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PARAMETER OPTIMIZATION FOR A PEMFC MODEL WITH PARTICLE SWARM OPTIMIZATION

M. Sedighizadeh[1] , A. Rezazadeh[2], M. Khoddam[2] and N. Zarean[2]
1-Faculty of Engineering and Technology, Imam Khomeini International University, Qazvin, Iran
2-Faculty of Electrical and Computer Engineering, Shahid Beheshti University,Tehran, Iran,
Email: m_sedighi@sbu.ac.ir

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Abstract

There are many steady state models of polymer electrolyte membrane fuel cells (PEMFC). However, rarely the methods for parameter optimization of PEMFC stack model were discussed. In this paper an electrochemical-based fuel cell method is used and parameters of this PEMFC model are optimized by means of Particle Swarm Optimization (PSO). The target of this paper is to show how PSO apply for parameter optimization of fuel cells. At the end of paper the PSO test result are compared with Genetic Algorithm.

Keywords: PEM fuel cell modeling, parameter optimization, particle swarm optimization

1. Introduction

Nowadays, because of air quality matters, the demand for clean energy has kept increasing. Polymer Electrolyte Membrane Fuel Cell (PEMFC) is widely researched for power generation system. Fuel cells have various advantages compared to conventional power sources, such as internal combustion engines or batteries. Fuel cells eliminate pollution caused by burning fossil fuels; the only byproduct is water and if the hydrogen used comes from the electrolysis of water, then using fuel cells eliminates greenhouse gases. Fuel cells do not need conventional fuels such as oil or gas and can therefore eliminate economic dependence on politically unstable countries. Since hydrogen can be produced anywhere where there is water and electricity, production of potential fuel can be distributed.

Two main modeling approaches can be found in literature. The first approach includes mechanistic models, which aim at simulating the heat, mass transfer and electrochemical phenomena encountered in fuel cells [1,2,3,4]. These models usually analyses specific components of the fuel cell stack, such as the anode, cathode, and membrane. The second approach deals with empirical or semi-empirical model equations, which are used to predict the effect of different input parameters on the voltage–current characteristics of the fuel cell. Generally, they are applied assumptions and approximations in PEMFC modeling thus there will be some errors between the models and the actual performance of them [5,6,7]. In spite of advances in PEM fuel cell modeling, the PEM fuel cell system is a complex nonlinear, multi-variable system that is hard to model by conventional methods . In order to improve the accuracy of the models and make the models reflect the actual PEM fuel cell performance better, it is necessary to identify the parameters of the models using optimization techniques. In recent years, the evolutionary computation technique based on genetic algorithm (GA) or its variation has

attracted much attention in the investigation of fuel cell systems [8]. For example, the GA was proposed for improving the accuracy of the fuel cell model parameter identification [9]. Nevertheless, there are still some deficiencies in GA performance [10]. The degradation in efficiency is apparent in applications with highly epistatic objective functions, i.e. where the parameters being optimized are highly correlated. In this case, the crossover and mutation operations cannot ensure better fitness of offspring because chromosomes in the population have similar structures and their average fitness is high toward the end of the evolutionary process. As an alternative to GA, particle swarm optimization (PSO) [11] is a recently invented high-performance algorithm.

The focus of this work is to identify fuel cell model parameters using the PSO method through fitting the mathematical model to actual experimental data.

2. Particle Swarm Optimization

Particle Swarm Optimization (PSO) is an extremely simple algorithm that seems to be effective for optimizing a wide range of functions. The swarm is typically modeled by particles in multidimensional space that have a position and a velocity. These particles fly through hyperspace and have two essential reasoning capabilities: their memory of their own best position (pbest) and knowledge of the global or their neighborhood's best (gbest). In a minimization optimization problem, problems are formulated so that "best" simply means the position with the smallest objective value. Members of a swarm communicate good positions to each other and adjust their own position and velocity based on these good positions. So a particle has the following information to make a suitable change in its position and velocity:

- A global best that is known to all and immediately updated when a new best position is found by any particle in the swarm.
- Neighborhood best that the particle obtains by communicating with a subset of the swarm.
- The local best, which is the best solution that the particle has seen.

