Development of an Integrated Fuel Cell System Simulator "FC-DynaMo"

- Toward Acceleration of Advanced Research and Product Development -

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ABSTRACT: A 1-dimentional (1D) model to simulate the dynamic behavior of an integrated fuel cell (FC) system was developed. The model consists of the physical models of the FC stack and the hydrogen (H_2), air, and coolant systems. To ensure numerical simulation of the entire FC system in life-long system operation (> 10 years) in acceptable calculation time, a proper model resolution is selected. The subsystem models are integrated with the FC stack model and controllers to build a closed-loop simulator of an integrated FC system. The dynamic system behavior of the FC system and the overall system performance, such as fuel economy and thermal balance, are simulated. It was demonstrated that the complicated relationships between the specifications of the fuel cell materials, system components, and the overall system performance could be quantified. In recent, the developed simulator has been extended with the models to estimate the rate of the FC catalyst degradation. It is expected that considerable efforts on development of various FC system products by the topological investigations with the costly prototypes can be replaced with the numerical simulation.

KEY WORDS: fuel cell, system, simulation, model based development, MBD

1. INTRODUCTION

Decarbonization is gathering attention in response to accelerating global warming in recent years and many countries have announced the declarations and policies toward it (1). Hydrogen (H_2) is considered as one of the most promising alternative energy sources to the fossil fuel. H_2 has high portability and can be produced from various renewable energy sources such as solar, wind, hydroelectric, and geothermal energies. Fuel cell (FC) is expected to play a main role of the energy conversion methods from H_2 because of its high efficiency (> 40%) compared with the conventional internal combustion engines (< 30%). A wide adoption of the FC system in various industries must be accommodated with the extension of the H_2 fueling stations network unlike the conventional fossil fuel and electric power sources. The applications of the FC system to a variety of purposes such as commercial vehicle, railway, construction, maritime, and aviation purposes as well as passenger vehicle are investigated to promote H_2 utilization in an entire industry (1). The FC system manufacturers are demanded to develop a variety of products in parallel and in shorter development period. Despite such expectation from the market and industries, the development and optimization of the FC system are conducted in a trial-and-error based process, which requires a significant amount of lead time, cost, and headcounts by manufacturing and testing the prototypes and calibration of controllers. Though studies on the entire FC system are of such great importance, the fuel cell itself has been more intensively investigated (2)–(4), much less research has been done on the FC system including the FC stack, the system components of H_2, air, and coolant systems as well as the FC system controllers. In addition, the system simulator that can estimate the dynamic behavior of the comprehensive FC system with an acceptable computational speed and accuracy has not been proposed yet. The objective of this study is to develop the integrated system simulator including the comprehensive FC system component models and controllers in the entire FC system, which can be utilized as a design platform for the wide range of

applications such as automotive, railway, marine, aviation, and stationary power generation purposes. The developed simulator can estimate the dynamic behavior of the entire FC system with the acceptable computational speed and accuracy. The developed simulator is easy to modify according to system requirements of the various applications.

2. Modeling

The configuration of the integrated FC system simulator, named "FC-DynaMo," is shown in Fig. 1. The physics in the FC stack and system components were formulated and implemented by MATLAB functions, and they were integrated as a comprehensive FC system component model by Simulink as shown in Fig. 1(a). The integrated FC system model is combined to the FC system controllers to build the closed-loop simulator shown in Fig. 1(b). The models and controllers are designed to reproduce the dynamic behaviors of 2nd-generation MIRAI (MIRAI-2), state-of-the-arts fuel cell electric vehicle (5)–(6). It has a modular configuration and is easy to modify for different system components or applications. The dynamic operating patterns including the setpoint of FC system net power and ambient conditions of temperature, pressure, and wind speed are inputs to the FC system simulator in Fig. 1(b). The controllers of the electric power system, FC stack, and system components calculate the setpoint of fuel cell current, state variables, and operating condition of each system component. The setpoints are inputs to the FC system model in Fig. 1(a). Based on the given setpoints the actual distribution of total pressure, flowrate, partial pressure, and temperature in each system component are calculated. The fuel cell current and the state variables at the inlet and outlet boundaries of FC stack are given to the FC stack models of mass transport and polarization and the actual polarization of the FC stack such as the current, voltage, and resistance are calculated. The actuation values of the FC system components and FC stack polarization are given to the electric power system model in Fig. 1(b) as the input arguments, and the actual FC system net power is calculated considering the power generation by the FC stack and power consumption by the FC system components. The calculated values at current time step are saved and used as the initial values in the calculation of next time step. The accuracy of the simulation results were validated by the data collected in a wide range of operating conditions using the test vehicle and system testbeds, where the additional sensors of pressure, flowrate, temperature, and gas composition are installed to the product system.

