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Short communication

An algorithm for optimum design and macro-model development in PEMFC with exergy and cost considerations

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Abstract

Previous algorithms in the term of designing mostly focused on separate sections of fuel cells. They addressed purpose of optimization, which only includes individual specific terms of fuel cells (such as membrane, electrodes, channels, electrolyte, . . .).

New comprehensive algorithm presented in present study is based on global optimization and macro-model development which covers all detail correlations with boundary limitations. The exergy–cost model is an additional tool for results evaluation which may lead to shifting optimum results.

The approach steps are:

- identification, categorization and formulating of irreversibilities cause voltage drops;
- founding optimum operational working point, based on power and efficiencies maximization;
- sensitivity analysis and quantification for potential drop effects in proposed macro-model;
- optimum engineering design for two case studies of 97 kW and 60 W;
- comparison of the model results with experimental data as well as previous literature test running results by HPR and efficiency targets;
- re-evaluating the results with exergy–cost model for design optimization.

Keywords: Fuel cell stack; Mathematical model; Engineering design; Fuel cell productivity; Proton exchange membrane fuel cell (PEMFC); Exergy analysis

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1. Introduction

Previous algorithms which have been drawn and developed before are shown in Fig. 1. Usually, these algorithms cover design case of fuel cells only in individual items, like membrane or electrodes and do not fully consider interaction of parts working together. In addition, optimized results are local and there is not enough attention to global optimum answer in those previous models.

New comprehensive algorithm presented in this paper is aiming for global optimization and macro-model development with assistance of micro-previous models. There are three major advantages as follows:

(I) In simulation stage of model, considering the impact of irreversibilities which cause voltage drops, predicts the level (amount) of real voltage drops (so close to experimental data).
(II) Thermo-exergetic system modeling analyzes and exergy-economy pattern are new additional applied tools for comparison of the models. Using these tools, calculations can be re-evaluated again.
(III) Cost consideration is another factor in order to avoid excess expenses, which will cause displacement of optimum results.

The main problem for existing micro-models in literature is the lack of ability to predict phenomena such as flooding,

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Nomenclature

B_a	anode B
B_c	cathode B
$\bar{c}_p$	molar specific heat $(J\,(mol\,k)^{-1})$
e^{-1}	electron charge
E_1	total produced energy (liquid water) $W\,cm^{-2}$
E_2	total produced energy (steam) $W\,cm^{-2}$
E_e	total produced electricity
F	constant number $(C\,mol^{-1}\,e^{-1})$
$\Delta\bar{g}_f$	molar Gibbs energy $(kJ\,mol^{-1})$
$\Delta\bar{h}_f$	molar enthalpy $(kJ\,mol^{-1})$
HHV	higher heating value
HPR	heat power ratio
i	current density $(mA\,cm^{-2})$
i_L	maximum current density $(mA\,cm^{-2})$
i_n	internal currents (A)
i_o	current exchange density
I_{total}	fuel cell current
LHV	lower heating value
OCV	open circuit voltage
Opt. index	optimum value of index
P_e	output electricity power (W)
P1	pressure in point no. 1
P2	pressure in point no. 2
Q	total heat produced
Q_{loss}	total heat loss
Q_{steam}	total steam generation energy
r	specific surface resistance $(k\Omega\,cm^2)$
req. index	required value of index
ROCV	reversible open circuit voltage
$\bar{R}$	gas constant, 8.314 $(kJ\,mol^{-1})$
$\Delta\bar{S}_f$	molar entropy $(kJ\,mol^{-1})$
v	voltage (V)
V_{total}	fuel cell voltage
Z	atomic number
Greek symbols	
α	charge transfer coefficient
α_n	partial to total pressure ratio, Pn/Po
δ_{T_0}	exergetic loss
ε_{el}	electric efficiency
ε_I	current efficiency
ε_{th}	maximum theorem efficiency
ε_v	voltage efficiency
ε_C	DC to AC transfer ratio
ε_R	thermal efficiency
$\eta_{max.\ ideal}$	ideal maximum efficiency
$\eta_{therm.\ real}$	real thermodynamic efficiency
η_{EX}	exergetic efficiency

