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VALIDATION OF SEMI-EMPIRICAL TEMPERATURE MODEL OF PEMFC USING ATOM SEARCH OPTIMIZATION ALGORITHM

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Proton Exchange Membrane Fuel Cell (PEMFC) has unique thermal characteristics. The change in PEMFC temperature directly effects the PEMFC performance. The voltage and temperature of PEMFC at different loading/ambient conditions is not easy to predict. In this work a newly developed semi-empirical model is used and the parameters of the model are optimized for single cell PEMFC (base-case) by using atom search optimization. The semi-empirical model was developed and tested for stack PEMFC system but any model developed for PEMFC cannot be validated unless it is effective for single-cell PEMFC system. The new parameters show promising results and hence the model works is considered as good model. Previously due to unknown base-case parameters the ranges selected for parameters are extremely large. In this model by considering the base-case parameters and previously extracted parameters the new short ranges for parameters are given so that in future the optimization of parameters will take less time and this increases the chances of this model to be used in online prediction of PEMFC temperature.

Key words:
Thermal, modelling, optimization, semi-empirical, PEMFC, algorithm.

Introduction

Proton Exchange Membrane Fuel Cell (PEMFC) is a clean alternate energy source that uses oxygen and hydrogen as fuel. There are two types of PEMFCs: low temperature LT-PEMFC which operates under 373,13 K while high temperature HT-PEMFC operates above 373,13 K. Most commercial PEMFCs are LT-PEMFC for small scale power. HT-PEMFC is also getting popular and in near future both types of PEMFCs will be used for commercial uses [1–3].

LT-PEMFC which is commonly referred as PEMFC has more application now-a-days than HT-PEMFC. The thermal characteristics are of extreme importance for PEMFC, the heat is produced during exothermic reaction and the portion of this energy is converted into electricity and rest of it is lost as heat energy. Due to this feature the PEMFC temperature increases, this is the main issue with PEMFC that must be operated at certain temperature range which enhances the its efficiency. Very low and very high temperature is not good for PEMFC performance. Ambient temperatures also effect the PEMFC temperature directly that is why most of the thermal/temperature models consider the ambient temperature as well [4–7].

There are various techniques to model the PEMFC temperature. They are listed in Table 1 [8].

Table 1. *PEMFC thermal modelling techniques*
Таблица 1. *Методы термического моделирования ТЭПОМ*

Sr no. № Sr	PEMFC thermal/temperature modelling approach Подход к тепловому/температурному моделированию PEMFC	Implementation procedure Процедура внедрения
1	Analytical/mechanistic approach Аналитический/механистический подход	Implemented through numerical/analytical techniques by having deep knowledge of chemical/electrical and mechanical structure of PEMFC Реализовано с помощью численных/аналитических методов благодаря глубоким знаниям химической/электрической и механической структуры ТЭПОМ
2	Semi-empirical approach Полуэмпирический подход	Implemented through less complex linear and non-linear equations which are combination of mechanistic and empirical approach Реализуется с помощью менее сложных линейных и нелинейных уравнений, которые представляют собой комбинацию механистического и эмпирического подхода
3	Empirical approach Эмпирический подход	Implemented through artificial intelligence, statistical analysis and electrochemical impedance spectroscopy (EIS) etc. Реализовано с помощью искусственного интеллекта, статистического анализа, спектроскопии электрохимического импеданса (EIS) и т. д.

The analytical approach of thermal modelling has been done in [9], the model considers one-dimensional flow of gases and PEMFC temperature model, the results are promising but the model is too much complex and cannot be used for online purposes. The numerical model/investigation of PEMFC is given in [10], this model is also very complex. The modern thermal models are moved towards empirical approach, in [11, 12] the empirical thermal models of PEMFC are given, the empirical models are not that reliable as compared to mechanistic/analytical approach. The thermal model of PEMFCs require extensive study and most empirical models use data driven approach which is not adequate for modelling the complex system of PEMFC. Semi-empirical approach is therefore a good option for thermal modelling of PEMFC. A good semi-empirical approach has been used in [6] but more effective and simpler approach was used in [13], this approach is further updated in [14] where Area A and number of cells N in the PEMFC stack are used in the modelling equations.

