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Modeling the Performance of Polymer Electrolyte Membrane Fuel Cells and the Challenges Involved

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Abstract:** Renewable and sustainable energy sources are being demanded more by the energy sector. The Polymer Electrolyte Membrane Fuel Cell (PEMFC) is an effective technique to produce power because it produces nearly minimal pollutants. PEMFC produces electrical energy and water as a byproduct by combining hydrogen and oxygen on the anode and cathode sides. The state of the art in simulation and performance modeling of polymer electrolyte membrane fuel cells is presented in this paper. The commercialization of fuel cells and their deployment in the transportation, industry, encounter numerous challenges. Water control, eat management, cost reduction, and increased cell reliability are the main issues hindering commercial viability of fuel cells. This paper provides an overview of some important realistic models as well as a comparison of them. The difficulties that fuel cell-based systems encounter are also explored. Any urban energy system must meet the demand side of the population while also guaranteeing reliable and efficient energy output. PEMFCs are also being explored as a forthcoming sustainable energy source. This chapter also covers the economic evaluation of fuel cell-based power generation systems.

Keywords: Urban Energy System, PEMFC, Performance Modeling, Fuel Cells.

1. INTRODUCTION

Due to the excessive usage of fossil fuels, the need for facilitating better energy-harvesting technology is becoming increasingly important. In this field, fuel cell technology is gaining a lot of momentum. The fuel and oxidizer are delivered to the electrodes of a fuel cell to generate energy in the external circuit. The fuel cell will create voltage as long as the reactants are available, with minimal environmental impact. Fuel cell energy production is based on an electrochemical reaction; hence combustion is not involved in the process. The fundamental block diagram of a fuel cell system, in general, is shown in Figure 1.

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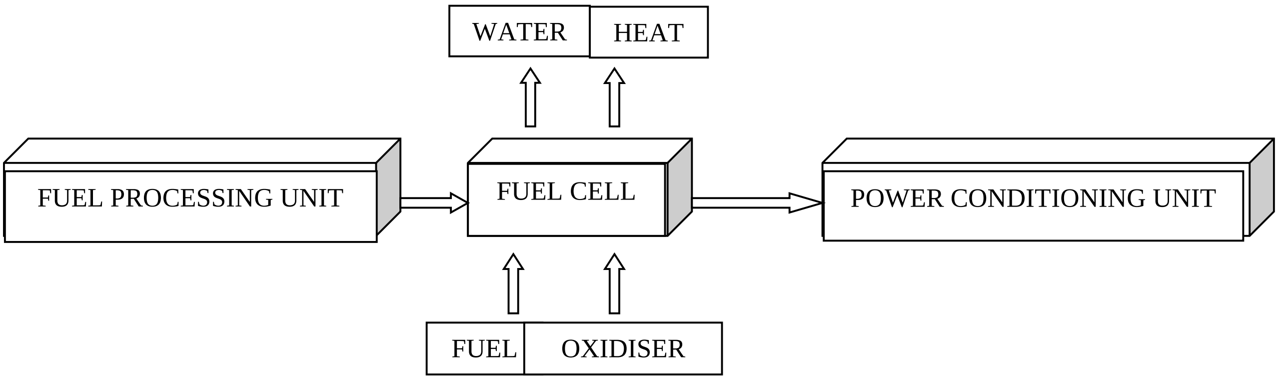

Fig 1: Basic representation of a fuel cell system

In fuel cell based power-plants, to achieve the required power rating, fuel cells are combined in series to form a fuel cell stack. Depending on the fuel supplied at the anode, there are different categories of fuel cells. They are summarized in Table I [1].

