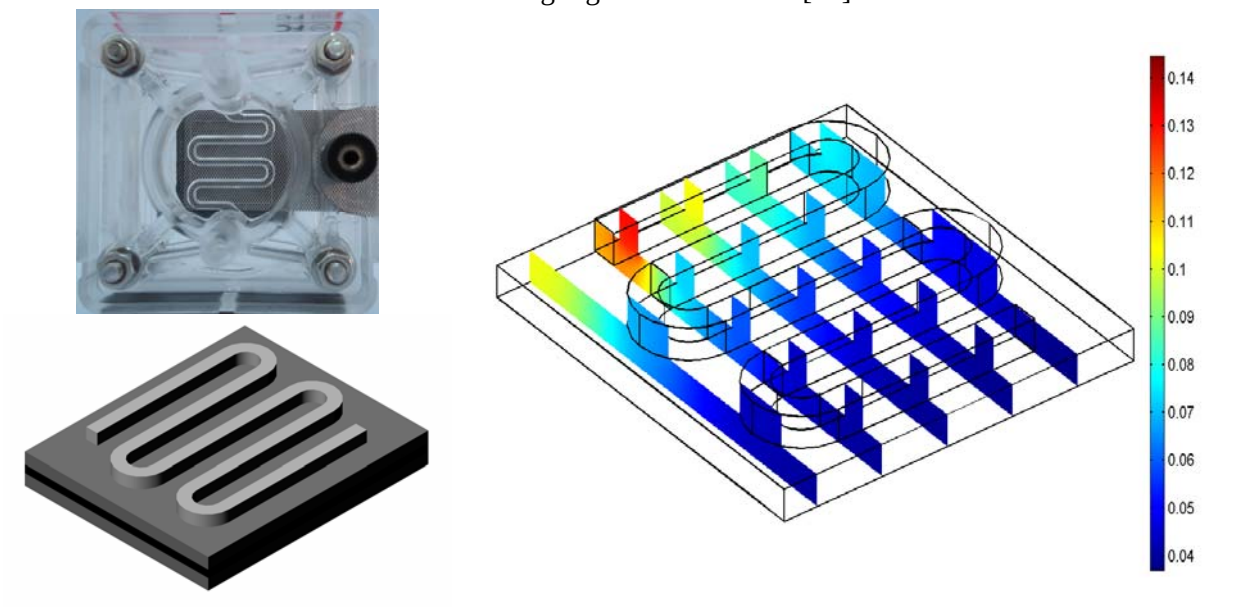


Figure 6. Three-dimensional computational domain and oxygen weight fraction distribution in micro PEM fuel cell with serpentine gas flow channels [21].

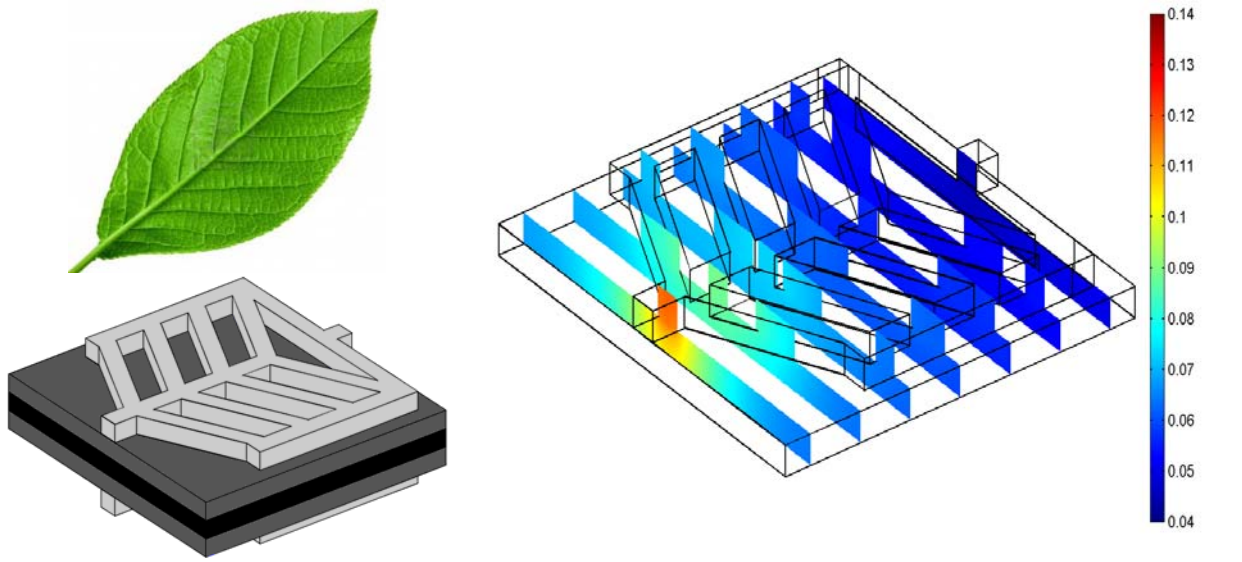


Figure 7. Three-dimensional computational domain and oxygen weight fraction distribution in micro PEM fuel cell with nature inspired gas flow channels. The design inspired from the existed biological fluid flow patterns in the leaf [22].

Although the small fuel cells have provided significant advantages in portable electronic applications over conventional battery systems. However, the typical PEM fuel cell system with its heavy reliance on subsystems for cooling, humidification and air supply would not be practical in small applications. The air-breathing PEM fuel cells without moving parts (external humidification instrument, fans or pumps) are one of the most competitive candidates for future portable-power applications. Three-dimensional, multi-phase, non-isothermal CFD models of different novel designs, simple to construct, PEM fuel cell which work in still or slowly moving air have been developed [23-28]. The novel geometries enables optimum air access to the cathode without the need for pumps, fans or similar devices. To the author's knowledge, these are the first novel designs. The results are presented and analyzed with a focus on the physical insight and fundamental understanding (see some examples in Figures 8-9). They can provide a solid basis for optimizing the geometry of the PEM fuel cell stack running with a passive mode [29-32].

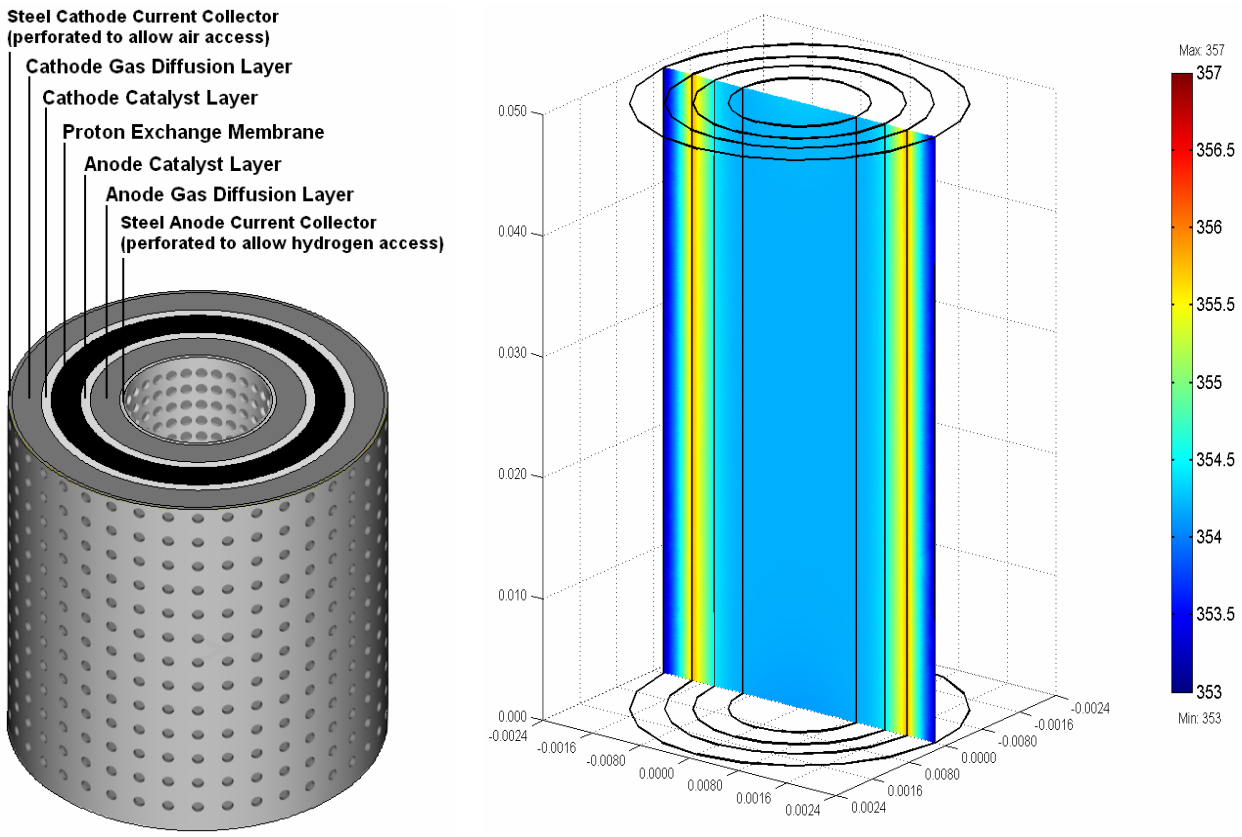


Figure 8. Three-dimensional computational domain of a tubular-shaped ambient air-breathing PEM fuel cell and the temperature distribution inside the cell at nominal current density of 1 A/cm^2 [29].