Good PEMFC models such as [15] model is first tested on single cell PEMFC and then the models are extended towards PEMFC stacks where cells are attached in series to get high voltage. But due to commercial use of PEMFCs most models now-a-days are tested and validated on stack system. The models in [13, 14] are tested on PEMFC stacks. These models are never tested/validated on single PEMFC system. It is necessary to test the models on single PEMFC especially in case of mechanistic/semi-empirical models.

In this research the model of [14] is tested on single cell PEMFC, the parameters of the model are optimized by using Atom Search optimizer (ASO) presented in [16] which is better and modern optimization technique as compared to Lightening Search Algorithm and Quantum Lightening Search Algorithm which were used for optimization in [13, 14]. The results show that the new parameters give good results and the model seems to fit with root mean square error (RMSE) less than 0,5. The parameters varied so much from the previous research work, however there is no bifurcation for low and high currents as explained in [14], single cell PEMFC exhibit different characteristics than stack of PEMFC. The model parameters can be considered as the base ones which were missing in previous research work.

The research work first explains the mechanistic thermal model of PEMFC, then details the semi-empirical model of [14] along with the implementation algorithm, next briefly explains the Atom Search Optimization, after that introduces the results and discussions, and finally the conclusion/future prospects of the research.

Mechanistic (theoretical) thermal model of PEMFC

PEMFC is an electrochemical cell that provides electricity by consuming hydrogen and oxygen as fuel. The hydrogen and oxygen are supplied at a specified pressure and they react in the presence of the platinum catalyst. The reaction produces energy which is converted into electricity and heat. The by-product of reaction is water and no carbon emission occurs during the reaction. The energy balance (thermodynamic) of PEMFC is given in equation (1) :

$$q_{net} = q_{chem} - q_{elec} - q_{sens+latent} - q_{loss}\,, \qquad (1)$$

where q_{net} is the net energy produced; q_{chem} is the chemical energy produced during reaction; q_{elec} is the electrical energy produced; $q_{sens+latent}$ is the sensible and latent heat of PEMFC; q_{loss} is the heat energy loss. The PEMFC temperature is strongly dependent upon the q_{net} and if PEMFC mass m_{fc} and specific heat capacity C_{fc} of PEMFC are known the PEMFC temperature can be easily extracted [6]. These equations are for air cooled PEMFC system, if special cooling mechanism is adopted then the equations can be modified accordingly. The equation for extracting PEMFC temperature is given in equation (2):

$$T = \int \frac{q_{net}}{M_{fc}C_{fc}}dt\,. \qquad (2)$$

The temperature profile along with heat generation and thermal properties of different parts of PEMFC are given in Fig. 1 [17].

Semi-empirical thermal model of PEMFC

The semi-empirical models of PEMFC simplified the equation (2) and convert it into first order exponential equation. The researchers in [18–20] adopted this first order exponential based equation. The simple exponential equation doesn't fulfil all the requirement hence some other supplement equations are used in [19] along with the detailed algorithm in order to mode the PEMFC stack temperature. The equation and algorithm are further simplified in [14]. The equations and algorithm for [14] model are given in equation (3):

$$T_{mod}(k) = L_1 I_{t\,(k)} + L_2\big(I_{t\,(q)} - I_{t\,(k)}\big)e^{-L_3(t_k - t_q)} + T_{amb}(t_k) - L_4$$
$$K = 1,2,3\ldots \quad . \qquad (3)$$

Here $T_{mod}(k)$ in Celsius scale is the initial modelled PEMFC temperature; $I_{t\,(q)}$ is the load current at a sample which is recorded before the last significant change in current referred as q sample; $I_{t\,(k)}$ is the current at the running sample k; T_{amb}refers to ambient temperature in Celsius scale.

The following expressions in equations (4), (5) are added to first order exponential equation of PEMFC, this may be due to cooling and other complex thermal effects present in PEMFC system:

$$T_{mod1}(t_k) = T_{mod}(t_k) - L_5\frac{\left[T_{mod1}(t_k) - T_{mod}(t_q)\right]}{(t_k - t_q)}\,, \qquad (4)$$

$$T_{mod2}(t_k) = T_{mod1}(t_k) + L_6\left\{T_{mod1}(t_k) - T_{mod}\big(t_q\big)\right\}. \qquad (5)$$

Here T_{mod2} is the final modeled temperature, and L_1 to L_6 are optimized using ASO while $t_k$is the time at sample k. Table 2 shows the range values of parameters L (1 to 6) taken from [13], [14] used in the model equations. Parameters $L_1$and L_2 are used to convert the current and its difference into temperature; L_3 controls the decay of exponent; L_4 is an offset from the temperature model; L_5 and L_6 are the constant parameters in the differential equations (4) and (5).