Table I: Different types of fuel cells[1]

TYPE	PEMFC	AFC	PAFC	MCFC	SOFC
Electrolyte	Hydrated Polymeric Ion Exchange Membranes	Mobilized or Immobilized Potassium Hydroxide in asbestos matrix	Immobilized Liquid Phosphoric Acid in SiC	Immobilized Liquid Molten Carbonate in $LiAlO_2$	Perovskites (Ceramics)
Electrodes	Carbon	Transition metals	Carbon	Nickel and Nickel Oxide	Perovskite and perovskite / metal cermet
Catalyst	Platinum	Platinum	Platinum	Electrode material	Electrode material
Interconnect	Carbon ormetal	Metal	Graphite	Stainless steel or Nickel	Nickel, ceramic, or steel
Operating Temperature	40 – 80 °C	65°C – 220 °C	205 °C	650 °C	600-1000 °C
ChargeCarrier	H^+	OH^-	H^+	$CO3^=$	$O^=$
External Reformer for hydrocarbon fuels	Yes	Yes	Yes	No, for some fuels	No, for some fuels and cell designs

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External shift conversionof CO to hydrogen	Yes, plus purification to remove trace CO	Yes, plus purification to remove CO and CO_2	Yes	No	No
Prime Cell Components	Carbon-based	Carbon-based	Graphite-based	Stainless-based	Ceramic
Product Water Management	Evaporative	Evaporative	Evaporative	Gaseous Product	Gaseous Product

The Polymer Electrolyte Membrane Fuel Cell (PEMFC) or Proton Exchange Membrane Fuel Cell (PEMFC) has risen to prominence among various fuel cell types. It has the high energy density 39.7 kWh/kg [2] and high conversion efficiency. Low temperature operation, high power density, fast start-up, system robustness, fuel type adaptability (with reformer), and reduced sealing, corrosion, shielding, and leaking problems are only a few of the benefits of PEM fuel cells over other fuel cell types [3]. Gas Diffusion Layer (GDL) provides mechanical support to the electrodes of PEMFC. The entire structure of PEMFC is depicted in Fig 2. PEMFC gaskets help to restrict fuel leaks within the system [4]. Bipolar plate helps to distribute the reactant gases inside the fuel cell [5].

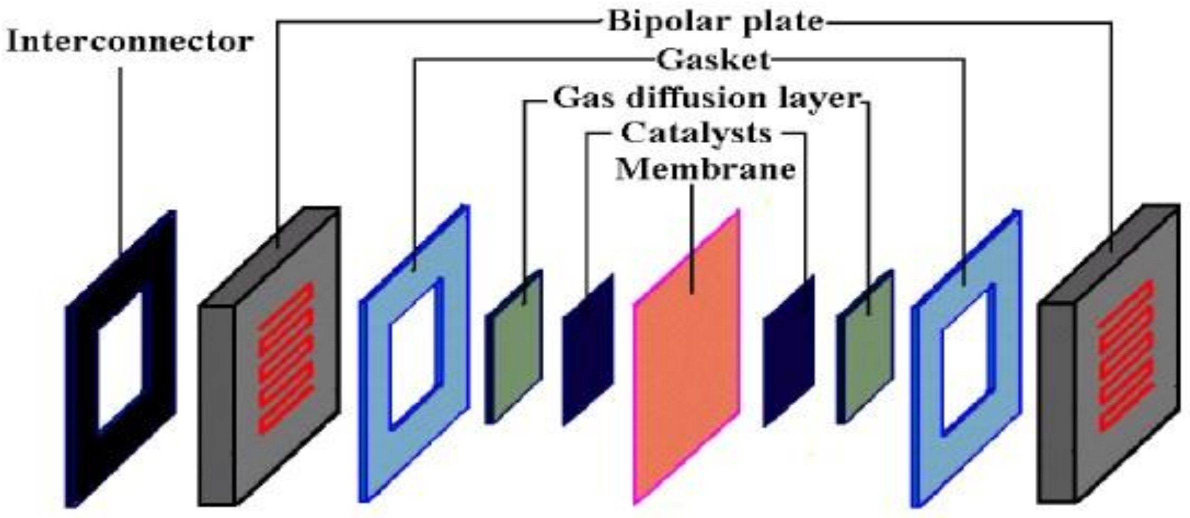

Fig 2: Different layers of a unit of PEMFC

The anode side of a PEMFC receives hydrogen, while the cathode receives oxygen. The reactions inside PEMFC are expressed in the following equations.