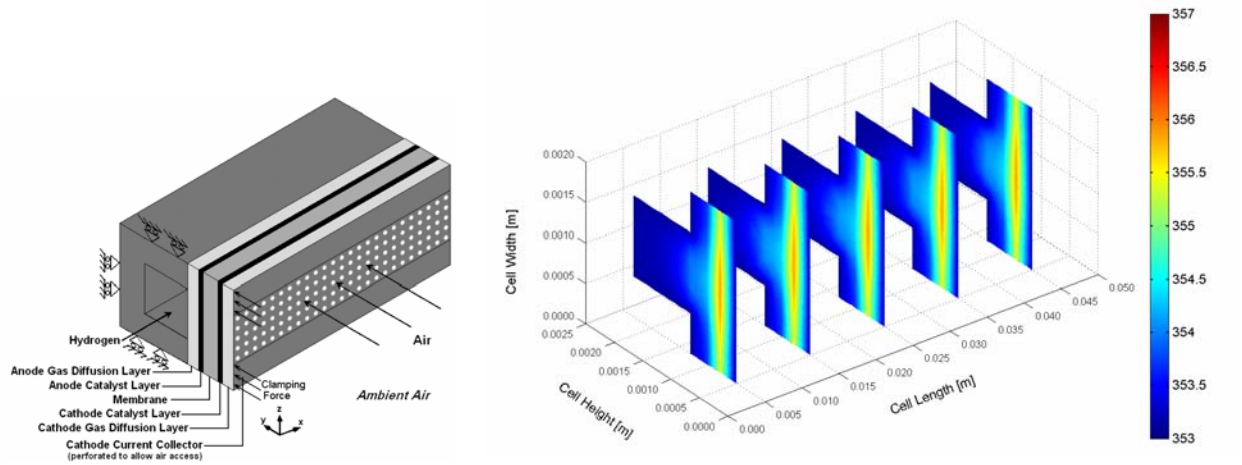


Figure 9. Three-dimensional computational domain of a planner ambient air-breathing PEM fuel cell and the temperature distribution inside the cell at nominal current density of 0.8 A/cm^2 [30-32].

The appearance of portable microelectronic devices and off-the-grid sensors employed for biological, environmental and security monitoring leads to the high demand for miniaturized and reliable power sources. For such applications, having miniaturized high-energy-density power sources to provide long-term operation is a critical requirement. Micro air breathing fuel cell technology can take advantage of fuels with energy densities of an order of magnitude higher than the energy stored in batteries. To bring in the high energy density of fuels, the miniaturization and integration of fuel cell systems are inevitable.
Different novel geometries of air-breathing PEM micro fuel cell operating with hydrogen fed at the anode and air supplied by natural convection at the cathode have been designed [33-36]. There are several reasons that make these novel designs more advantageous than the usual one for medium to high power stacks: (i) elimination of the flow field: lower pressure drop at the anode fields and no time-consuming machinery due to shorter flow fields, (ii) uniform pressure applied to the MEA by the cathode, (iii) quicker response when switching from fuel cell mode to electrolyser mode in a unitized regenerative fuel cell, (iv) greater cathode surface that increases the amount of oxygen reduction, the rate of which is slower than the hydrogen oxidation rate. In addition, (v) these designs can achieve much higher active area to volume ratios, and hence higher volumetric power densities.
A non-isothermal, fully three-dimensional CFD models of different novel designs for ambient air-breathing PEM micro fuel cell are presented with some examples in Figures 10-12. The informative results obtained can help in understanding of the local gas transports and electrochemical characteristics in air-breathing PEM micro fuel cells. Also, they can provide a solid basis for optimizing the geometry of the passive PEM micro fuel cell stacks. To the author's knowledge, these are the first new designs of air-breathing PEM micro fuel cells.

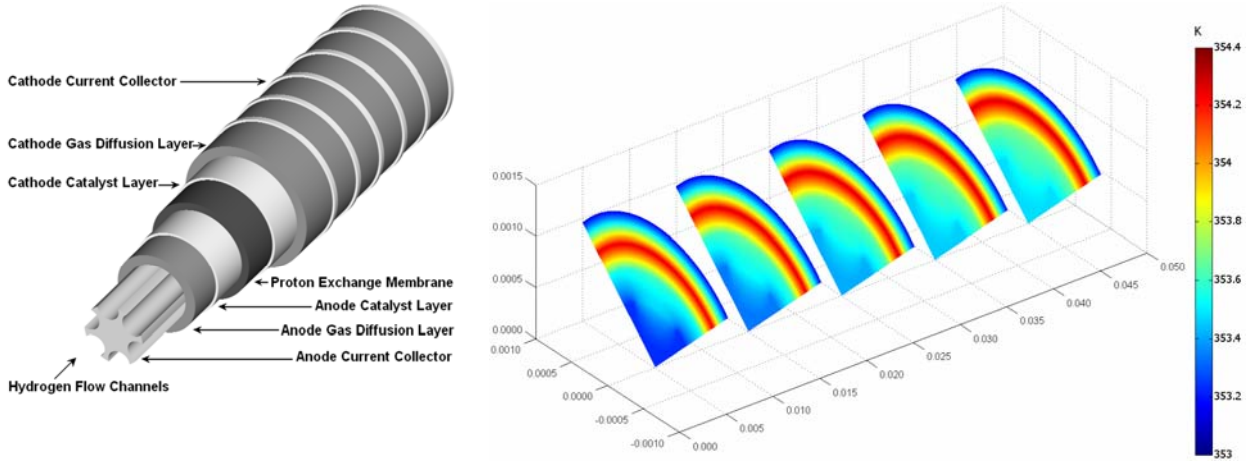


Figure 10. Three-dimensional computational domain of a tubular-shaped ambient air-breathing PEM micro fuel cell and the temperature distribution inside the cell [33, 34].

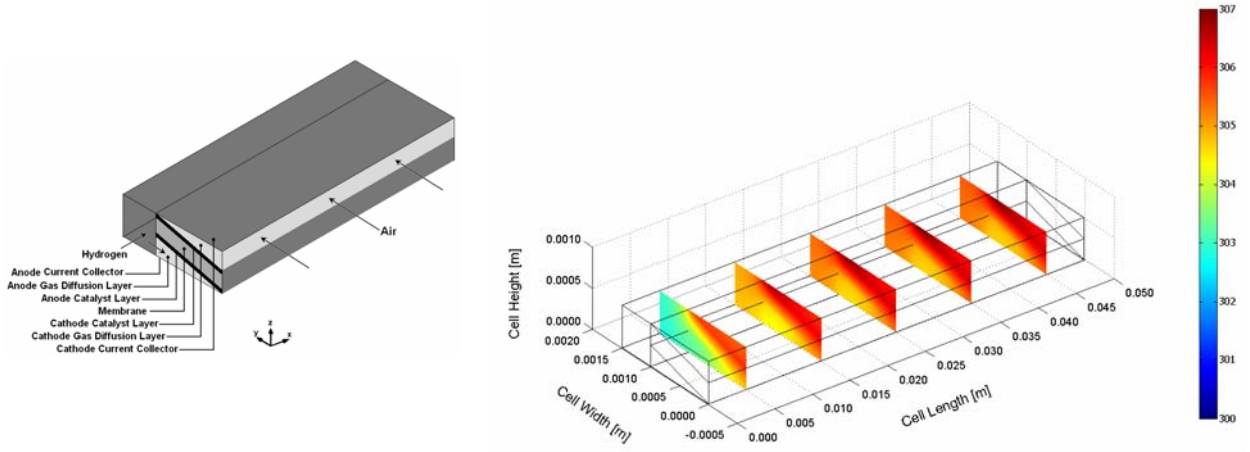


Figure 11. Three-dimensional computational domain of a planar compacted-design micro-structured ambient air-breathing PEM micro fuel cell and the temperature distribution inside the cell [35].

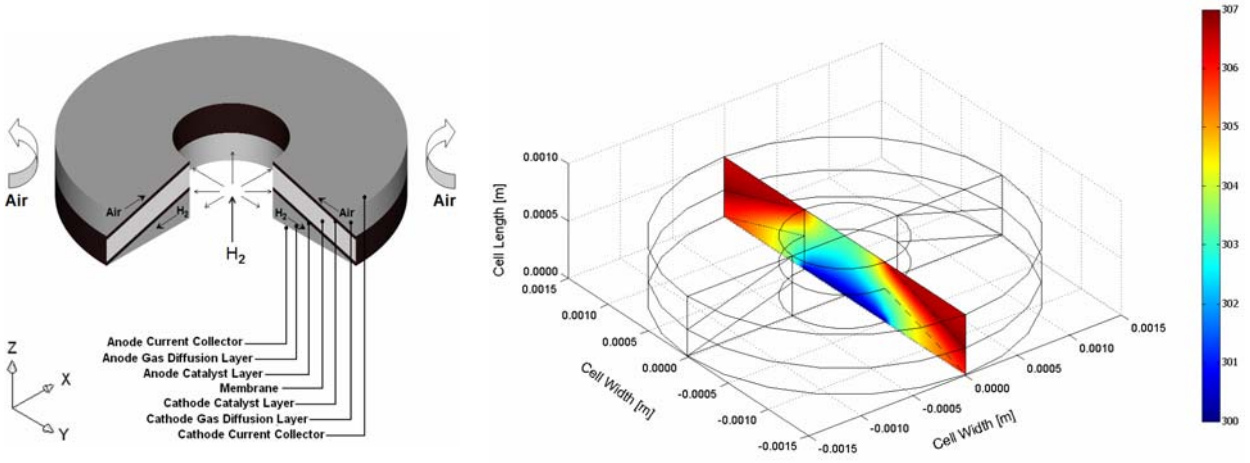


Figure 12. Three-dimensional computational domain of a disk-shaped micro-structured ambient air-breathing PEM micro fuel cell and the temperature distribution inside the cell [36].