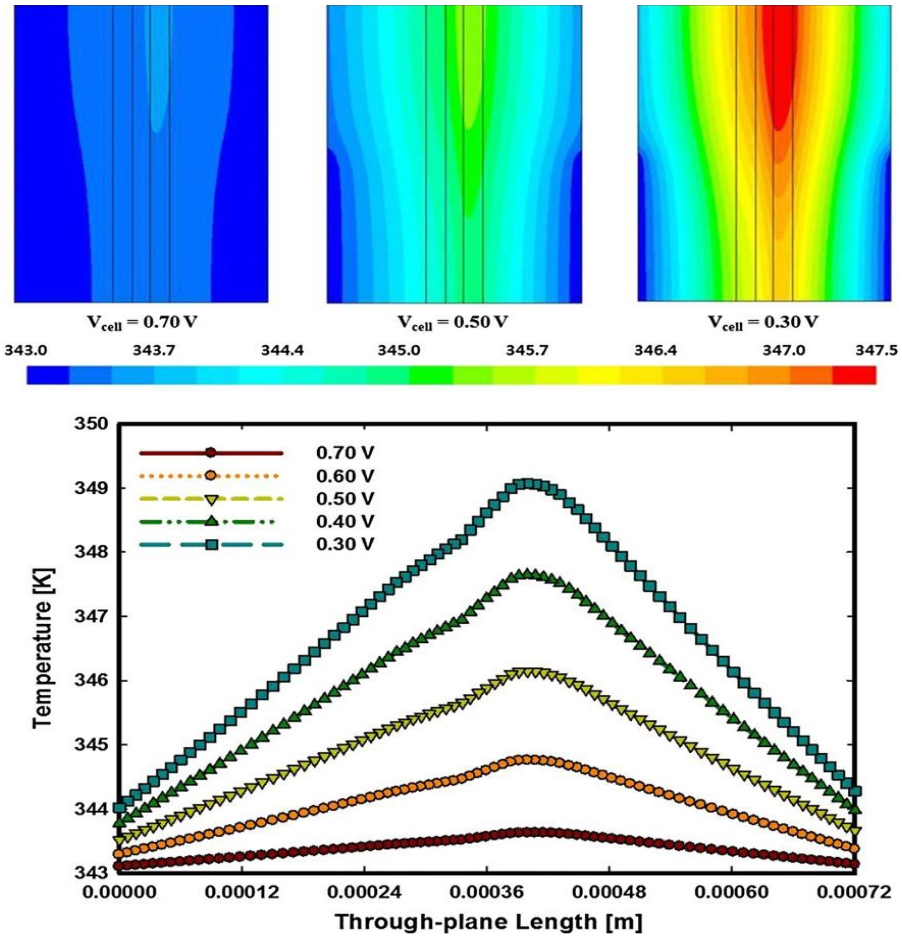


Fig. 1. *Thermal profile of PEMFC*
Рис. 1. *Тепловой профиль ТЭПОМ*

Table 2. *Parameter ranges for ASO*
Таблица 2. *Диапазоны параметров для оптимизации поиска атомов (ОПА)*

Parameter Параметр	Min	Max	Parameter Параметр	Min	Max
L_1	$1*10^{-6}$	5	L_4	–400	400
L_2	$1*10^{-6}$	5	L_5	–200	200
L_3	$1*10^{-6}$	5	L_6	–200	200

The code for implementing the temperature model is given in Table 3 from [14], here filtering is not required for single PEMFC as small variations must not be neglected. The modelled temperature and ambient temperature will be in Celsius scale.