At anode, $H_2 \rightarrow 2H^+ + 2e^-$ ……………………………………………………………..(1)

At cathode, $\frac{1}{2} O_2 + 2H^+ + 2e^- \rightarrow H_2O$ …………………………………………………...(2)

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The first section of this chapter will provide an overview of practical PEMFC mathematical models. The second portion focuses on the problems that the PEMFC market faces in terms of commercialization. In the third phase, we look at PEMFC's cost management.

Realistic Models for PEMFC

Mathematical models are equations that represent the physical and chemical processes of a system. Numerical models can also be used for representing any system. For the design and optimization of fuel cells and fuel cell power systems, mathematical models and simulations are necessary [6].

A. Steady state PEMFC Models

Some preliminary work was carried out in the early 1990s by [7]. They outline a one dimensional, isothermal, steady state model of PEMFC. The cell's resistance was investigated under various operating situations. The performance characteristics of PEMFC was captured by [8] also. The transport phenomena inside the solid PEMFC were captured well by this steady state model. The model was also validated against various experimental conditions.[9] Outlines a steady state model of PEMFC and proposes control strategies during application of step increase in current to PEMFC. But the model ignores water transport mechanism inside the fuel cell. Experiments and steady state modeling of PEMFC performance was carried out by [10]. They presented models from electrical and thermal point of view. [11] Present steady-state and dynamic modelling of hydrogen and air-fueled PEMFCs. They test the models under different loads and operational situations. A steady state and dynamic model of PEMFC was outlined by [11]. The dynamic model captures voltage response during load variations. PEMFCs operating at high temperature was also modeled in steady state by [12]. The model was isothermal, single phase and one dimensional. In the model suggested by [13], membrane of PEMFC is taken as an interface between the anode and cathode domains. They also depict the water content inside PEMFC for various operating conditions. In [14], the authors investigated a PEMFC model simulated in 'scilab' software. Safiye [15] presents a three dimensional model of PEMFC in computational fluid dynamics.

B. Transient models of PEMFC

A realistic transient model of PEMFC was proposed by [11]. They present a clear flow chart indicating the entire modeling procedure which makes the model user friendly. The load variations and its influence on the response is also captured. [16] present a transient model of PEMFC subject to step variations in load. Even when the dynamics is captured, water transport inside the cell is neglected. The model is one dimensional too. The [17] introduces a multi-physics model of PEMFC based on electrical, pneumatic and thermal properties of parameters within the cell. The methodology captures most of the features; but the model is complex.[18] provided a one-dimensional single phase model of PEMFC. Degradation model of PEMFC was described in [19] .The analysis and validation signifies the importance of the model. [20] present a dynamic model of PEMFC during failure of temperature sensor. The paper concludes by proposing the possibility of a control strategy to tolerate the sensor failures. The dynamic response analysis of PEMFC under load variations achieved by step changes in current is put forward by [21]. The effect of membrane hydration and

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stoichiometry of reactants in the dynamic response is also monitored. [22]reported a two dimensional transient model of PEMFC. Control using voltage and current modes were also studied. The porous layers were also modeled using wettability model. In their review on transient response of PEMFC, [22] discusses the categorisation of transients occurring in PEMFC. And the dynamic response during start up and shutdown.

C. Water transport models of PEMFC

The steady state water flux was examined by [7] in their steady state isothermal mathematical model. But the model was one dimensional and isothermal. In the article [23], a three dimensional lattice Boltzmann model is formulated to depict the transport of water inside the fuel cell. Special attention is given to the oxygen transport at cathode side, where water generation occurs. [24] signifies the importance of gas diffusion layer and its porous structure on water transport inside PEMFC. A disturbance rejection based control strategy for controlling humidity inside the fuel cell is proposed by [25]. The work compares the control with PID and fuzzy-PID controllers and concludes the benefit of active disturbance rejection control strategy. Some recent models are specified in Table II.