3. Mechanical and hygro-thermal stresses modeling of PEM fuel cell

The Membrane-Electrode-Assembly (MEA) is the core component of PEM fuel cell and consists of membrane with the gas-diffusion layers including the catalyst attached to each side. The fuel cell MEA durability plays a vital role in the overall lifetime achieved by a stack in field applications. Within the MEA's electrocatalyst layers are three critical interfaces that must remain properly intermingled for optimum MEA performance: platinum/carbon interface (for electron transport and catalyst support); platinum/Nafion interface (for proton transport); and Nafion/carbon interface (for high-activity catalyst dispersion and structural integrity).

The MEA performance shows degradation over operating time, which is dependent upon materials, fabrication and operating conditions [37-47]. Mechanical degradation is often the cause of early life failures. Mechanical stresses which limit MEA durability have two origins. Firstly, this is the stresses arising during fuel cell assembly (bolt assembling). The bolts provide the tightness and the electrical conductivity between the contact elements. Secondly, additional mechanical stresses occur during fuel cell running because PEM fuel cell components have different thermal expansion and swelling coefficients. Thermal and humidity gradients in the fuel cell produce dilatations obstructed by tightening of the screw-bolts. Compressive stress increasing with the hygro-thermal loading can exceed the yield strength which causes the plastic deformation. The mechanical behaviour of the membrane depends strongly on hydration and temperature [37-47].

An operating fuel cell has varying local conditions of temperature, humidity. As a result of in the changes in temperature and moisture, the membrane, GDL and bipolar plates will all experience expansion and contraction. Because of the different thermal expansion and swelling coefficients between these materials, hygro-thermal stresses are introduced into the unit cell during operation. In addition, the non-uniform current and reactant flow distributions in the cell result in non-uniform temperature and moisture content of the cell which could in turn, potentially causing localized increases in the stress magnitudes, and this leads to mechanical damage, which can appear as through-the-thickness flaws or pinholes in the membrane, or delaminating between the polymer membrane and gas diffusion layers. Therefore, in order to acquire a complete understanding of these damage mechanisms in the membranes and the gas diffusion layers, mechanical response under steady-state hygro-thermal stresses should be studied under real cell operation conditions.

Three-dimensional computational fluid dynamics (CFD) model of a PEM fuel cell has been developed to simulate the stresses distribution and deformation inside the cell, which are occurring during fuel cell assembly (bolt assembling), and membrane swelling and cell materials expansion during fuel cell running due to the changes of temperature and relative humidity. To the author's knowledge, Maher A.R. Sadiq Al-Baghdadi's work [37] is the first to incorporate the effect of mechanical and hygro-thermal stresses into actual fuel cell model with three-dimensional effect.

The behavior of the whole cell during operation has been studied and investigated under real cell operating conditions [48]. The results show that the non-uniform distribution of stresses, caused by the temperature and relative humidity gradient in the cell, induces localized bending stresses, which can

contribute to delaminating between the membrane and the gas diffusion layers. These stresses may explain the occurrence of cracks and pinholes in the membrane under steady–state loading during regular cell operation. Figure 13 shows stress distribution and total displacement inside the PEM fuel cell during operation. To the author's knowledge, this has not been specifically described before.

PEM fuel cell assembly pressure is known to cause large strains in the cell components. All components compression occurs during the assembly process of the cell, but also during fuel cell operation due to membrane swelling when absorbs water and cell materials expansion due to heat generating in catalyst layers. Additionally, the repetitive channel-rib pattern of the bipolar plates results in a highly inhomogeneous compressive load, so that while large strains are produced under the rib, the region under the channels remains approximately at its initial uncompressed state. This leads to significant spatial variations in GDL thickness and porosity distributions, as well as in electrical and thermal bulk conductivities and contact resistances (both at the ribe-GDL and membrane-GDL interfaces). These changes affect the rates of mass, charge, and heat transport through the GDL, thus impacting fuel cell performance and lifetime.

Figure 14 illustrates the changes suffered by the porosity field during the compression process as a result of assembly process of the stack, and also as a result of membrane swelling, and cell materials expansion due to the temperature and relative humidity cycles during operation [49]. The GDL intrusion into the channel and the compressive stress applied at the rib symmetry plane are also indicated for illustrative purposes. The inhomogeneity associated with the repetitive channel-rib pattern is perfectly reflected, showing a region of large porosity reduction under the rib, a region of unperturbed porosity under the channel, and an intermediate fan like transition region below the channel-rib wall. Note in particular the accumulation of stresses under the rib corner, which results in high porosity reduction in this particular region. The simulations also show that the upper edge of the GDL experiences slight tensile strains in the region below the channel, thereby increasing the GDL porosity above its initial value 0.4.

In a real PEM fuel cell stack, the contact pressure on the GDL is different from the clamping pressure because of the channels in the bipolar plate. Furthermore, due to the round corners of the bipolar plate, the contact behavior at the interface is hard to predict without a CFD analysis. Figure 15 shows the interfacial contact resistance a long the rib width.

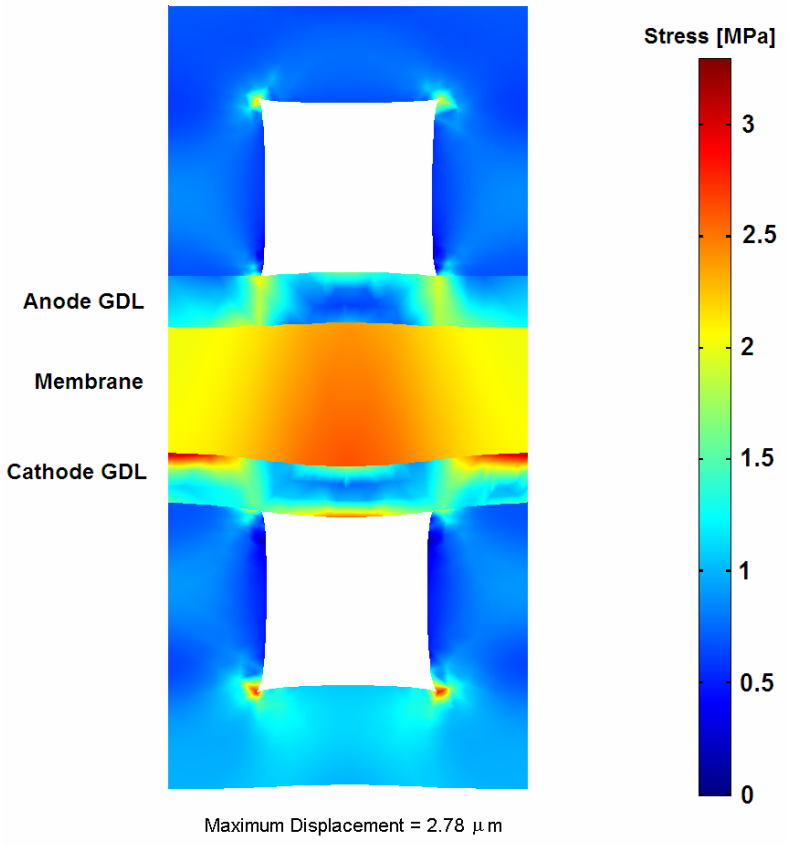


Figure 13. Von Mises stress distribution inside the cell (contour) and total displacement (deformed shape plot, scale enlarged 200 times) on the y-z plane at x=10 mm [48].

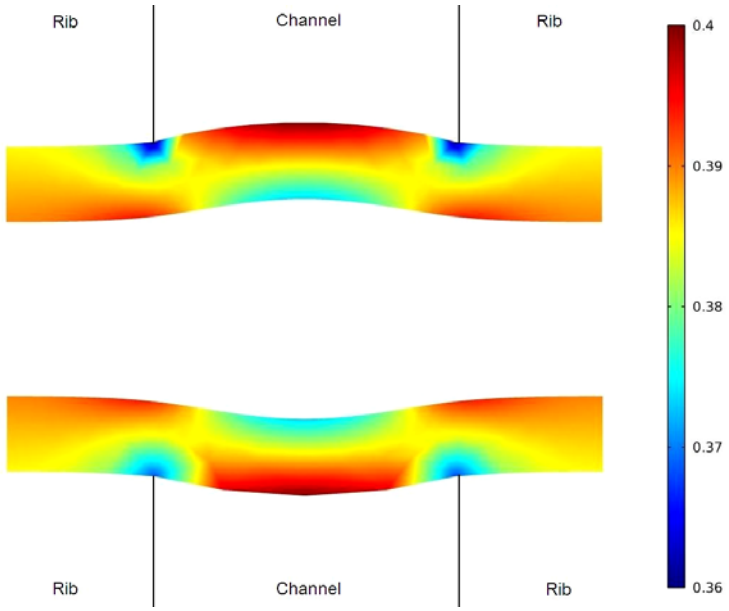


Figure 14. Porosity distribution in the GDLs (contour) and total displacement (deformed shape plot, scale enlarged 250 times) on the y-z plane at x=10 mm [49].