Atom Search Optimization

Atom Search Optimization (ASO) is also a population-based heuristic algorithm which is inspired by basic molecular dynamics. ASO mimics the atomic motion controlled by interaction and constraint forces to design an effective search mechanism for global optimization problems. The time and accuracy of ASO is better than all well-known optimization algorithms such as Particle Swarm Optimization (PSO), Lightening Search Algorithm (LSA), Gravitational Search Algorithm (GSA) etc. as mentioned in [16]. The atoms join together in a molecule due to force of attraction among them, some atoms have force of repulsion among them as well. Both attraction and repulsion forces are used in this algorithm. The mass of the atom is varied in this algorithm and the heavier atom is close to the main solution. The movement of heavier atoms is slower than that of lighter ones. At first the initial population have been selected randomly where number of atoms, i. e. solutions, have given different values within the range given above. The objective function which is to be minimized is the root mean square error (RMSE) and it is given in equation (6):

$$\mathrm{RMSE} = \sqrt{\frac{\sum e_t{}^2}{n}}. \qquad (6)$$

Here e_t is the error between the experimental and modelled values of temperature. At first the repulsion force is dominant in order to scatter the initial population and with the time when some of the atoms are close to the solution the force of attraction dominates. The heavier atoms start to attract the other atoms in order to find the best optimum solution. The formulae for mass calculations, randomizing the initial population, calculating the forces, velocity, acceleration and position can be taken from [16], the Matlab code for ASO is also given on Mathworks (Matlab) website. The pesudocode for ASO is given in Table 4.

Table 3. *Code to implement the semi-empirical temperature model*

Таблица 3. *Код для реализации полуэмпирической температурной модели*

Data: Experimental measurements of Temperature of PEMFC and current at sample k, set q as unity for initial value
Данные: Экспериментальные измерения температуры ТЭПОМ и тока в образце k, q задана как единица для начального значения
Output: Semi-empirical modelled temperature T_{mod2} (k)/Результат: Полуэмпирическая смоделированная температура T_{mod2} (k)
$T_{mod,1} \rightarrow T_{amb,1}$**;** Set modelled temperature equal to ambient temperature at start/Установите смоделированную температуру равной температуре окружающей среды при запуске
j → k ; set value of **j** equal to present value of sample/установите значение **j** равным текущему значению выборки
While j>1/Когда j>1
If absolute (**It(k)–It(j)**)>1 **then/Если абсолютное (It(k)–It(j))>1, то**
It(q)→It(j); Save previous value of load current before sufficient deviation
Сохраните предыдущее значение тока нагрузки до достаточного отклонения
tq→tj; Save time value for last significant deviation of current
Сохраните значение времени для последнего значительного отклонения тока
j→1;
end if/завершите, если
j→j–5 instead of one j can be reduced to five samples for reducing runtime as skipping ten samples have negligible effects on results/вместо одного j может быть уменьшено до пяти выборок для сокращения времени выполнения, поскольку пропуск десяти выборок оказывает незначительное влияние на результаты
end while/завершите, когда
It(k)<It
Li→Li, **low curren/малый ток**; low current parameters are to be used
должны использоваться параметры низкого тока
Else/Иначе
Li→Li, **high current/большой ток**; high current parameters are to be used
должны использоваться параметры большого тока
Tmod,2 (tk) → Calculate final value of modelled temperature from equations (3) to (5)
Вычислите конечное значение моделируемой температуры Tmod,2 (tk) из уравнений (3)–(5).

Table 4. *ASO general pseudocode*

Таблица 4. *Общий псевдокод ОПА*

Randomly initialize a set of atoms X (solutions) and their velocity v, and FitBest=Inf.
Случайным образом инициализируйте набор атомов X (растворов) и их скорость v, и FitBest=Inf.
While the stop criterion is not satisfied do/**Пока** критерий остановки не удовлетворен
For each atom Xi do/**Для** каждого атома Xi
Calculate the fitness value Fiti/Рассчитайте значение пригодности Fiti;
If/Если Fiti< FitBest **then/то**
FitBest= Fiti;
XBest= Xi;
End if/Закончите, если
Calculate the mass using equations/Вычислите массу, используя уравнения
Determine the atom neighbors/Определите соседей атома
Calculate the forces/Рассчитайте силы
Calculate the acceleration and update the velocity and position/Рассчитайте ускорение и обновите скорость и положение
End for/Закончите
End while/Закончите, когда
Find the best solution so far XBest/Найдено лучшее решение на данный момент XBest

Experiment performed

The experiment is performed on single cell PEMFC (Fischertechnik) of 300 mW power. The pressure of hydrogen remains at 1 atm while pressure of oxygen is 0,9 atm. The maximum limiting current is 0,9 A and the area of PEMFC is 4 cm^2. The experiment is performed at normal room temperature, i. e. 298,13 K. The load current varies from 0 to 0,7 A, the voltage of PEMFC varies from 1,2 to 0,3 V. Fig. 2 shows the experimental setup and current, voltage and temperature waveform.