Table II: Recent mathematical models of PEMFC

Authors,year	**Type of model**	**Software/ tool used**	**Main features**
Ahmed H[26],2021	Steady state model	Marine Predators Algorithm	• Semi-empirical model • Optimization done • Comparison with other optimization techniques
Arun[27],2021	Dynamic model	Matlab	• System Identification • Validation with real time data • Voltage response analysis
Venkateswaralu[28], 2021	Numerical model	Ansys Fluent	• Comparison of various flow fields • Steady state performance characteristics • Water transport captured
Ansari[29],2021	Steady state and dynamic model	Simulink	• Combined generation using rankine cycle • Waste heat recovery • Enhanced efficiency
Alessandro[30], 2021	Dynamic model	Computational Fluid Dynamics	• Three dimensional model • Serpentine flow fields • Water transport, temperature plots

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Dang[31],2021	Water transport model	Volume Of Fluid	• Focuses on flow field design • Liquid water content inside flow field
Yuan[32],2021	Water transport model	Matlab	• Models flow in GDL,CCL,ACL • Ficks diffusion model
Yunjin[33] ,2021	Catalyst degradation model	Catalyst transformation theory	• Pt catalyst durability • Model applicability discussed • Validation with data set
Tao[34] ,2021	Transient model	Experimental	• Captures transient behavior • Analyses different modes of operation
Zheng [35] ,2021	Lifetime prediction model	Artificial neural network optimized using particle swarm optimization	• Back propagation ANN • Voltage degradation of on-road vehicle for comparison
Abdulla [36],2021	Steady state model	Moth flame optimization	• Parameter estimation • MFO,PSO,SCA used for optimization
Omran [37] ,2021	Steady state model	Matlab, Simulink	• Isothermal, one dimensional model • Efficiency calculation • Experimental comparison
Zhang [38],2021	Multi-scale model	Ansys Fluent	• Pt loading effects • Optimization of ionomer content
Dongmin [39],2019	Steady state model	Matlab	• Fluid search optimization • Efficiency analysis • System identification
Wang [40], 2020	Steady state model	Computational fluid dynamics	• Genetic algorithm • Optimization
Loureiro[41] ,2020	Steady state and transient model	PSCAD, EMTDC	• Thermal analysis • transient loading profiles of voltage
Zhang [42],2020	Steady state model	Ansys Fluent	• Metal foam flow fields • Performance enhancement • Accounts for losses in fuel cell

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Xie [43],2020	Steady state model	Computational fluid dynamics	• Optimization by partition • Scale up analysis

[44] Presents a detailed picture of the importance of water management inside PEMFC. The work also analyses two phase flow inside GDL, channels, and catalyst layer of PEMFC. The hydration level of fuel cell is predicted using the artificial neural network based model of [45]. The water management and distribution inside the fuel cell is regulated by collecting water produced at the cathode side in [46].

Challenges in PEMFC Commercialization
Being a green technology, PEMFC based power production is attracting considerable attention. Fuel cells also outshine batteries because they have a higher energy density.

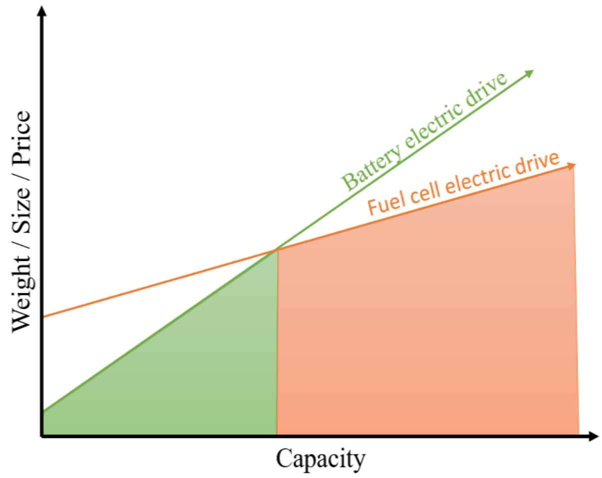

Fig 3: Fuel cell and battery drives for different capacities [47]

The key roadblocks to fuel cell commercialization are discussed below.

D. Cost
Fuel cells' purchase price and management cost will be a key factor in their commercialization. The total cost for running the PEMFC based power plant originates from the cost of procurement of fuel. For the cell, water is generated as the by product in cathode catalyst layer. In their seminal review article on water management strategies,[44] gives the effect of water content variations in membrane, flow channels, and gas diffusion layers of PEMFC.