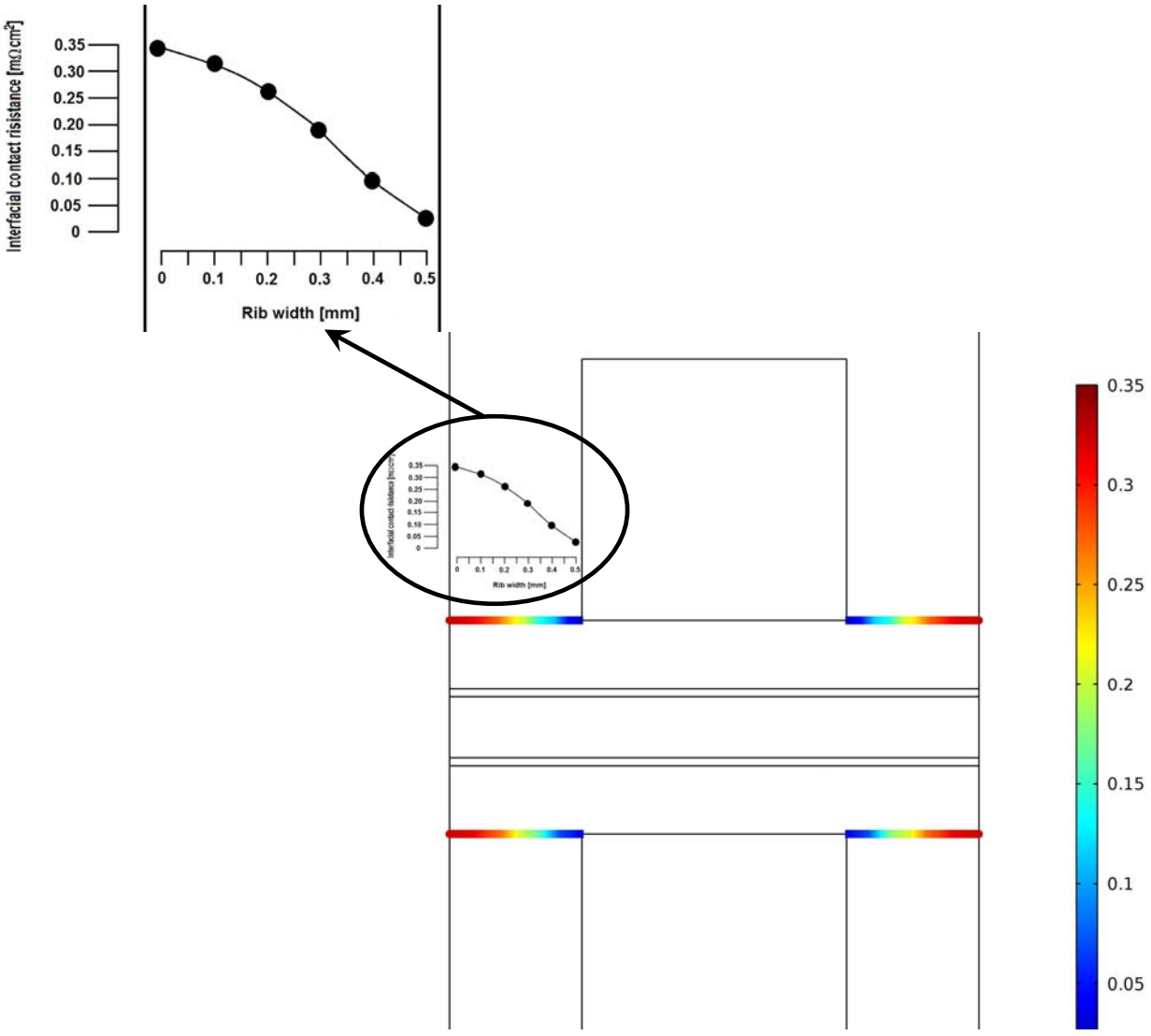


Figure 15. Interfacial contact resistance GDL/bipolar plate a long the rib width [49].

Optimization study of a PEM fuel cell durability has been performed to achieve long cell life [50]. The study quantifies and analyses the impact of operating, design, and material parameters on fuel cell durability and get an optimal conditions for PEM fuel cells to achieve long cell life. In these optimum conditions, the maximum deformation (displacement) reduction by about 50% than the base case operating conditions (Figure 16). To the author's knowledge, this has not been modeled before, and this is the first work that shows how to optimize a PEM fuel cell to achieve long cell life.

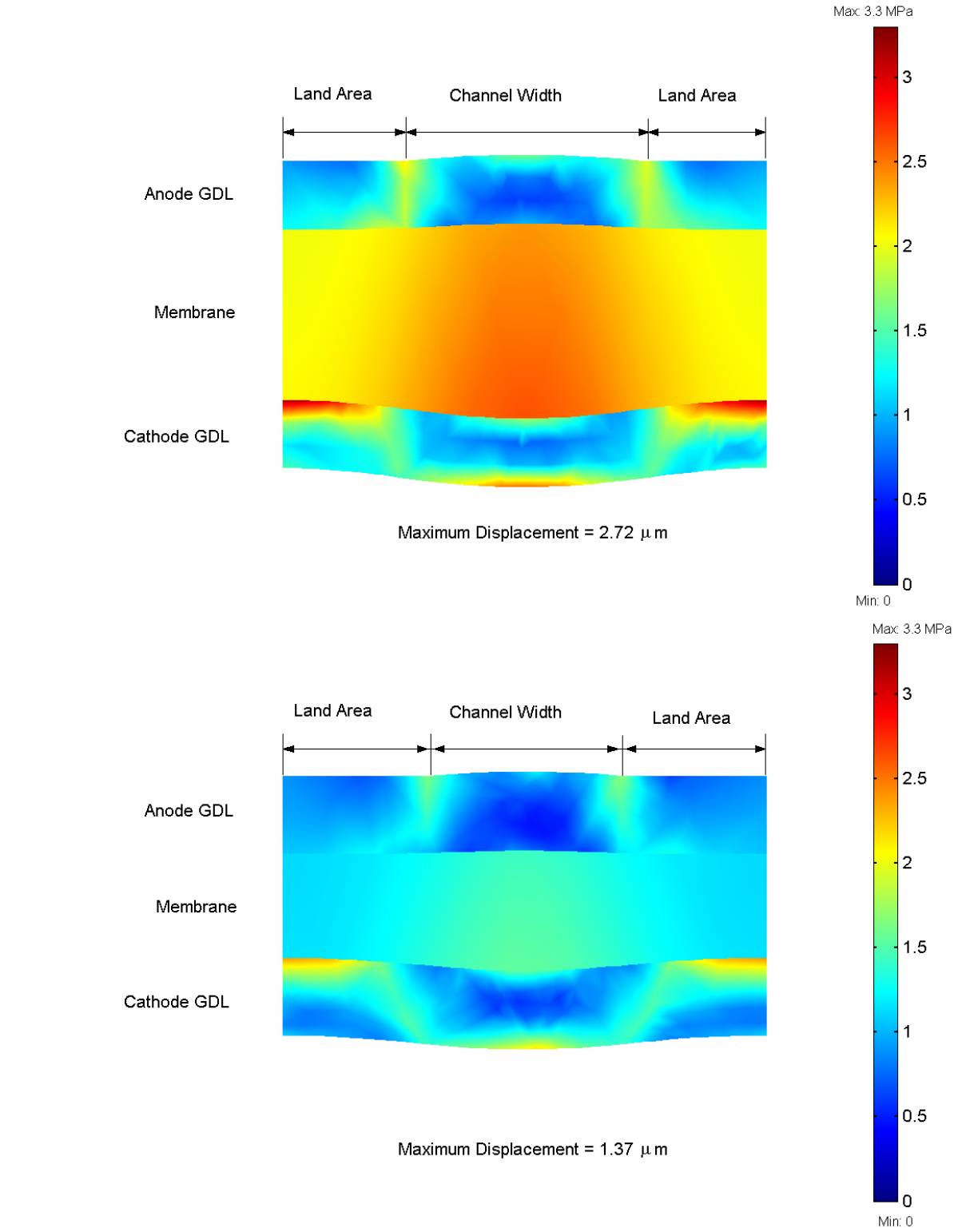


Figure 16. Mises stress distribution (contour) and total displacement (deformed shape plot, X200) in the MEA: at base case conditions (upper), and for optimum design, material, and operating conditions (lower) [50].

4. Assembly modeling of PEM fuel cell stack

Many parameters must be considered when designing a PEM fuel cell stack. Some of the most basic design considerations include power required, size, weight, volume, cost, transient response, and operating conditions. From these initial requirements, the more detailed design requirements (such as the number of cells, material and component selections, flow field design, etc.) can be chosen.

PEM fuel cell stack assembly process, including clamping pressure, material properties of each component, design (component thickness and cell active area), and number of cells in the stack are important factors influencing the performance and durability of the PEM fuel cell stack. Furthermore, when temperature and relative humidity increase during operation, the membrane absorbs water and swells. Since the relative position between the top and bottom end plates is fixed, the polymer membranes in the stack are spatially confined. Thus the gas diffusion layers (GDLs) in the stack will be further compressed under the land and the intrusion into channel becomes more significant. Assembly pressure, contact resistance, membrane swelling and operating conditions, etc., combine to yield an optimum assembly pressure. The clamping pressure is therefore a critical parameter for optimal fuel cell stack performance and durability. Too high, too low, or inhomogeneous compressions have negative effects on the performance and durability of the stack.

