ARTICLE IN PRESS

INTERNATIONAL JOURNAL OF HYDROGEN ENERGY XXX (2016) 1–14

Available online at www.sciencedirect.com

ScienceDirect

journal homepage: www.elsevier.com/locate/he

Mathematical modeling and dynamic Simulink simulation of high-pressure PEM electrolyzer system

Tevfik Yigit [a,b], *Omer Faruk Selamet* [a,b,*]

[a] *Mechatronics Engineering Department, Nigde University, Nigde 51245, Turkey*
[b] *Dr. T. Nejat Veziroglu Clean Energy Research Center, Nigde University, Nigde 51245, Turkey*

ARTICLE INFO

Article history:
Received 16 March 2016
Received in revised form
29 May 2016
Accepted 4 June 2016
Available online xxx

Keywords:
PEM electrolyzer
Hydrogen generation
Simulink model
Dynamic model
Mathematical model
System simulation

ABSTRACT

PEM electrolysis based hydrogen generator system model is developed by using Simulink in MATLAB. The model covers the following system components: PEM electrolyzer stack, water pump, cooling fan, storage tank, water tank, power supply, control unit and sensors. In simulation, PEM electrolyzer stack model is the most complex component and consists of four parts; anode and cathode modules, membrane and finally voltage calculations module. Efficiency drops and voltage losses in the PEM electrolysis stack are estimated. The overpotentials are investigated as anode and cathode activation, electronic and ionic ohmic resistances. In addition, the loss of the other components is considered. The model is tested against the dynamic changes and it responded with quick outputs. The cell and stack behavior under different conditions (i.e. ranging of temperature and pressure) are examined. The loss of each system component at different current densities is added to the simulation. The study shows that the loss of stack dominates the losses of other components at higher current densities. The simulation counts that the stack and system model can run with different cases and scenarios. It is run for the scenario that it consumes constant power for a high pressure operation. Results show that current drawn by the stack decreases as the voltage increases because of the increasing pressure.

The model is also compared with the experimental results and the model is found to be consistent with the experimental data.

Introduction

On earth, hydrogen is the most abundant chemical element, but not easily accessible to its monatomic form. The pure hydrogen is needed to be produced with the least energy consumption possible [1]. Being one of the most environmentally friendly, efficient and independent from hydrocarbon-based fuels, Proton Exchange Membrane (PEM) electrolysis as a hydrogen production technique is recently drawing researcher's attention. Among other electrolysis techniques, it has many advantages such as high working current densities, production at high pressure, pure gas generation and compact design. PEM electrolysis is relatively new and promising technology. Since PEM electrolysis has many aspects remain unstudied, it's being investigated by more researchers by time, as expected [2,3].

* *Corresponding author*. Mechatronics Engineering Department, Nigde University, Nigde 51245, Turkey.
E-mail address: omerfarukselamet@nigde.edu.tr (O.F. Selamet).
http://dx.doi.org/10.1016/j.ijhydene.2016.06.022

There are numerous experimental studies investigating the PEM electrolyzers in different aspects. However, modeling a PEM electrolyzer is also necessary. Modeling a cell or stack has uttermost importance in understanding the operational behavior of a PEM electrolyzer [4]. Many mathematical models/calculations exist for characterizing the cell component(s), using own code [5], employing statistical methods [6] available software [7,8]. Gorgun has proposed a PEM electrolyzer stack model containing 3 cells at the atmospheric pressure using Simulink/MATLAB [9]. Awasthi et al. investigated the effects of changing the temperature and pressure on the cell performance and polarizations [10]. Lee et al. developed a PEM electrolyzer model to investigate the effect of the temperature, the water flow rate and the flow field on the performance of a PEM electrolyzer and compared the results with an experimental study [11]. Han et al. developed an electrochemical model which is able to compute the diffusion overpotential in a PEM electrolyzer [12]. Abdin et al. also developed a PEM electrolyzer model that employs Simulink to represent the ohmic resistances in electrolyzers with an electrical circuit model [13]. They also investigated the effect of temperature and pressure on PEM electrolyzer performance and compared their results with the published experimental ones.