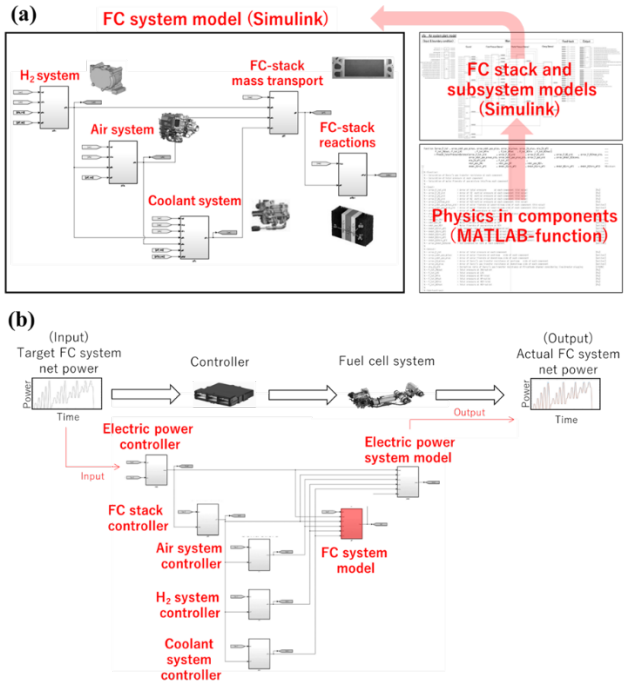

Fig. 1. The configuration of an integrated FC system simulator "FC-DynaMo", (a) FC system component models and (b) closed-loop FC system simulator including controllers.

3. Simulation results

The setpoint of FC system net power shown in Fig. 4 and the constant ambient temperature of 25 °C, ambient pressure of 100 kPa, and ambient wind speed of 80 km/h are also inputs to the simulator. This operating pattern was designed so that the dynamic and steady conditions are combined and a wide range of power load and temperature conditions appear. The simulation results of the dynamic system behavior are shown in Fig. 3. The actual FC system net power and FC stack gross power are shown in Fig. 3(a). The difference between FC stack gross power and FC system net power attributes to the power consumption rate of the system components such as the pumps, valves, and DC-DC converters. The power consumption rate of the system component reaches 23.6 kW for 100 kW of FC system net power under a maximum load condition at 670 s. Coolant temperatures at the inlet and outlet of FC stack are shown in Fig. 3(b). The FC stack outlet temperature reaches 91 °C at the end of the continuous high-load operation at 670 s. The heat generation rate from the FC stack and air intercooler and the heat emission rate from the radiator are shown in Fig. 3(c). The heat generation rate and emission rate at 670 s were 128.5 and 104.6 kW, respectively, and they were not balanced. It means that the coolant temperature will continue to rise if the similar high-load operation is continued. The cumulative H_2 consumption amount is shown in Fig. 3(d). The fuel economy

for the operating pattern shown in Fig. 2, which is one of the most important system performance indicators, was estimated to be 0.605 kg in this case. Fig. 4(a) shows the polarization curve and the breakdown of overpotentials during the operating pattern shown in Fig. 2. The fuel cell voltage and ohmic, cathode activation, and cathode concentration overpotentials at the highest load were 0.611, 0.152, 0.346, and 0.056 V, respectively. The anode overpotential was negligibly low. The cathode activation overpotential accounted for 62.4 % in the overall overpotential and it suggests that the improvement in the cathode catalyst activity is the prior material development research to be carried out. Fig. 4(b) shows the fuel cell resistance and the breakdown of the resistance at each fuel cell component. The resistance of PEM, anode GDL and MPL, and cathode GDL and MPL were 8.3, 15.9, 14.1, 16.3, and 15.1 mΩ cm2, respectively, at the highest load of 2.2 A/cm^2. The PEM resistance accounted for 12 % in the overall fuel cell resistance as a result of the PEM thickness being reduced to less than 10 μm in MIRAI-2 (5)–(6). It suggests that the reduction in the resistance of the GDL and MPL is the prior material development research target to reduce the ohmic overpotential. The computational time for the simulation of the operating pattern in Fig. 2 is shown in Table 1. The simulation environment where the model in this study was deployed is as follows: Intel Core i9-10900 CPU 2.80 GHz/2.81 GHz; 32.0 GB RAM; Windows 10 Enterprise; MATLAB 2015a Service Pack 1 Update 3 with Simulink ver. 8.5.1. The computational speed was 50 times faster than the actual time and an acceptable computational speed for the future application of the year-long durability simulation was confirmed. It was demonstrated that the relationships among the system and controller specifications, dynamic behaviors of the comprehensive system, and an overall system performance such as fuel economy and thermal balance and the detailed breakdown of the overpotential and resistance in the FC stack could be calculated quantitatively in a remarkable computational speed.