Modeling and simulations at the early stage of the stack architecture development are mandatory to lower the costs of the stack and to contribute in designing component dimensions and forms, particularly of stamped bipolar plates or clamping systems. CFD modeling is a great tool for the design and analyses of fuel cell stack. CFD model of a PEM fuel cell stack has been developed to simulate the pressure distribution inside the stack, which are occurring during fuel cell assembly (bolt assembling), and membrane swelling and cell materials expansion during fuel cell running due to the changes of temperature and relative humidity [51, 52]. A five cells stack with clamping plate and rod assembly has been modeled and analyzed during assembly process and also during operation (Figure 17). The five cells stack model simulated includes the following components; two end-plates, two current plates, and in each cell includes; two bi-polar plates, two GDLs, two gaskets and, an MEA (Figures 18 and 19). A detailed analysis of the stack performance and durability during operation and assembly process, including clamping pressure, material properties of each component, stack design (component thickness and cell active area), and number of cells in the stack has been conducted and examined. This can be demonstrated by some examples in Figures 20 and 21. To the author's knowledge, this is the first study to apply a multiphysics computational fluid dynamics for calculating mechanical and thermal stresses in PEM fuel cell stack during operation.

In practice, multiple single cells are usually connected in series to form a PEM fuel cell stack to provide the sufficient power and desired voltage. This configuration results in a high requirement of assembly accuracy for the adjacent bipolar plates. Otherwise, the assembly error will affect the perfect alignment of the adjacent bipolar plates and there will be an assembly position deviation, which leads to the assembly force transmitting asymmetrically and in turn makes the contact pressure distribution between the bipolar plate and MEA non-uniform. Moreover, such assembly error brings an extra moment to the MEA, which may deform the MEA seriously and produce stress concentration even cracks. Once the stress of MEA exceeds its yield strength, the plastic deformation will happen, and in turn, results in residual stresses in MEA after unloading, which are believed to be a significant contributor for the stress failure of MEA. Hence, it is very important to control the assembly error of the Bipolar plate to a low level in order to maintain a proper pressure distribution and avoid stress failure of the MEA.

However, the assembly error for the PEM fuel cell stack has not received enough attention currently, and in particular manual assembly processes are still widely applied for most of the stacks, which results in large assembly errors of the bipolar plates. Furthermore, during the running of a PEM fuel cell stack, the unavoidable vibration may aggravate the assembly error, especially for the automotive application due to more vibrations. In addition, for the PEM fuel cell stack of metallic bipolar plate, the bipolar plate exhibits larger manufacturing error because of its plastic characters (for example spring-back), which in turn makes the influence of assembly error more serious.

On one hand, the assembly error of bipolar plate should be controlled and decreased in order to improve the performance of the PEM fuel cell stack. On the other hand, based on the current assembly process and manufacturing process, it is very hard to control the assembly error to a very low level. And moreover if the assembly error required is too small, the assembly and manufacturing cost of the PEM fuel cell stack will increase dramatically, which is unacceptable and conflict with the cost reduction of the PEM fuel cell. Therefore, there is a need to investigate the effect of the assembly error of the bipolar

plate on the contact behavior of PEM fuel cell stack in order to guide the assembly process, and furthermore obtain a trade-off between the performance and the assembly accuracy.

An example result of the misalignment (the channel alignment of the bipolar plate on the anode side is not be in the perfect match of the channel on the cathode side in the first cell) during the process of fuel cell stack assembly are shown in Figure 22. To the author's knowledge, this has not been modeled before during operation conditions.

A PEM fuel cell stack is laminated with a number of plate-type cells, and the latest model is assembled by compression from both ends of plates. PEM fuel cells are exposed to high magnitude vibrations, shocks, and cyclic loads in many applications. Vibrations during operation show significant impact in the longer run of the fuel cells. Frequencies which are not close to the resonant frequencies or natural frequencies show very little effect on the overall performance. However, if the frequency ranges of operation approaches the resonant frequency range, the probability of component failure increases. It is possible that there will be lateral transition of cells or leakage of fuel gas and coolant water. Therefore, it is necessary to evaluate the effects vibration has on the fuel cell.

Vibration characteristics are required to understand the vibration behaviour of PEM fuel cell stack components such as the membrane, catalyst layer, gas diffusion layers, bi-polar plates, gasket, current plates, and end plates. Vibrating at resonance frequency can lead to the initiation and acceleration of defect formation, which may ultimately result in operational failure. Vibrations may exacerbate defects such as pinholes, cracks, and delamination, which can result in fuel crossover, leakage of fuel gas and coolant water, performance degradation, and reduced durability.

Natural frequencies and mode shapes of the PEM fuel cell stack has been modeled using finite element methods (FEM). The work aims to understand the vibration characteristics of a PEM fuel cell stack and to evaluate their seismic resistance under a vibration environment. A parametric study has been conducted to investigate how the natural frequency varies as a function of thickness, Young’s modulus, and density for each component layer. In addition, this work provides insight into how the natural frequencies of the PEM fuel cell stack should be tuned to avoid high amplitude vibrations by modifying the material and geometric properties of individual components [53]. The mode shapes of the PEM fuel cell stack provide insight into the maximum displacement exhibited under vibration conditions that should be considered for transportation and stationary applications. The natural frequencies and the mode shapes of the PEM fuel cell stack are shown in Figure 23 at the base case conditions.

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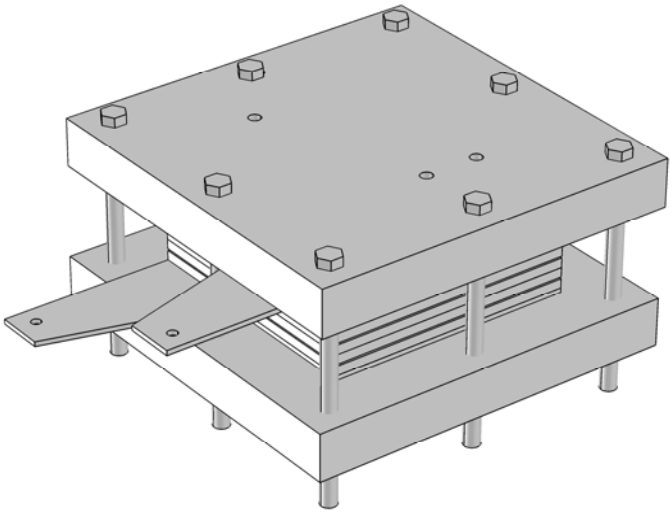


Figure 17. A PEM fuel cell stack assembly.

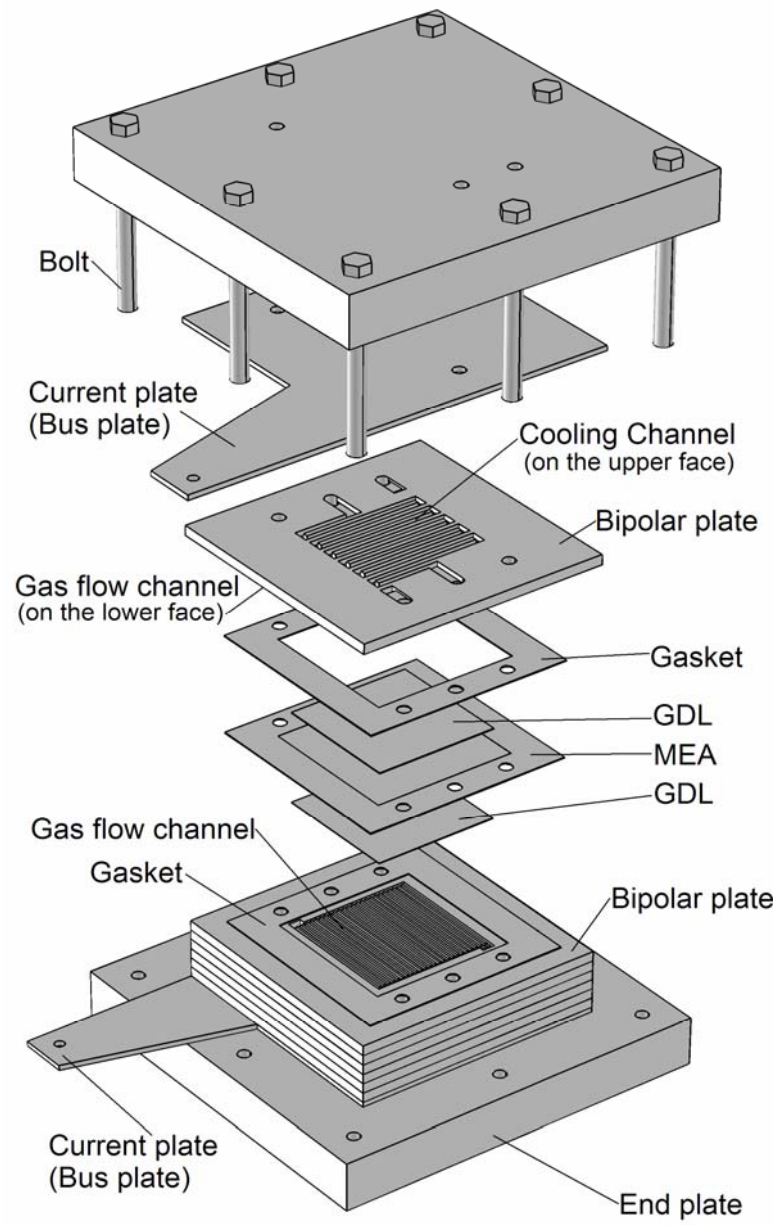


Figure 18. Expanded view of a PEM fuel cell stack.