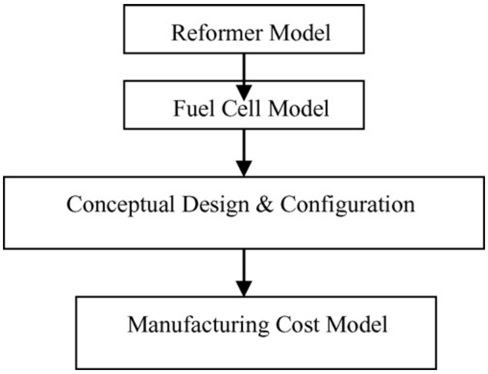

Fig. 1. General methodology and previous algorithms developed before.

poisoning, and unwilling accidents, which cause high drops in output power and efficiency. The proven advantage of this macro-model which runs by non-linear mathematical programming is not affected by the inner boundary condition of each cell parts. Because the in–out equations in inner boundaries are linked together so the number of non-basic variables will be reduced in solution procedure. The basic variables related to outer boundary layers will be solved and optimized without troubles of statistical variation of non-basic ones.

The complete algorithm which combined macro- and micro-models is explained in Table 1. (1) Rapid conversion in model solution and (2) ability for self upgrading in model by any new approved invention are another advantage of specified model.

2. Identification, categorization and formulating of irreversibilities cause voltage drops

Voltage formula with zero level current density condition is known as open circuit voltage, therefore [1,2];

$$\Delta v = \Delta v_{activation} + \Delta v_{fuel\ crossover} + \Delta v_{ohmic} + \Delta v_{concentration} \quad (1)$$

$$\text{OCV} = \text{ROCV} - \Delta v_{(i=0)} \quad (2)$$

Thus:

$$\begin{aligned} \Delta v_{activation+fuel\ crossover} &= 0.032 \times \ln \frac{i+3}{0.07} \\ \Delta v_{ohmic} &= 30 \times 10^{-6} \times i \\ \Delta v_{concentration} &= -0.024 \times \ln \left(1 - \frac{i}{800}\right) \end{aligned} \quad (3)$$

$$V = 1.167 - 0.032 \times \ln \left(\frac{i+3}{0.07}\right) - 30 \times 10^{-6} i + 0.024 \times \ln \left(1 - \frac{i}{800}\right) \quad (4)$$

Eq. (4) is explained in Fig. 2 which explains real voltage path based on current density.

3. Optimum operational working point, based on power and efficiencies maximizing

The mathematical programming model is a non-linear type and its objective function is to maximize the output power (Pe).

Table 1
New informed table algorithm for Fuel Cell Model Development and Engineering Design [3]

Steps	Descriptions
Reformer model	Fuels, fuelling, fuel storage systems, reforming processes, reforming description, reforming PFD's, reforming model and optimization (mathematical programming)
Cell simulation	Cell simulation based on *irreversibilities causes voltage drops*
Fuel cell model	
Macro	Potential, efficiencies, pressure and temperature effects, losses (Tafel, Nerst, . . .), control volume, balances, simulation (output power density graph), modeling (graphs and correlation math programming)
Element	Differential equation of element assembling, ions current and balances, potentials, concentrations, mass transfer, heat transfer, momentums, energy balances, total model equations of system, solving procedure, logical assumptions in boundary conditions, numerical methods, running test for boundary conditions fixing, finalizing
Conceptual design and configure	Design algorithm (initial i, v)
	Sizing and configurations
	Redesigning and modification (based on optimized i, v)
	Finalizing (based on comparison of results)
Thermo exergetic system modeling	
Thermo-dynamic system model	Static model
	Dynamic model
	Optimization with mathematical programming
	Exergy concepts, exergy considerations, exergy modeling and optimization (techniques) η_{EX}, Δ_{Ex} (techniques)
Manufacture cost model [US\$ kW^{-1}]	Fixed cost, running cost, total cost, cost comprehensive model, cost minimizing as an objective function, design displacement (based on cost considerations)