The particle position and velocity update equations in the simplest form that govern the PSO are given by:

$$c_o v_{i,j} + c_1 r_1 (\text{global best}_j - x_{i,j}) + c_2 r_2 (\text{local best}_{i,j} - x_{i,j}) + c_3 r_3 (\text{neighborhood best}_j - x_{i,j}) \rightarrow v_{i,j}$$

$$x_{i,j} + v_{i,j} \rightarrow x_{i,j}$$

In Standard PSO, the parameter c_1 is set to zero. And when $ighborhood\ best_j = local\ best_{i,j}$ then r_3 is also (temporarily) set to zero. As the swarm iterates, the fitness of the global best solution improves. The selection of coefficients in the velocity update equations affects the convergence and the ability of the swarm to find the optimum. It is highly dependent on stochastic processes, like evolutionary programming. The adjustment toward ***pbest*** and ***gbest*** by the particle swarm optimizer is conceptually similar to the ***crossover*** operation utilized by genetic algorithms. It uses the concept of fitness**,** as do all evolutionary computation paradigms.

3. Basic Operation Principle of a PEMFC Stack

A proton exchange membrane fuel cell transforms the chemical energy liberated during the electrochemical reaction of hydrogen and oxygen to electrical energy, as opposed to the direct combustion of hydrogen and oxygen gases to produce thermal energy. A stream of hydrogen is delivered to the anode side of the membrane electrode assembly. At the anode side it is catalytically split into protons and electrons. The newly formed protons permeate through the polymer electrolyte membrane to the cathode side. The electrons travel along an external load circuit to the cathode side of the MEA, thus creating the current output of the fuel cell.

Meanwhile, a stream of oxygen is delivered to the cathode side of the MEA. At the cathode side oxygen molecules react with the protons permeating through the polymer electrolyte membrane and the electrons arriving through the external circuit to form water molecules.

The electrochemical reactions occurring electrodes of a PEMFC are as follows:

Oxidation half reaction in the anode: $2H_2 \rightarrow 4H^+ + 4e^-$ (1)

Reduction half reaction in the cathode: $O_2 + 4H^+ + 4e^- \rightarrow 2H_2O$ (2)

Total electrochemical cell reaction: $2H_2 + O_2 \rightarrow 2H_2O$ (3)

Electrochemical energy comes from last reaction. We can assemble many single cells into a fuel cell stack system in order to provide the required amount of power [12].

3. Electrochemical Models of The Fuel Cell

In an electrochemical model the behavior of the voltage as the function of the current is presented; i.e. the polarization curve. It's mentioned that the actual cell potential is decreased from its equilibrium potential because of irreversible losses.

The losses, originate usually from three sources:1) the activation overvoltage,2) ohmic loss and 3) concentration overvoltage.

Vapor pressure for water mentioned as a function of the temperature:

$$\log_{10}\left(P_{H_2O}^{sat}\right) = 2.95 \times 10^{-2}.(T - 273.15) - 9.18 \times 10^{-5}.(T - 273.15)^2 + 1.44 \times 10^{-7}.(T - 273.15)^3 - 2.18 \quad (4)$$

If the reactants are air and H2, then

$$P_{N_2}^{channel} = \frac{0.79}{0.21} P_{O_2} \quad (5)$$

$$P_{O_2} = P_c - \left(RH_c.P_{H_2O}^{sat}\right) - P_{N_2}^{channel}.\exp\left(\frac{0.291.(i/A)}{T^{0.852}}\right) \quad (6)$$

If the reactants are O2 and H2, then

$$P_{O_2} = \left(RH_c.\ P_{H_2O}^{sat}\right).\left[\frac{1}{\exp\left(\frac{4.192.\left(i/A\right)}{T^{1.334}}\right).\frac{\left(RH_c.P_{H_2O}^{sat}\right)}{P_c}} - 1\right] \quad (7)$$

In both reactive conditions

$$P_{H_2} = 0.5\left(RH_a.\ P_{H_2O}^{sat}\right).\left[\frac{1}{\exp\left(\frac{1.653\left(i/A\right)}{T^{1.334}}\right).\frac{\left(RH_a.P_{H_2O}^{sat}\right)}{P_a}} - 1\right] \quad (8)$$

Where P_a, P_c are anode and cathode inlet pressure terms in atm, $P_{N_2}^{channel}$ is $the\ N_2$ partial pressure at the cathode gas flow channel in atm, P_{O_2}, P_{H_2} are the O_2, H_2effective partial pressure terms in atm and T is temperature in Kelvin. A is the effective electrode area (cm2) and i is the cell current (A).