Results and discussion

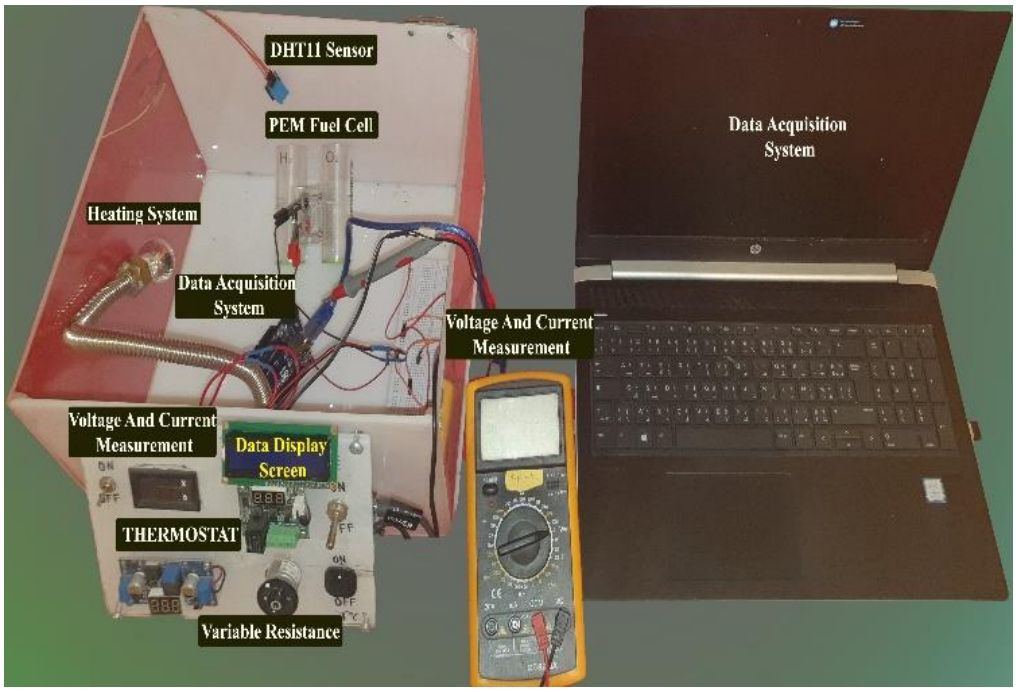
The parameters are already extracted for 1200 and 500 W PEMFC stack in [13, 14]. The parameters are listed in Table 5.

The temperature model extracted from the parameters P-1 and P-2 is shown in Fig. 3. The RMSE is extremely high for these parameters so the new parameters are extracted by using ASO. The new parameters are the baseline parameters (B-1) for single cell PEMFC.

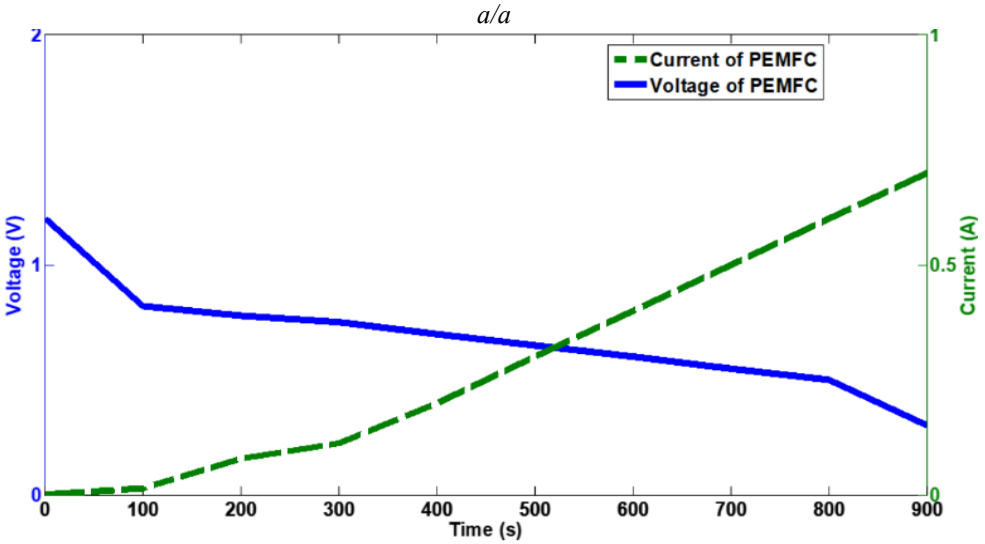
Table 5. *Parameters extracted for 1200 and 500 W PEMFC stack*