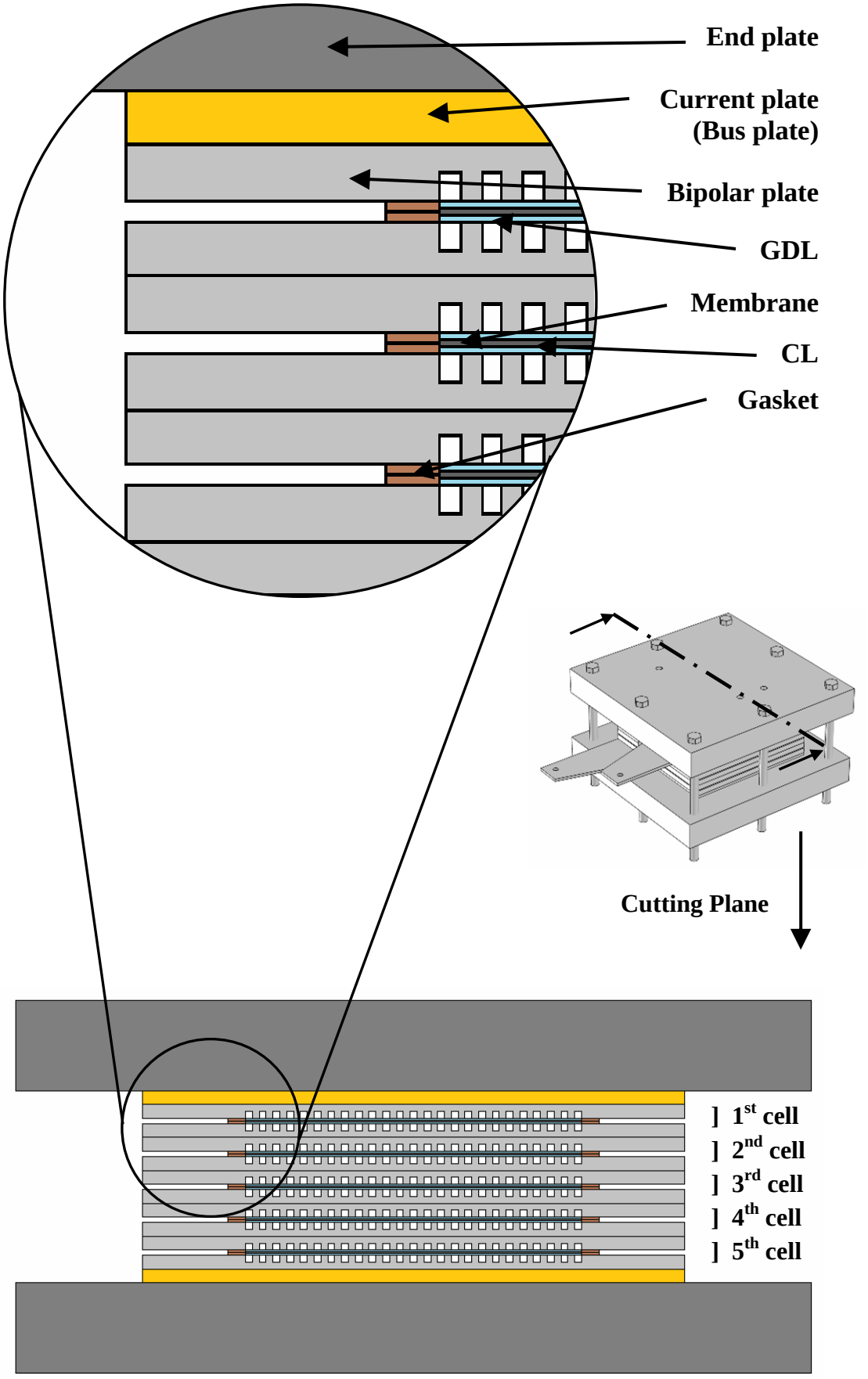


Figure 19. Description of the different stack components (Five cells).

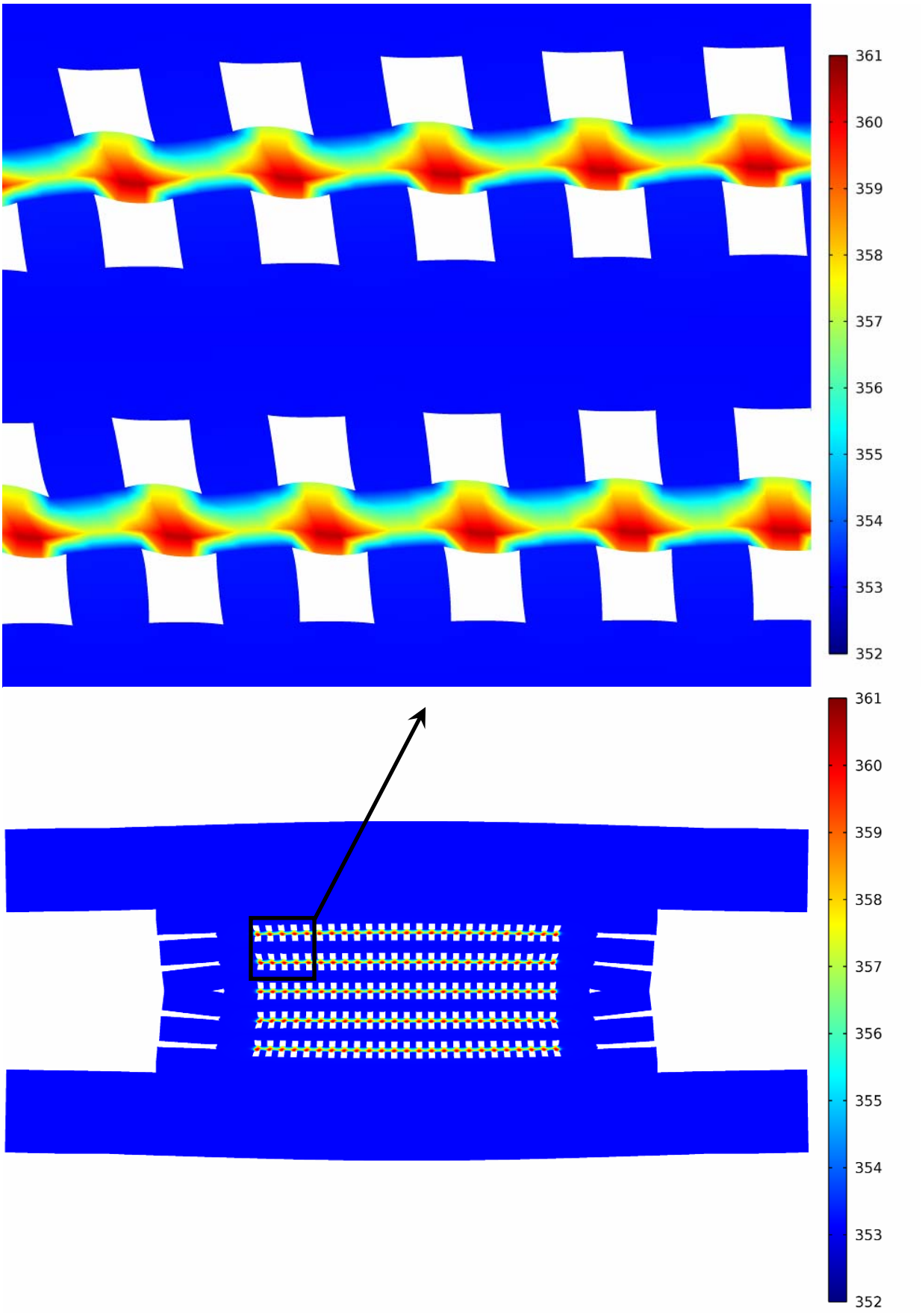


Figure 20. Temperature distribution [K] in the PEM fuel cell stack during operation, (deformed shape plot: stack = X50, part = X100) [51].