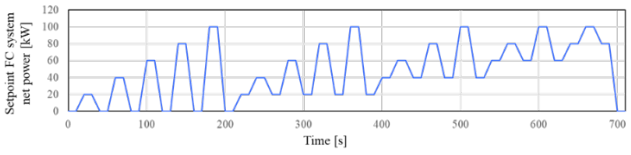

Fig. 2. Setpoint of FC system net power as an input to the FC system simulator

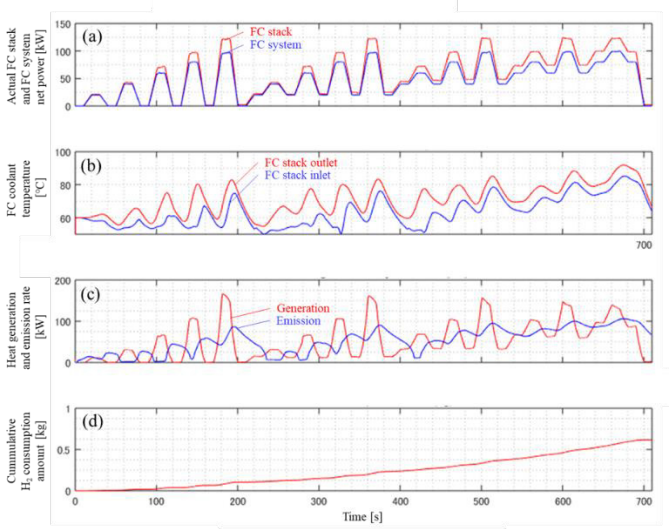

Fig. 3. Simulation results of (a) the fuel cell voltage and overpotentials and (b) the resistance at each fuel cell component

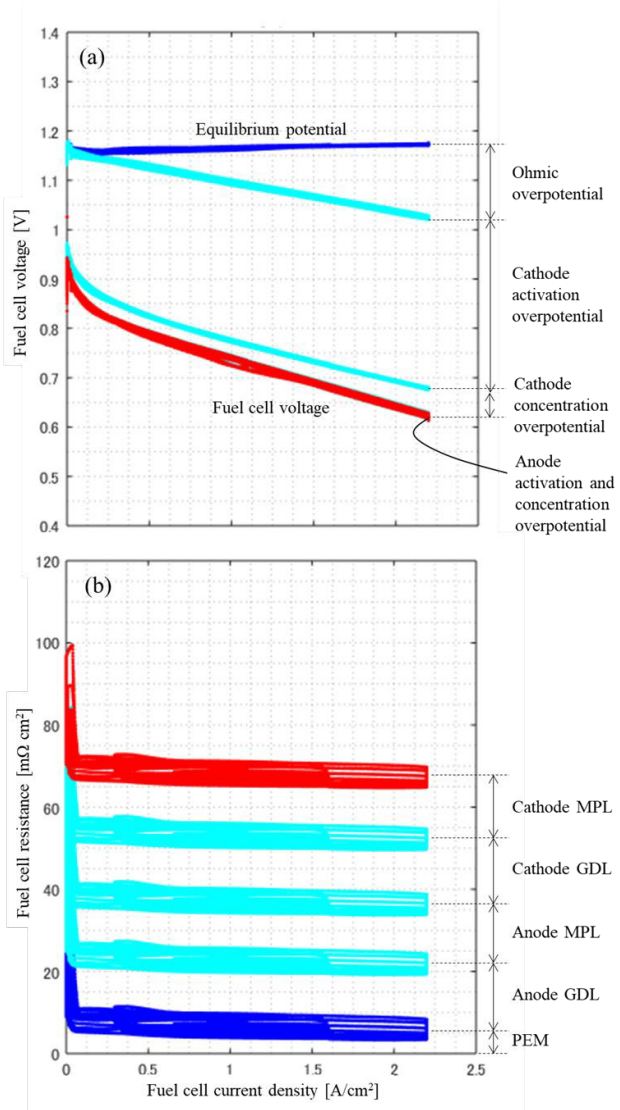

Fig. 4. Simulation results of (a) the fuel cell voltage and overpotentials and (b) the resistance at each fuel cell component