E. Thermal Management
Oxygen undergoes reduction reaction at cathode of PEMFC, where it combines with the protons from hydrogen side. This reaction produces water, together with heat energy liberation. This may heat up the stack. So, thermal management must be properly done. Cooling systems are associated with balance of plant .[48] Presents a critical review on the topic of thermal management and its significance in PEMFC.

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F. Durability
The durability issues associated with different layers of PEMFC, together with the strategies to eliminate the adverse effects is depicted in the review of [49].The probable failure modes of each component is outlined by reviewing the literature available. The lifetime of the fuel cell within the repair rates and maintenance is referred to its durability [50].

G. Membraane Degradation
The reactant crossover at the polymer electrolyte membrane during the electro-chemical process inside the PEMFC may result in the release of radicals. These can harm the membran e and cause it to break down. This corresponds to the chemical degradation of membrane. Thinning of the membrane or de-lamination [51] can affect the operation of PEMFC and its durability.

H. Reliability
Reliability of PEMFC refers to the ability of the cell to work in the stated conditions, to deliver required power output. It is related to the rate of failure also. Increased probability of failure of the cell reduces its reliable operation.
Table III outlines dominating works addressing the challenges faced for commercialization of PEMFC.

Table III: Pioneering works addressing challenges in fuel cell commercialization

Author, year	Background	Improvement strategies proposed
Du [52],2021	High cost of Platinum Group Metal catalysts	• Fe-N-C ,Co-N-C, and Mn-N-C Catalysts • PGM free cathode catalysts
Kurnia [53],2021	Complexity at cathode side configuration	• Ambient air as oxidant • Open cathode PEMFC • Air supply subsystem simplified
Cullen [54], 2021	Extend focus beyond light duty vehicle transport application of fuel cells	• Heavy duty transport application based review • Discusses state of art materials for enhancing stability and durability of fuel cells
Xia [55], 2019	Increased cost on using PGM based catalysts	• Options for choosing catalysts • Alternative materials used as PGM free catalysts
Nguyen [56] ,2021	Durability of fuel cells	• Degradation of GDL, CL, Bipolar plate, membrane and gasket analyzed separately • Water and thermal management aspects • Stress testing for durability
Haider [57] ,2021	Development of high	• Materials and component

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	temperature fuel cells	development • Combined heat and power generation
Ren [58] ,2020	Performance improvement	• Pt/C catalyst development
Kongkanand [59] ,2016	Develop market affordable fuel cells	• Low level of Platinum loading in PEMFC
Jiao[60] ,2021	Future directions for PEMFC development	• High power density achievement • MEA, water and thermal management, design and development
Wang [61],2021	Performance enhancement of PEMFC	• Molecular dynamics simulated • Transport phenomena in the catalyst layer
Luo [62],2021	Combined Heat and Power generation using PEMFC	• Fueling options from hydrogen • Hydrogen content and efficiency of PEMFC
Pahon[63] ,2021	Aging of PEMFC	• Temperature influence on durability of PEMFC • Open cathode cell
Huang [64],2021	Thermal management	• Vapor chambers to support heat management • Open cathode fuel cell
Vasilyev [65] ,2021	Reliability of fuel cell	• Operating conditions influence on reliability • Survival time calculated
Heinzel [66] ,2021	Water management	• Fuzzy logic approach • Optimization of cell performance
Chiara [67] ,2021	Cost, durability	• Multi-objective optimization • Life span increase
Wang [68], 2021	Lifetime of fuel cell and degradation	• Predict degradation trend using rated voltage • Aging tests and model development
Kavya[69], 2023	Heat recovery	• Waste heat utilization • Organic Rankine cycle

Fuel Cell Cost Management

The top most concern regarding the establishment of fuel cell based systems worldwide is their cost. Fig 2. Represents the cost evolution report of PEMFC stacks.