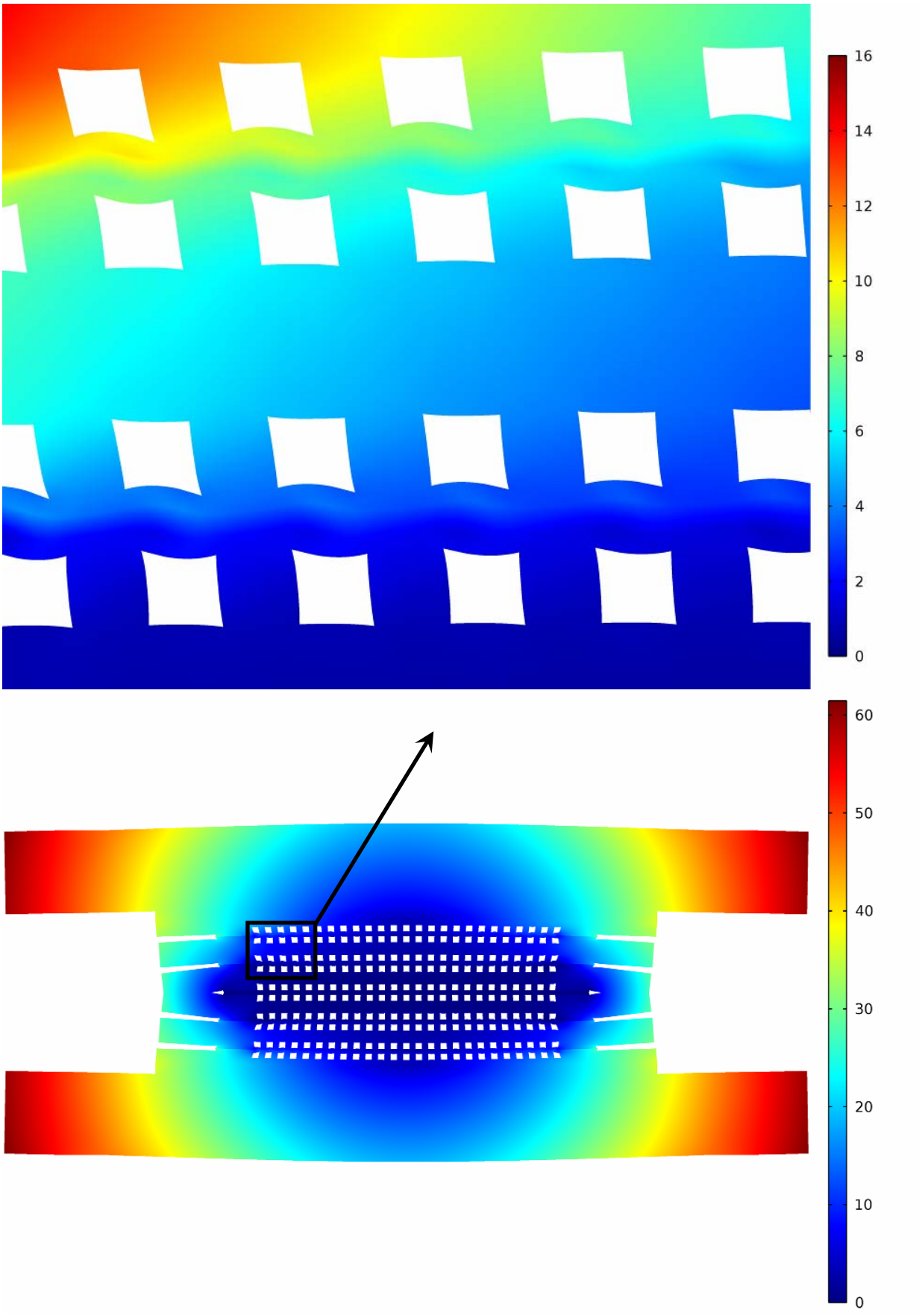


Figure 21. Total displacement [μm] in the PEM fuel cell stack during operation, (deformed shape plot: stack = X50, part = X100) [51].

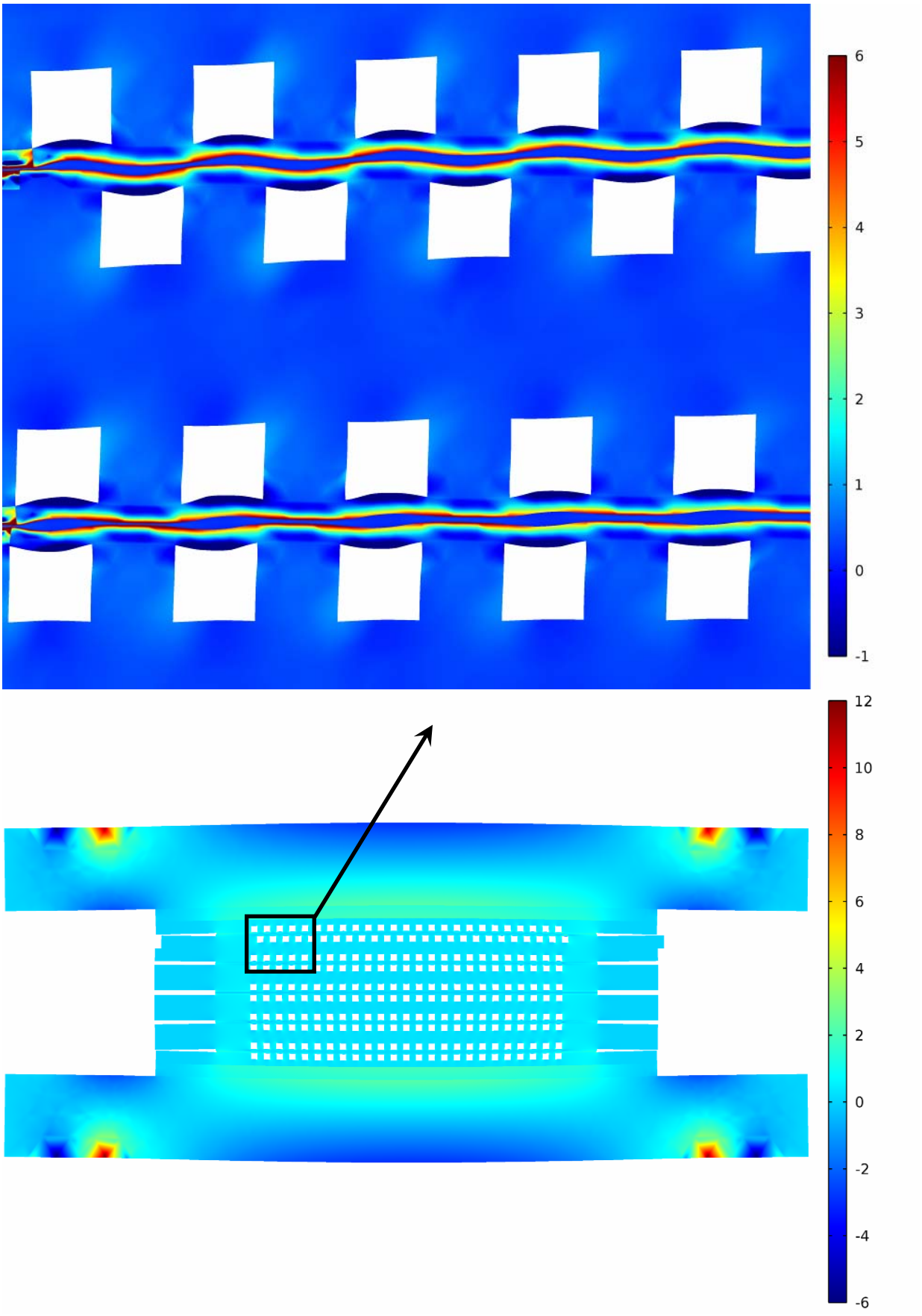
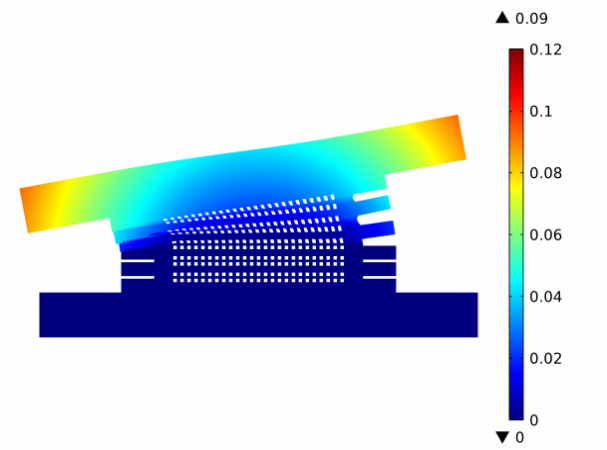
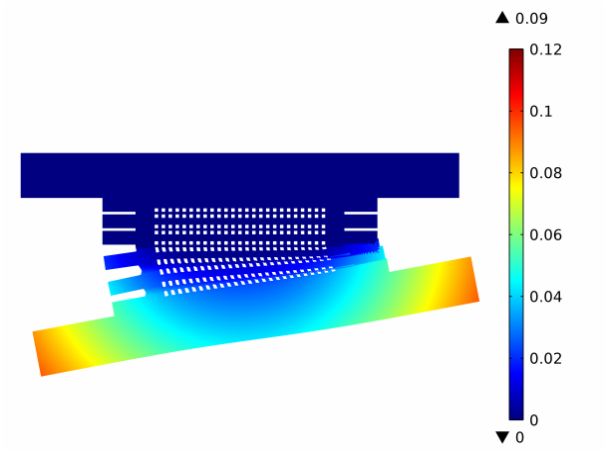


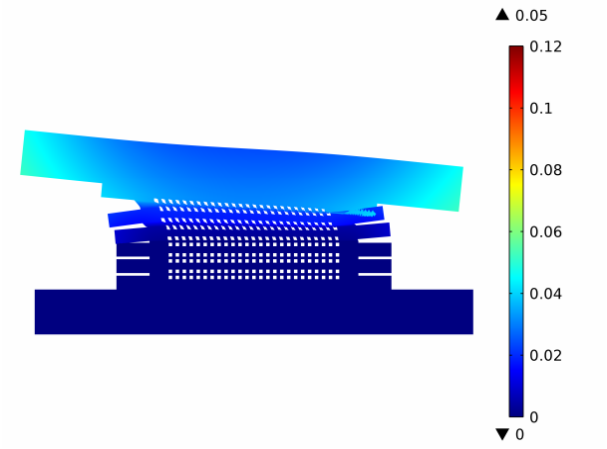
Figure 22. Pressure distribution [MPa] in the PEM fuel cell stack, (deformed shape plot: stack = X200, part = X400), (with assembly error during assembly process) [51].