Most of the modeling studies are mainly focused on the physics or the behavior of a cell or a stack. The behavior of a PEM electrolyzer depending on the operating conditions should be investigated when designing a system. Moreover, building a system using the optimized parameters of a cell/stack is also quite important. Sometimes, the operating parameters of the cell/stack may subject to change according to the other system components properties. Obviously, the properties of other components such as power supply, water pump, water tank, cooling system, control unit, gas managing subsystem etc. should also be considered when deciding system components and the range of operating parameters. Literature has various system modeling studies regarding fuel cells [14–20]. However, a study dedicated to system modeling including a PEM electrolyzer is scarce and as far as author's knowledge. Dale et al. [21] modeled a commercial PEM electrolyzer stack in a system containing balance of plant, but they didn't include the system components to the model. Such a system should continuously decide on the operating conditions according to environmental conditions and previous operating conditions while it is running.

Furthermore, designing and customizing another system with higher or lower hydrogen flow rate, the stack and the other components behavior in the system may change. Instead of performing all the experiments over and over for each case, a Simulink model can help to estimate the losses and required parameters such as the heat dissipation, the water flow rate and the working current density for failsafe operation.

Even though well-established simulations [9,10,22,13,12,23] are available in the literature, there is a limited number of system modeling related to PEM electrolysis in the literature.

Therefore, a basic PEM electrolyzer system model is introduced using Simulink/MATLAB in this study. The system components modeled by using Simulink/MATLAB is taken after a laboratory scale in house made PEM electrolyzer.

PEM electrolyzer system and model

The simplified schematic view of a PEM electrolyzer system is shown in Fig. 1. The system consists of a 100 cm^2 PEM electrolyzer cell/stack, an AC-DC power supply, a cooling fan, a water circulating pump, a water vessel, a hydrogen storage tank, a controller, a display and sensors. Simulink model of the system is depicted in Fig. 2. The power supply is thought to be the source for the energy required for cracking the water in the electrolysis process. Besides, all the other components such as controller, pump, fan and sensors which need electric power are connected to this power supply. The controller and the sensors have very low power consumption. The energy consumption of commercial compatible components has been taken into consideration by assigning an average constant value to the calculations. The controller collects the values of the current, the temperature, the pressure and the water level in the vessel and decides whether everything is neat for starting the system. The cooling fan is responsible for removal of heat dissipation from the stack. The controller also decides the fan speed according to the stack temperature. The model includes a clock, thus, the transient response of the system can also be collected.

PEM electrolysis stack model

The Simulink model of the main component in the system, the PEM electrolyzer stack, is given in Fig. 3. It consists of four modules and each module has its own model which can be run separately, but, all the modules are linked to each other. These modules are the anode, the cathode, the membrane and the voltage. The model is based on electrochemical, electrical and flow calculations. It also can optionally work in atmospheric or pressurized conditions.

Before modeling the system, a flow diagram is formed to design mathematical calculations and interactions between each module in Simulink. In the model, the flow of water at the anode inlet and outlet, electro-osmotic drag and diffusion of water are calculated dynamically in real time. Hydrogen ions evolved from the anode catalyst layer pass to the cathode, combine and produce H_2 gas at the catalyst layer. The hydrogen production rate depending on the current density is calculated in the model.

The behavior of the PEM electrolyzer considering different conditions is obtained for different cases. A production scenario for higher pressure or temperature are planned and simulated on the model.

Anode module

The water cracking and the oxygen evolution reaction take place in the anode compartment. The half-cell reaction is given as;

$$2H_2O \rightarrow O_2 + 4H^+ + 4\bar{e} \quad (1)$$

Oxygen evolves as gas, the hydrogen ions travel to the cathode through the membrane, while the electrons are driven by the power supply to the outer circuit. The total

Please cite this article in press as: Yigit T, Selamet OF, Mathematical modeling and dynamic Simulink simulation of high-pressure PEM electrolyzer system, International Journal of Hydrogen Energy (2016), http://dx.doi.org/10.1016/j.ijhydene.2016.06.022