Таблица 5. *Параметры, полученные для ТЭПОМ мощностью 1200 и 500 Вт*

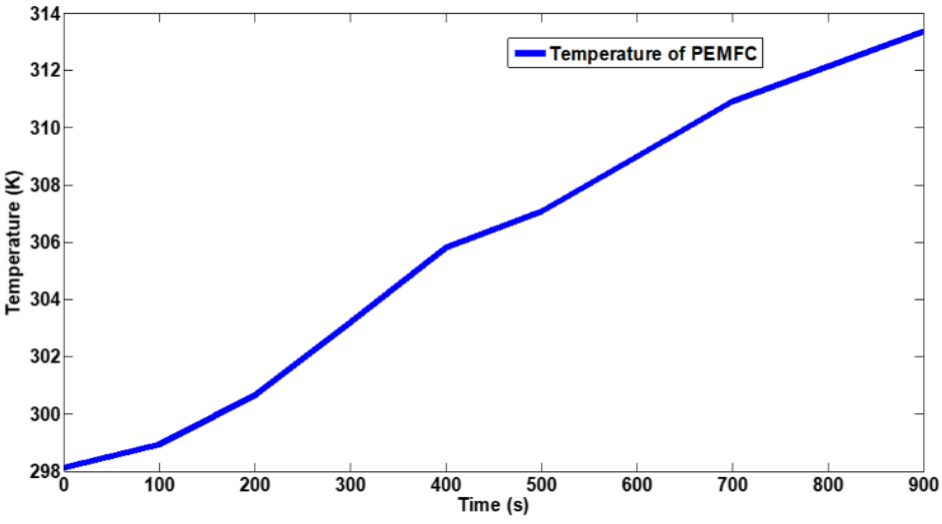
Parameter Параметр	Parameter extracted for PEMFC Параметр, полученный для ТЭПОМ	
	1200 W (P-1) мощностью 1200 Вт (P-1)	500 W (P-2) мощностью 500 Вт (P-2)
L_1	2,6278	0,995
L_2	2,7825	1,429
L_3	0,0112	0,031
L_4	–4,2894	4,461
L_5	13,0207	0,405
L_6	–0,36143	0,166



a/а



b/б



c/в

Fig. 2. *(a) experimental setup (b); voltage-current curve; (c) temperature curve*

Рис. 2. *(а) экспериментальная установка; (б) кривая зависимости напряжения от тока; (в) температурная кривая*

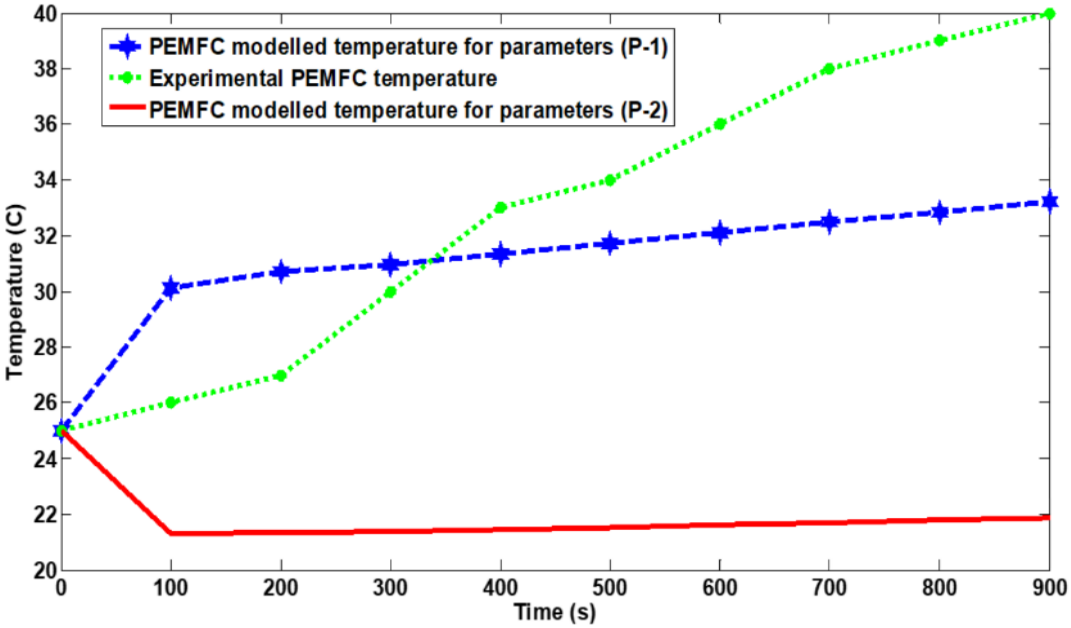


Fig. 3. *Temperature model for parameters P-1 and P-2 comparison with experimental temperature*