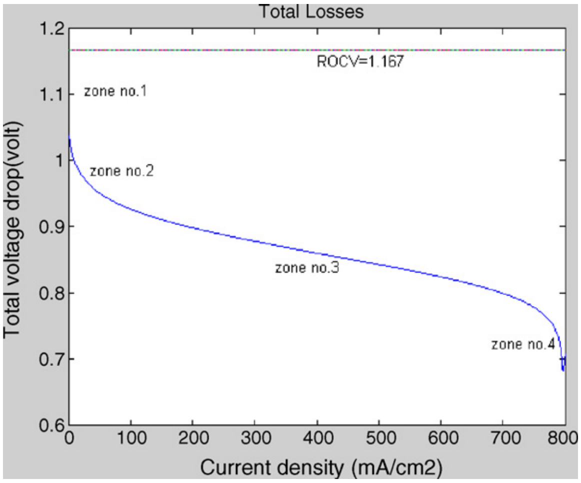

Fig. 2. Total real voltage variation vs. current density in macro-model simulation.

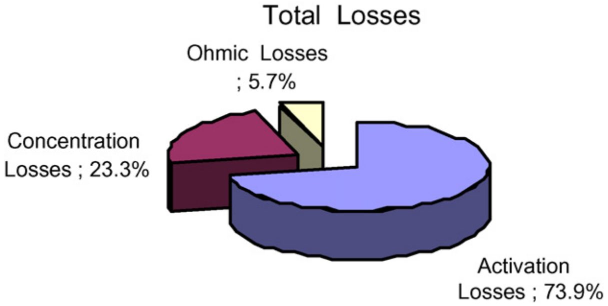

Fig. 3. Total losses onion diagram shows losses in percentage.

Optimizing technique is based on gradiant method as a mechanism to solve the model. The objective function is defined as a function of voltage and current density. Mathematical model presents the optimization of procedure in order to evaluate the effects of parameters in ranking the potential drops. Following above steps, GAMS software [7] were used for optimization, and the optimum voltage and current density of cell at optimum point were concluded. In other words in this section, modeling and best operational cell condition based on output power maximization has evaluated. By this means, quantification tool of losses effects is achieved.

Objective function:

$$\begin{aligned} f(i) &= -60\times10^{-6}\times i + 1.16691 - \frac{0.032\times i}{i+3} - \frac{0.024\times i}{800-i} \\ &\quad -0.032\,\ln\left(\frac{i+3}{0.07}\right) + 0.024\,\ln\left(1-\frac{i}{800}\right) \end{aligned} \tag{5}$$

By integrating non-linear mathematical model and GAMS optimizer the summary of calculation results are as follows:

$$\begin{aligned} i_{\text{opt.}} &= 770.894\,\text{mA cm}^{-2} \\ v_{\text{opt.}} &= 0.7637\,\text{V} \\ P_{\text{opt.}} &= 588.733\,\text{W cm}^{-2} \\ \Delta v_{\text{act.+fuel crossover}} &= -0.298\,\text{V} \\ \Delta v_{\text{ohm.}} &= -0.023\,\text{V} \\ \Delta v_{\text{con.}} &= -0.082\,\text{V} \end{aligned} \tag{6}$$

4. Sensitivity analysis and quantification for potential drop effects in proposed macro-model

The onion diagram in Fig. 3 shows the quantitative analysis results of irreversibilities due to voltage drops. Sensitivity analysis of effects percentage in performance increasing is defined as:

$$\text{Effect percentage index} = \frac{\text{OCV} - \Delta v_{\text{total}}}{\overline{\Delta g_{\text{f}}}} \times 100 \tag{7}$$

This new index informed by this research is used to identify the effects of voltage drops on the performance, as shown in Table 2.

Table 2
Effective items on performance based on defined effect percentage index

Effective items on performance	Effect percentage index = OCV $-\Delta v_{\text{total}}/\Delta g_{\text{f}} \times 100$ (%)
Pressure increasing	35.5
Concentration increasing	33.5
Temperature decreasing	27.9
Catalyst	25.9
Electrodes effective surface increasing	23.9
Electrolyte thickness reducing	6.1
Electrodes conductivity increasing	4.2
Connections	2.0

5. Optimum engineering design for two case studies of 97 kW and 60 W

Engineering design of a fuel cell is described in the present section based on the conclusion of model results in previous sections. As depicted in following sections, fuel cell stack, which consists of an assembly group of cells, is defined as an energy producing system. Its nominal capacity is a function of energy demand rate. In order to estimate the design parameters, such as number of cells, total required cell area and stack specifications, it is assumed that the output power would be 97 kW and the cell would be operated at optimal point. Total fuel cell volume, voltage and current as well as mass and energy balance were then concluded. The electrical energy, thermal loss and produced energy can then be calculated. Finally, the major indicators were derived.

