A model-based approach to set the future target of fuel cell performance for heavy-duty applications

Takao Watanabe [1)] Masao Shibata [1)] Norihiro Fukaya [1)] Tomoyuki Nagai [1)] Takahisa Suzuki [1)]

1) Toyota Central R&D Labs, Inc., Nagakute, Aichi, Japan
E-mail: twatanabe@mosk.tytlabs.co.jp

ABSTRACT: This paper proposes a modeling and optimization method that enables a fuel cell performance target to be derived from the system requirements of various fuel cell applications, such as heavy-duty trucks (HDTs), buses, and industrial machinery. We developed a comprehensive model of the fuel cell system, comprising a fuel cell performance model, catalyst degradation model, and power management control model of the hybrid system containing a fuel cell and a battery. The model predicts the end-of-life fuel cell performance based on the initial performance of the fuel cell and how the fuel cell system is operated, allowing the simultaneous optimization of the hardware and software. By conducting the optimization calculation assuming various fuel cell performances, the model derives the required fuel cell performance with the optimal system components that satisfy durability and performance requirements.

KEY WORDS: fuel cell, heavy-duty vehicles, I-V polarization curve, model-based development

1. INTRODUCTION

Fuel cells play an important role in achieving carbon neutrality in the transportation sector of a future hydrogen society. To this end, much research is being conducted on using proton exchange membrane fuel cells (PEMFCs) in heavy-duty trucks (HDTs), buses, and industrial and agricultural machinery. A recent review paper by Cullen et al.[(1)] summarizes the research challenges of fuel cells for heavy-duty applications. To promote the use of PEMFCs in these heavy-duty applications, it is essential to improve the efficiency and durability of PEMFCs. However, the performance improvements that can be achieved by PEMFCs for these heavy-duty applications are unclear. An important is that the performance improvement of PEMFCs needs to be considered simultaneously with the performance improvement of hybrid system components, including batteries and cooling radiators, along with their varied applications.

In this paper, we propose a modeling and optimization approach for setting fuel cell performance targets based on the system requirements. A mathematical model of a fuel cell system that comprises a fuel cell performance model, a catalyst degradation model, and a hybrid system model linked with optimal power management control is employed to bridge the gap between the components' properties and the system performance. Optimization calculations using this comprehensive model enable us to determine the candidates depicting required polarization curves with optimal system configurations of fuel cell stacks, batteries, and radiators and their control algorisms.

In the following sections of this paper, we describe the fuel cell performance model and the catalyst degradation model. A comprehensive model that includes the fuel cell system and the power management control system is then described. We show that optimization using the comprehensive model enables us to derive the performance improvement targets required for each element from the product and system requirements. To demonstrate an application of the proposed method, this paper describes the fuel cell performance target required to meet the HDT system targets.

2. FUEL CELL PERFORMANCE AND DEGRADATION

2.1. Fuel cell performance model

The performance of a fuel cell can be represented by a polarization curve model. As a simple model, we employed the following equation to obtain the cell voltage V

$$V = V_{OCV} - R_{\Omega} I - \frac{RT_{cl}}{\alpha F} log\left(\frac{I}{i_0}\right) - \frac{RT_{cl}}{\alpha F} log\left(\frac{C_{ref}}{C_{O2} - R_{MT}\frac{I}{4F}}\right) \quad (1)$$

where the parameters are listed in Table 1. Among these parameters, i_0, R_{Ω}, and R_{MT} describe the material properties of a membrane electrode assembly (MEA), which is the main component of the PEMFC. The exchange current density i_0 represents the catalyst activity, ohmic resistance R_Ω represents the resistance component in the membrane and catalyst layer, and mass transport resistance R_{MT} represents the resistive component involved in the transfer of the reactant gas. Accordingly, these parameters provide design guidelines for MEA materials and components such as catalysts, supports, ionomers, membranes, gas diffusion layers, and separators that compose the cell. Although Eq. (1) is too simplified to accurately capture the overpotentials due to in-plane or through-plane inhomogeneity, the equation can reproduce the overall fuel cell performance by using the empirical values of i_0, R_Ω, and R_{MT}[(2)]. In this study, we used this model to evaluate various polarization curves without any iterative calculation. Fig. 1 shows the polarization curves for different values of each of these parameters. Hereafter, we denote these parameters collectively as $\Theta_{mat} = \{i_0 \quad R_\Omega \quad R_{MT}\}$.

Table 1. Parameters of the polarization curve model.