The basic expression for the voltage for a single cell is:

$$V = E_{Nernst} - V_{act} - V_{ohm} - V_{conc} \quad (9)$$

The reversible voltage of the cell (E_{Nernst}) is the potential of the cell obtained in an open circuit thermodynamic balance (without load). It can be defined via a Nernst equation in expanded form as (Mann et al., 2000)

$$E_{Nernst} = 1.229 - 0.85\ .\ 10^{-3}(T - 298.15) + 4.3085\ .\ 10^{-5}T\ \ln(P_{H_2}P_{O_2}^{0.5}) \quad (10)$$

The concentration of dissolved oxygen *(CO,)* in mol/cm3 at the gas/liquid interface can be defined by Henry's Law expression of the form

$$C_{O_2} = P_{O_2}/\left(5.08 \times 10^6 \exp\left(-498/T\right)\right) \quad (11)$$

The activation overpotential is mentioned below :

$$V_{act} = -\left[\xi_1 + \xi_2 T + \xi_3 T\ln(i) + \xi_4 T\ln(C_{O_2})\right] \quad (12)$$

R_M is the equivalent resistance of the membrane and is calculated by:

$$R_M = \frac{\rho_M . l}{A} \quad (13)$$

Where R_M is the specific resistivity of the membrane for the electron flow and l is the thickness of the membrane. The following numeric expression for the resistivity of the membranes is used

$$\rho_M = \frac{181.6 \cdot \left[1+0.03 \cdot \left(\frac{I}{A}\right)+0.062 \cdot \left(\frac{T}{303}\right)\left(\frac{I}{A}\right)^{2.6}\right]}{\left[\lambda-0.634-3 \cdot \left(\frac{I}{A}\right)\right] \cdot exp\left[4.18 \cdot \left(\frac{T-303}{T}\right)\right]} \quad (14)$$

The ohmic loss follows the equation

$$V_{ohm} = -i(R_M + R_C) \quad (15)$$

V_{con} can be determined by

$$V_{con} = -b \ln\left(1 - \frac{I}{I_{max}}\right) \quad (16)$$

I_{max} is the maximum current value where fuel is used and applied at its maximum rate. Above, ξ_1, ξ_2, ξ_3, ξ_4, R_M, R_C and b are the optimized parameters.

the output voltage of a PEMFC stack can be determined by:

$$V_S = n \cdot (E_{Nernst} - V_{act} - V_{ohmic} - V_{con}) \quad (17)$$

n is the number of series cells which are connected in the stack, so V_S is the stack voltage.
The Stack parameters are shown in Table 1. The upper and lower bounds of these parameters are given in Table 2.

5. Objective Function

A sum of the squared error between the output voltage of the PEMFC stack model and the experimental output voltage of the actual PEMFC stack can be served as an objective function for optimization to determine these model parameters

$$\min_{(\xi_1,\xi_2,\xi_3,\xi_4,\lambda,R_C,b)} \left(y = \Sigma_{j=1}^{J}(V_{sm} - V_s)^2\right) \quad (18)$$

Where y is the objective function, Vsm is the experimental data of stack voltage, Vs is output voltage of the model and J is the number of the experimental data point.

6. Calculation and Simulation Results

A stack whose parameters and operational range are described in Table I is examined and the result are shown in table 3. PSO code is developed with MATLAB software. The parameter optimizations of PSO were compared to the solutions of the Genetic algorithm reported in [9].The contrast results are shown in table 3. From results it is clear that model output voltage agrees well with experimental data. PSO has many advantages: (1) it has convergence of this optimization problem, (2) it provides a stable and global optimization solution; (3) PSO is more accurate than GA as the results shown in table 3.

Mainly errors are caused in the area of concentration loss and ohmic loss because I_{max} and R_M are changed at the different operating condition. Error corrections can be implemented by other advanced control schemes.

Table 1. Stack parameters

	Stack parameters		
Number of series cells n	48	Stack temperature T (K)	323
Cell's effective area A (cm2)	62.5	pressure of hydrogen (atm)	1.47628
thickness of membrane l(cm)	.0025	pressure of oxygen (atm)	.2095
maximum current I_{max}	42	Anode relative humidity RH_a	1

Table 2. Bounds of model parameter

Model parameter	ξ_1	ξ_2	ξ_3	ξ_4	λ	R_C	b
Upper bound	-0.944	0.005	-0.0000954	0.000098	24	0.0008	0.5
Lower bound	-0.952	0.001	-0.00026	0.000036	14	0.0001	0.0136

Table 3. Values of the optimized parameters

Model parameter	ξ_1	ξ_2	ξ_3	ξ_4	λ	R_C	b	y
PSO	-0.9479	0.0030	-0.0001	0.0002	20.5256	0.0003	0.1099	17.5675
GA	-0.94731	0.0030641	-0.0001939	0.000077134	19.767	0.00027197	0.023981	20.81

7. Conclusions

An electrochemical steady state PEMFC model is developed in this paper. The model parameters are optimized globally by using PSO in the operating region, because traditional gradient-based optimization methods are difficult to solve this global optimization problem. According to the results, PSO is a good choice for parameter optimization because it has convergence of this optimization problem, it provides a stable and global optimization solution, and PSO is more accurate than GA.

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