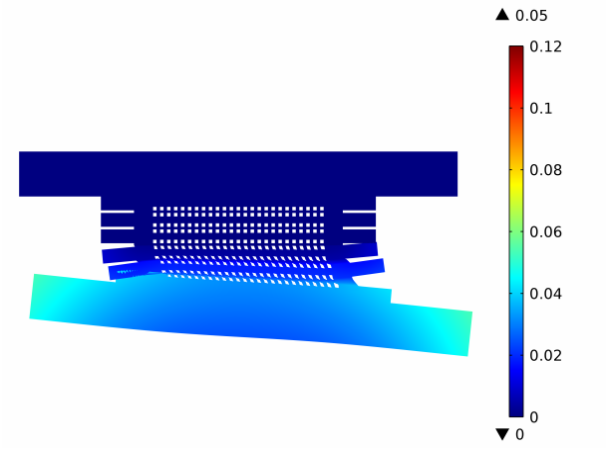
Mode 1, frequency 1777.615 Hz



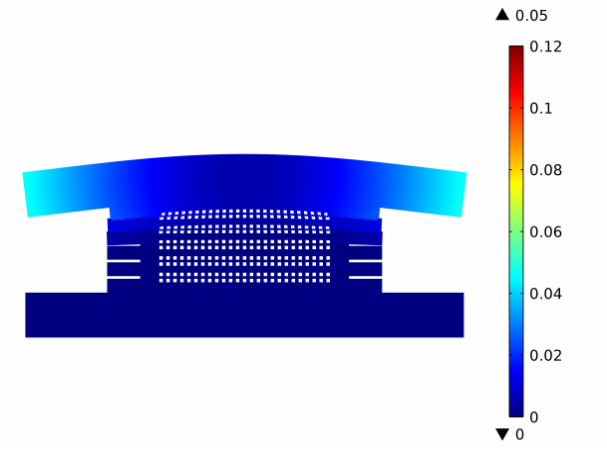
Mode 2, frequency 1777.683 Hz



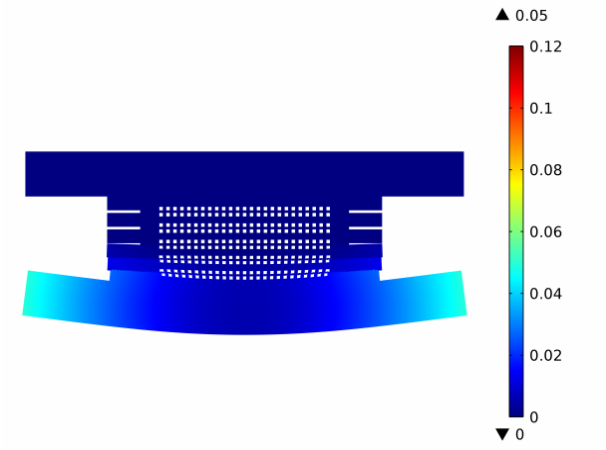
Mode 3, frequency 2735.020 Hz



Mode 4, frequency 2735.103 Hz



Mode 5, frequency 3315.592 Hz



Mode 6, frequency 3315.601 Hz

Figure 23. Natural vibration modeling of PEM fuel cell stack. First six natural mode shapes with total displacement [nm]. (Number of cells in the stack = 5) [53].

5. PEM fuel cells and hydrogen fuel

PEM fuel cells need hydrogen as fuel. Commercialization of PEM fuel cells, particularly for transportation and stationary electricity-generation markets, must be accompanied by commercialization of hydrogen energy technologies, that is, technologies for hydrogen production, distribution, and storage. In other words, hydrogen must become a readily available commodity (not as a technical gas but as an energy carrier) before fuel cells can be fully commercialized. On the other hand, it may very well be that the fuel cells will become the driving force for development of hydrogen energy technologies. PEM fuel cells have many unique properties, such as high energy efficiency, no emissions, no noise, modularity, and potentially low cost, which may make them attractive in many applications even with a limited hydrogen supply.

Hydrogen has some unique properties that make it an ideal energy carrier, namely [54-56]:

- It can be produced from and converted into electricity at relatively high efficiencies.
- Raw material for hydrogen production is water, which is available in abundance. Hydrogen is a completely renewable fuel, because the product of hydrogen utilization through electrochemical conversion is pure water.
- It can be stored in gaseous form (convenient for large-scale storage), in liquid form (convenient for air and space transportation), or in the form of metal or chemical hydrides (convenient for surface vehicles and other relatively small-scale storage requirements).
- It can be transported over large distances through pipelines or via tankers (in some cases more efficiently and economically than electricity).
- It can be converted into other forms of energy in more ways and more efficiently than any other fuel.
- Hydrogen as an energy carrier is environmentally compatible, its storage, transportation, and end use do not produce any pollutants, greenhouse gases, or any other harmful effects on the environment. Hydrogen itself is not toxic.
- Hydrogen is a relatively safe fuel if handled properly.

Production of hydrogen requires feedstock. Technologies for hydrogen production from fossil fuels have been developed and are used to produce industrial hydrogen. These include steam reforming of natural gas, partial oxidation of hydrocarbons, and coal gasification. However, these technologies will not help reduce dependency on fossil fuels and will not reduce CO_2 generation. The only method that can generate hydrogen from fossil fuels without generation of CO_2 is direct thermal (and catalytic) cracking of hydrocarbons. This method has been used to produce carbon, but for costeffective hydrogen generation it is in a rather early development phase, barely showing technical feasibility in the labs. Water electrolysis is a mature technology and was developed for hydrogen production capacities ranging from a few cm^3/min to thousands m^3/hr. It is relatively efficient, but because it needs high-quality energy (electricity), hydrogen produced by water electrolysis is expensive. Full benefits of hydrogen will be realized only in conjunction with renewable energy sources. Both hydrogen and electricity complement the renewable energy sources and allow their indirect utilization in almost every imaginable application. Such a system is in complete balance with the environment and can run as long as the energy source is available [54-56].

Hydrogen as an energy carrier must be stored to overcome daily and seasonal discrepancies between energy source availability and demand. Hydrogen can be stored either as a pressurized gas or as a liquid. It can also be stored in chemical or physical combinations with other materials, such as metal hydrides, chemical hydrides, glass microspheres, and cryoadsorbers.

Like any other fuel or energy carrier, hydrogen poses risks if not properly handled or controlled. The risk of hydrogen, therefore, must be considered relative to the common fuels such as gasoline, propane, or natural gas. The specific physical characteristics of hydrogen are quite different from those common fuels. Some of these properties make hydrogen potentially less hazardous, whereas other hydrogen characteristics could theoretically make it more dangerous in certain situations [57]. Table 1. compares hydrogen properties with other fuels and ranks their effect on safety.

In conclusion, hydrogen appears to pose risks of the same order of magnitude as other fuels. In spite of public perception, in many aspects hydrogen is actually a safer fuel than gasoline and natural gas.

Table 1. Summary of hydrogen safety related properties compared with other fuels.

Property	Compare with other fuels	Risk
Leak probability	Higher than other fuels	Dangerous
Volume of fuel released in leak	Higher than other fuels	Same as other fuels
Energy of fuel released in leak	Lower than other fuels	Safe
Diffusivity and buoyancy	Higher than other fuels	Safe
Lower flammability limit in air	Higher than other fuels	Same as other fuels
Minimum ignition energy	Lower than other fuels	Same as other fuels
Ignition energy at LFL	~Same as other fuels	Same as other fuels
Flame velocity	Higher than other fuels	Dangerous
Lower detonability fuel/air ratio	Higher than other fuels	Safe
Explosive energy per energy stored	Lower than other fuels	Safe
Flame visibility	Lower than other fuels	Dangerous
Flame emissivity	Lower than other fuels	Safe
Flame fumes toxicity	Lower than other fuels	Safe
Fuel toxicity	Lower than other fuels	Safe

6. Conclusion

Fuel cell system is an advanced power system for the future that is sustainable, clean and environmental friendly. Fuel cells are growing in importance as sources of sustainable energy and will doubtless form part of the changing program of energy resources in the future. Fuel cells are at the vanguard of emerging clean energy technologies, but must surmount a number of key challenges in order to successfully compete against incumbents such as IC engines and batteries. Among all kinds of fuel cells, PEM fuel cells have many superior advantages. These advantages have sparked development efforts in various quarters of industry to open up new field of applications for PEM fuel cells. PEM fuel cells are still undergoing intense development, and the combination of new and optimized materials, improved product development, novel architectures, more efficient transport processes, and design optimization and integration are expected to lead to major gains in performance, efficiency, reliability, manufacturability and cost-effectiveness.

The strategy of the Fuel Cell Research Center at the International Energy and Environment Foundation (IEEF) is developing the PEM fuel cells to improve their lifetime with a much higher power density and lower cost. An overview of innovations in the field of PEM fuel cells has been presented from the published results of the center over the last decade. There are some interesting and promising new results, that have been explored particularly for what concerns: innovative designs, innovative algorithm, maximum power and long cell life, air breathing PEM fuel cells, micro PEM fuel cells, micro air breathing PEM fuel cells, mechanical and hygro-thermal stresses in the PEM fuel cells, natural vibration of the PEM fuel cell stacks, and integrated PEM fuel cells. These innovative improvements will show a new scenario for the future fuel cell market of the next years.

Acknowledgements

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