1 Estimation of oxygen and hydrogen consumption per unit area and water generation [6]:

$$\begin{aligned} &\mathrm{O_2\ usage} = 6.4 \times 10^{-8}\,(\mathrm{kg\,(s\,cm^2)^{-1}}) \\ &\mathrm{H_2\ usage} = 0.8094 \times 10^{-8}\,(\mathrm{kg\,(s\,cm^2)^{-1}}) \\ &\mathrm{H_2O\ product} = 7.2 \times 10^{-8}\,(\mathrm{kg\,(s\,cm^2)^{-1}}) \end{aligned} \tag{8}$$

2 Technical specifications of cells and stack [6]:

$$\begin{aligned} &I_{\text{req.}} = 127.01\,(\mathrm{A}) \\ &\mathrm{Area} = 165766\,(\mathrm{cm^2}) \\ &\mathrm{No.\ of\ cells} = 65.9 \cong 66 \\ &\mathrm{No.\ of\ stacks} = \frac{66}{17} = 3.88 \cong 4 \end{aligned} \tag{9}$$

3 Assuming stack configuration of seventeen cells (1.56 mm thickness) each, and four parallel stacks in one FC pack, the results would then be [3]:

$$\begin{aligned} &V_{\text{total}} = 13\,(\mathrm{V}), \quad I_{\text{total}} = 32.76\,(\mathrm{A}) \\ &\mathrm{FC\ volume} = 0.10296\,(\mathrm{m^3}) \end{aligned} \tag{10}$$

Energy balance in prototype PEMFC based on Fig. 4 is as follows:

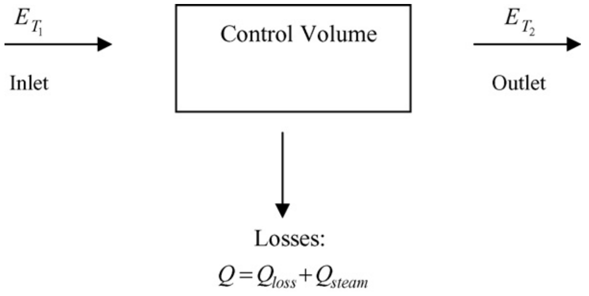

Fig. 4. Mass and energy balance.

$$\begin{aligned} &E_{T_1} = 1.1315\,(\mathrm{W\,h\,cm^{-2}}) \\ &E_{T_2} = 0.9573\,(\mathrm{W\,h\,cm^{-2}}) \\ &Q_{\text{loss}} = 0.3685\,(\mathrm{W\,cm^{-2}}) \\ &Q_{\text{steam}} = 0.1742\,(\mathrm{W\,cm^{-2}}) \\ &Q = 0.5427\,(\mathrm{W\,cm^{-2}}) \end{aligned} \tag{11}$$

4 Final indicators are concluded and summarized below [6]:

$$E_{\text{e}} = 0.588\,(\mathrm{W\,cm^{-2}}) \tag{12}$$

$$\begin{aligned} &\eta_{\text{max . ideal}} = 92.8\%, \quad \eta_{\text{real therm.}} = 60.6\% \\ &\varepsilon_{\text{el}} = 54.9\%, \quad \mathrm{HPR} = 1.1 \end{aligned} \tag{13}$$

6. Comparison of the model results with experimental data as well as previous literature test running results by HPR and efficiency targets

6.1. Model validation

Validation of the model has been based on experimental data obtained from a PEMFC running test [4]. Table 3 shows the comparison and bands of variation of model results with that PEMFC operational condition.

6.2. Model comparison verification

Comprehensive assessment of model requires a grid of data, which are taken from bench test results. Table 4 shows verification of model results with eight operated test cases taken of relevant literatures as specified in references [4,5,8–13].

7. Re-evaluating the results with exergy–cost model for design optimization

Selecting types and capacities of cells in different alternatives are covered by exergy analysis method as a comparison tool which is presented in this research.

Heat power ratio, electrical and exergetic efficiencies and exergy loss are effective parameters in decision making. Comparison between model results of present study and references [4,5] in HPR and global efficiency is shown in Table 5.