Table 1. Computational time of the integrated FC system simulator in Fig. 1 in the operating pattern in Fig. 2

Computational Conditions	Simulated time	710 s
	Time step	16 ms
Computational time		14 s

4. Recent updates

Fig. 5 shows the mechanism of the FC material degradation. It is considered that the major contributors of the FC material degradation are of Pt coarsening, carbon support corrosion, and PEM thinning by chemical and mechanical stresses. Pt and C degradation affects the polarization and PEM degradation affects the gas barrier property. In recent, the developed FC system simulator was updated by implementing Pt and C degradation models.

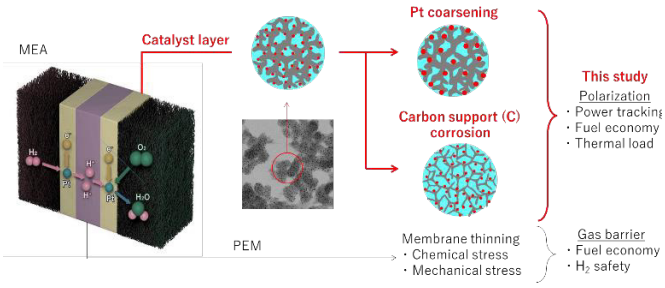

Fig. 5. The major contributor of the FC material degradation.

Similar as the FC mass transport and polarization models, the model parameters were determined by the test data collected with a test-piece MEA used in MIRAI-2. The accuracy of the developed model was validated by the polarization curves after the accelerated stress tests (ASTs) in the literature (7), which are measured with a FC stack having 13 FCs of MIRAI-2 under the operating patterns shown in Fig. 6.

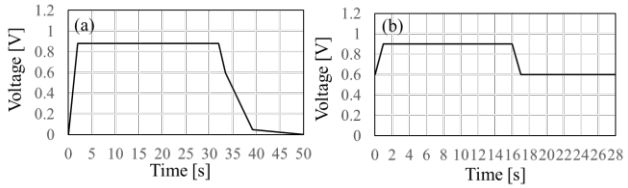

Fig. 6. The accelerated stress test (AST) Patterns for validation, (a) 30000 cycles of startup-shutdown cycles (AST1) and (b) 70000 cycles of acceleration-deceleration cycles (AST2)

Fig. 7 shows the validation results of the developed Pt and C degradation models. The simulation results of the polarization curves of biggening of life (BOL) state, after AST1, and after ASTs 1 and 2 agreed with the literature data and it was confirmed that the developed model can reproduce the actual degradation behavior of the product FC stack.

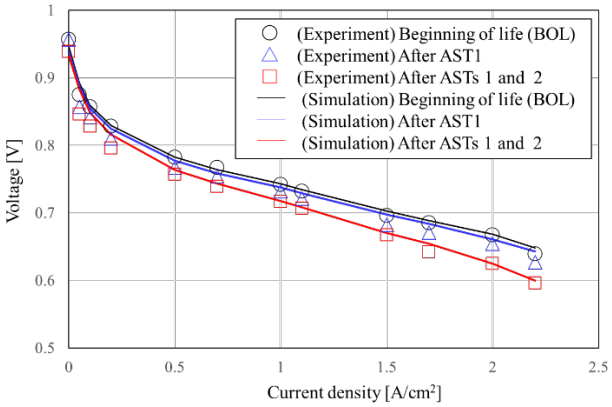

Fig. 7 The validation results of the developed Pt and C degradation models by the accelerated stress test results with a FC stack having 13 FCs used in MIRAI-2.

5. CONCLUSIONS

An integrated fuel cell (FC) system simulator "FC-DynaMo" was developed to reduce considerable efforts for the development of the various FC system products by the topological investigation using the costly prototypes. FC-DynaMo consists of the models of the FC stack, the H_2, air, and coolant systems, and the controllers. The simulator was capable to simulate the dynamics behaviors of the comprehensive system components and controllers. In the case study, It was demonstrated that the relationships among the system and controller specifications, dynamic behaviors of the comprehensive system, and an overall system performance such as fuel economy and thermal balance and the detailed breakdown of the overpotential and resistance in the FC stack could be calculated quantitatively. The computational time was more than 50 times shorter than the simulated. In recent, the developed simulator has been extended with the models to estimate the rate of the FC catalyst degradation. The developed model was validated by the data collected with a product FC stack.

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