Рис. 3. *Температурная модель для сравнения параметров P-1 и P-2 с экспериментальной температурой*

Table 6. *Parameters extracted for single cell PEMFC using ASO*

Таблица 6. *Параметры, полученные для одноэлементного ТЭПОМ с использованием ОПА*

Parameter Параметр	Parameter extracted for/Параметр, полученный для		
	single cell (B-1) отдельной ячейки (B-1)	1200 W PEMFC (P-1) PEMFC мощностью 1200 Вт (P-1)	500 W PEMFC (P-2) PEMFC мощностью 500 Вт (P-2)
L_1	1,90680	2,6278	0,995
L_2	1,94388	2,7825	1,429
L_3	3,29821	0,0112	0,031
L_4	–0,62803	–4,2894	4,461
L_5	93,36161	13,0207	0,405
L_6	–8,00470	–0,36143	0,166

Table 6 demonstrates that the parameters for single cell PEMFC show lot of variation as compared to the parameters extracted for PEMFC stack system. Fig. 4 gives the comparison of modelled temperature and experimental one. Here RMSE is less than 0,5 which is acceptable in this case.

The parameters change from single cell to 1200 W PEMFC stack in Table 6 are very haphazard. This is due to the cooling system and material choice in various commercial PEMFCs. The thermal characteristics change from one PEMFC to another. 500 W PEMFC stack was manufactured by Horizon while 1200 W – by NEXA. All air cooled PEMFC systems do not exhibit the same behavior, the materials used in PEMFCs are updating day by day [21]. Previously the model in [14] gave equations of the parameters based on the area A and number of fuel cells in the stack as given in Table 7. But these equations are not reliable as in this case the area of PEMFC is 4 cm^2 and number of fuel cell is 1 so it is not possible to apply the equation on single cell PEMFC. Moreover no such concept of threshold current that differentiate parameters for low and high current is witnessed in this case, parameters (B-1) fit the experimental temperature for all currents (low and high). Hence it is better to optimize parameters for new type of PEMFC systems again in order to validate the model.

Table 7. *Parameters prediction equation for semi-empirical thermal model*

Таблица 7. *Уравнение прогнозирования параметров для полуэмпирической тепловой модели*

Parameter Параметр	Function (in the low current) Функция (при низком токе)	Function (in the high current) Функция (при сильном токе)
L_1	0,403+1,071 NA	0,498+1,071 NA
L_2	2,182–3,08 NA	2,519–3,08 NA
L_3	0,1821–0,3237 NA	0,1777–0,3237 NA
L_4	–5,329+21,02 NA	–4,858+21,02 NA
L_5	3,3937–7,432 NA	3,5953–7,432 NA
L_6	1,3988–3,054 NA	1,4730–3,054 NA
It (threshold current) It (пороговый ток)	30,34–0,01029 P	

Still this model can fit all types of air-cooled PEMFCs but the parameters will change and these parameters can be tuned by using any good optimization techniques. But since after this research the base parameters are known and other stack parameters were also known, so the range of the parameters can decreas. This will reduce the optimization time and give better results in quick time. The new parameter range is given in the Table 8 based on the parameters variation in Table 6.