On the question of economical capability, shown in Table 6 fuel cell cost is the main obstacle in development and commercialization of this technology.

Table 3
Comparing model results with experimental data

Item (unit)	Test running results [4]	Presented model results	Bands of variation (%)
Working pressure (bar)	1.03	1.04	−0.9
Working temperature (°C)	80	100	−22
Hydrogen consumption (kg s^{-1})	2.91×10^{-3}	2.32×10^{-3}	+12.1[a]
Gibbs energy (kJ mol^{-1})	−329.9	−225.2	+24.7[a]
ROCV (cell) (V)	1.175	1.167	+0.6
Operating cell voltage (V)	0.668	0.7637	−14
Electric power output (kW)	107.3	97.24	+9.4
HPR	1.469	1.1	+25.1[a]
Total electrical efficiency (%)	52.9	55	+2.1

[a] It should be noted that, the variation are mostly due to assumption of linear increase in output power. Hence, items such as fuel consumption, Gibbs free energy, OCV, . . . will be different in two cases.

Table 4
Comparison between model results and experimental data of PEMFC test results

Item (unit)	Model results	TRR[a] [4]	TRR[a] [5]	TRR[a] [11]	TRR[a] [8]	TRR[a] [12]	TRR[a] [13]	TRR[a] [10]	TRR[a] [9]
Pressure	1.03 bar	1.03 bar	200 kPa	–	–	30 psi	10 psi	1.013 Bar	–
Temperature (°C)	80	80	70	50	–	80	60	52.5	–
ROCV (cell) (V)	1.167	1.175	–	–	–	–	–	1.01	–
OCV (cell) (V)	0.9357	0.668	0.75	0.72	–		0.6	0.7	–
Current density (A cm$^{-2)}$	0.77	–	0.4	1	–	0.4	1	–	–
Electric power output (kW)	97	107.3	1	1	–	250.5	20	27.5	–
HPR	1.1	1.469	1.62	–	1.25	–	–	1.12	1.43
Total elec. efficiency (%)	55	52.9	51	53	44	46.5	49.5	48.3	54.9

[a]TRR: test running results.

Table 5
Comparing between model results and two previous models in HPR and total efficiencies

Fuel cell cases	$\delta T_o^* = \delta T_o / P_e$	η_{Ex} (%)	HPR, $\eta_{electrical}$ (%)
Presented FC	1.77	36.1	1.1, 54.9
Virginia Tech. FC [4]	2.1	32.1	1.469, 52.9
Sharif University FC [5]	2.92	20.9	1.62, 51

Table 6
Comparison between final cost of FC vehicle and gasoline vehicle

	Item	FC vehicle	Gasoline vehicle
Specifications	Capacity (kW)	97	97
	Life cycle (h)	6000	4500
	Efficiency (%)	54.9	25
	Working hours (h)	1500	1500
Assumptions	Discounting rate (%)	8	8
	Increasing rate (%)	15	15
	Total life (years)	4	4

Costs	FC vehicle	Gasoline vehicle
Initial cost (US$)	38950	7910
Fuel cost (US$)	8470	3142.9
Maintenance cost (US$)	6826	8809.3
Final cost (US$)	54246	19862.2

8. Conclusions

Validation of model and verification of its results with empirical data is the main conclusion of the present paper. The model fits on experimental data with derivation of 2.1% in overall efficiency:

- Estimated efficiency is 55% and it is compatible with the cases reported in Table 3.
- Maximum efficiency is achieved with lowest heat production ratio of 1.1, which may be compared with estimated HPR reported in Table 4.

In addition, exergy analyze results shows increasing in exergy efficiency of 12.8%, and decreasing in exergy loss of 9.2%.

It should be noted that also the FC vehicle cost is three to four times more than gasoline vehicle, but the attraction of environmental aspects and higher efficiency in FC emphasize researches more in costs reduction and commercialisation. In fact economical justification of fuel cell technology requires identification of optimum operation and design point. Therefore, the present research has had the objective of developing a new method of modeling and engineering design, for higher productivity in fuel cell, i.e. an increase in the useful generated energy “electricity” for unit volume of fuel cell. is increased. Indirectly, this subject could explain some future steps and a good view point in fuel cell commercializing.

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