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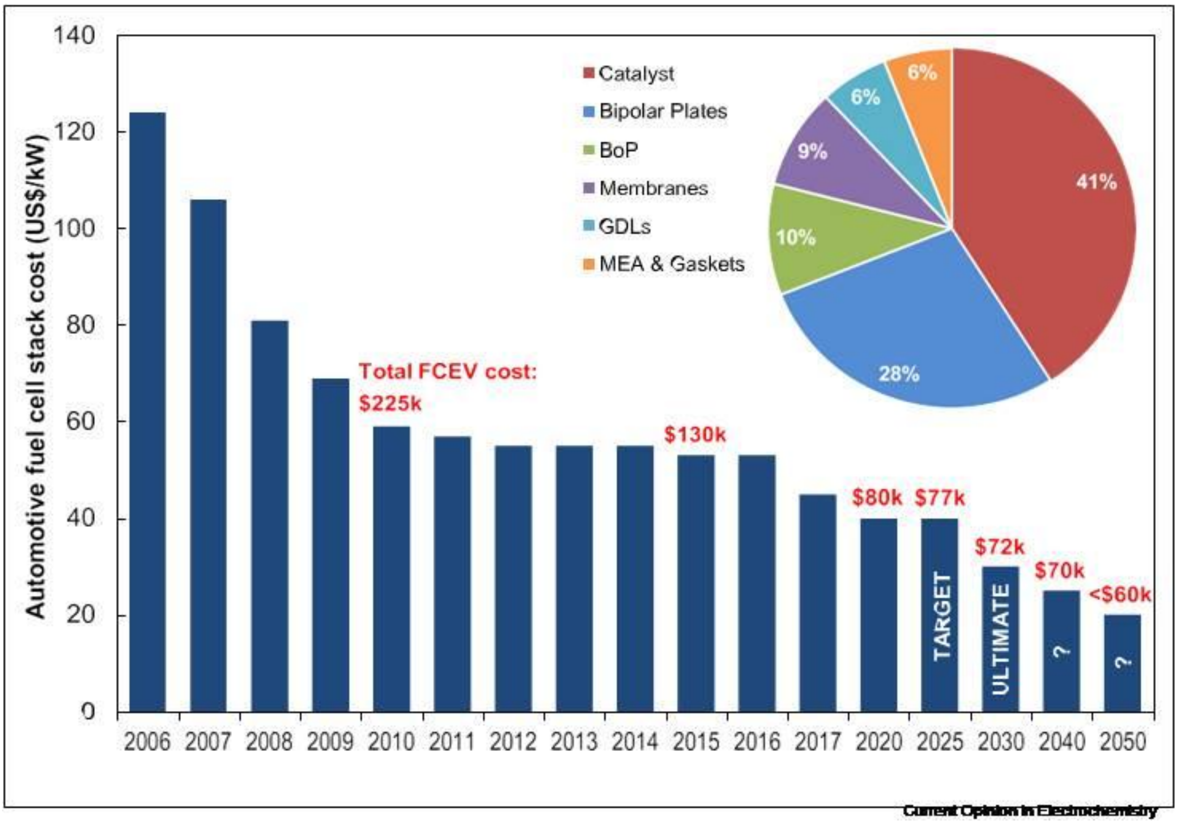

Fig 2: Cost evolution of PEMFC[70]

The total cost of Fuel Cell Electric Vehicle(FCEV) is represented in the bar graph. The cost is around 225k US Dollars in 2010. This total cost has reduced to 80k US Dollars in 2020. The cost per kilowatt also decreased to around 40.
For a single kilowatt of power generation from a fuel cell, the current price is roughly 300 INR . The relevance of cost control in PEMFC is thus pointed out clearly.

	Ranking (from list)		
	1st	2nd	3rd
Cost of Pt due to high PGM total loading	26	4	2
Cost of BPPs	4	7	12
Cost of membrane	1	14	8
Cost of air compression system	1	7	3
Cost of GDLs	1	3	5
Cost of heat exchangers	1		1
Cost of cathode humidifier		1	2

Fig 4: Ranking of hindrances to deduct PEMFC system cost[71]

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In Fig 4, the assessment of fuel cell cost in automotive area is outlined. The dark color of the cell indicates the assessment by more number of experts. The usage of Platinum Group Metals (PGM) in catalyst layer is one of the main factors causing hike in the cost.

2. CONCLUSION

Demands for 'green recovery' are gaining traction worldwide. PEMFCs present a pollution free chapter in the energy sector.

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