Table 8. *New parameter ranges for thermal modelling*

Таблица 8. *Новые диапазоны параметров для теплового моделирования*

Parameter Параметр	Min	Max	Parameter Параметр	Min	Max
L_1	0.1	5	L_4	–10	10
L_2	0,5	5	L_5	$1*10^{-2}$	150
L_3	$1*10^{-3}$	5	L_6	–15	5

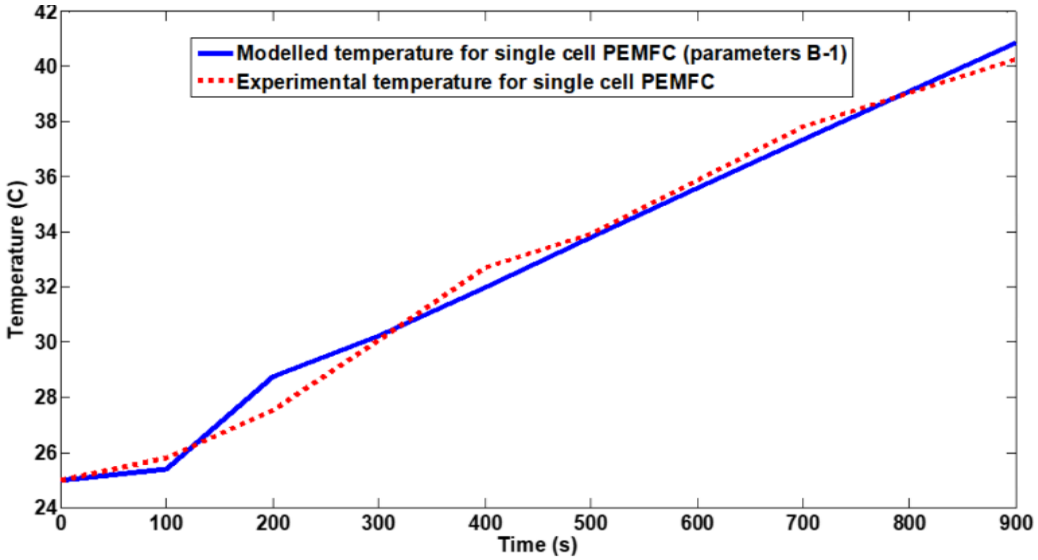


Fig. 4. *PEMFC temperature comparison by using parameter (B-1)*

Рис. 4. *Сравнение температуры ТЭПОМ с использованием параметра (B-1)*

Conclusion

In this paper the semi-empirical thermal model is validated for base case, i. e. single cell PEMFC. The model was only validated for large PEMFC stack systems. The model parameters are optimized by using newly developed optimization technique. The new parameters fit the experimental temperature well and can be considered as the base ones for all air-cooled PEMFC systems. Previously all parameters are optimized by using larger range for parameters, which cannot be useful for fast optimization. Now based on the previous and newly optimized parameters new parameters range is given. The new range of parameters will be extremely helpful for the future researchers in order to optimize the parameters for any air-cooled PEMFC system quickly. Future research is to apply this thermal model on various PEMFC system with different range of power, if large sample size is collected the change in parameters must be studied and this will be extremely helpful in predicting the model parameters for all types of PEMFCs and more reliable generic model can be designed.

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ПРОВЕРКА ПОЛУЭМПИРИЧЕСКОЙ ТЕМПЕРАТУРНОЙ МОДЕЛИ ТЭПОМ С ИСПОЛЬЗОВАНИЕМ АЛГОРИТМА ОПТИМИЗАЦИИ ПОИСКА АТОМОВ

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Топливный элемент с протонной обменной мембраной обладает уникальными тепловыми характеристиками. Изменение температуры топливного элемента с протонной обменной мембраной напрямую влияет на его характеристики. Напряжение и температуру топливного элемента с протонной обменной мембраной при различных условиях нагрузки/окружающей среды предсказать непросто. В этой работе используется недавно разработанная полуэмпирическая модель, параметры которой оптимизированы для топливного элемента с протонной обменной мембраной с одной ячейкой (базовый случай) с использованием оптимизации поиска атомов. Полуэмпирическая модель была разработана и протестирована для многоэлементной системы топливного элемента с протонной обменной мембраной. Но не каждая модель, разработанная для топливного элемента с протонной обменной мембраной, может быть утверждена, если она эффективна для одноэлементной системы топливного элемента с протонной обменной мембраной. Новые параметры показывают многообещающие результаты, и поэтому модель считается хорошей. Диапазоны, выбранные ранее для параметров базового случая, были чрезвычайно велики. В этой модели с учетом параметров базового случая и ранее извлеченных параметров задаются новые короткие диапазоны параметров, чтобы в будущем их оптимизация занимала меньше времени, что увеличивает шансы использования этой модели в онлайн-прогнозировании температур топливного элемента с протонной обменной мембраной.

Ключевые слова:
*Термический, моделирование, оптимизация, полуэмпирический,
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