Parameter	Parameter description
V_{OCV}	Open circuit voltage
i_0	Exchange current density
R_Ω	Ohmic resistance
R_{MT}	Mass transport resistance
I	Current density
T_{cl}	Coolant temperature
α	Constant
C_{ref}	Reference concentration
C_{O2}	Representative oxygen concentration
R	Gas constant
F	Faraday's constant

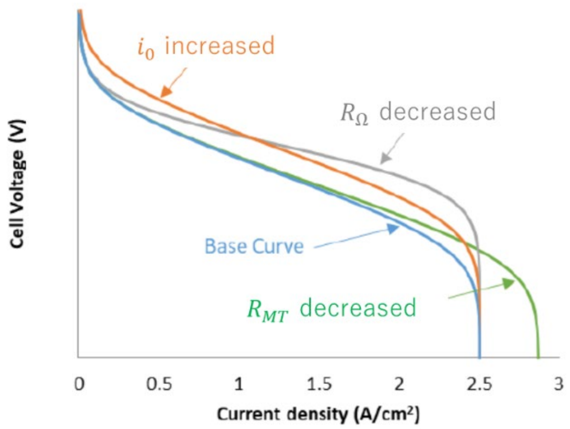

Fig. 1. Polarization curves with different parameters.

2.2. Catalyst degradation

Electrochemical surface area (ECSA) loss is one of the major sources of performance degradation in PEMFCs. In platinum-based fuel cells, the kinetic activity decreases as the surface area of the platinum available for the reaction decreases because of the repeated platinum dissolution and deposition. We employ the kinetics model of platinum dissolution and deposition reported in Ref. (3) to predict the ECSA loss using the time series data of cell potentials during system operation. The kinetic parameters in the model were determined by fitting them to experimental results. Based on an empirical relation between the ECSA and exchange current density i_0, this catalyst degradation model was utilized in the fuel cell performance model to estimate the degraded polarization curve. By using the fuel cell performance model and the catalyst degradation model, our model predicts the deterioration of the power generation performance of PEMFCs due to catalyst degradation. Fig. 2 shows our model structure.

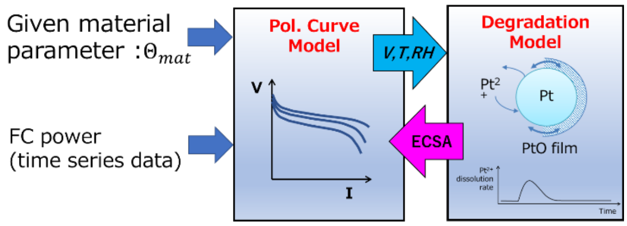

Fig. 2. Fuel cell polarization curve model coupled with catalyst degradation model.

3. FUEL CELL HYBRID SYSTEM AND POWER MANAGEMENT CONTROL MODEL

3.1 Fuel cell hybrid system

The operating conditions of a PEMFC depend on the application, system configuration, and control strategy used by the PEMFC. This implies that the durability of PEMFCs can be improved by properly applying the operating conditions obtained through the appropriate design of the system configuration and control strategy. This paper describes a hybrid system model with PEMFCs and batteries and a model for power management control, enabling us to find the optimal system configuration and control strategy. Fig. 3 describes the structure of the fuel cell hybrid system, where p_{req}, p_{fc}, and p_{bat} represent the required power, fuel cell generation power, and battery power, respectively.

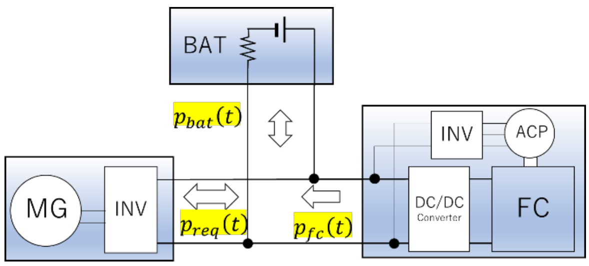

Fig. 3. Fuel cell hybrid system model.

3.2 Power management control

The role of the power management control is to split the vehicle's power requirement between generating power of a PEMFC and charging and discharging power of a battery. The splitting strategy influences the fuel efficiency and the durability of both PEMFCs and batteries. To determine the performance target of the fuel cell, it is required to select a controller that provides an appropriate power-splitting strategy. This paper provides a method to obtain the fuel cell performance targets needed to meet the product requirements of a fuel cell vehicle through optimization, including system configuration and control methods. In the following, we will discuss two optimization problems separately.

As a first step, an optimal control problem is formulated to obtain a set of candidate controllers that minimize the fuel consumption of a PEMFC while limiting the heat generation of a battery within an upper bound (UB).

(First step optimization)

Given: $p_{req}(t),\ \forall t \in \{t|\, 0 \le t \le t_f\} \subset \mathbb{R}$,

find $p_{fc}(t),\ \forall t \in \{t|\, 0 \le t \le t_f\} \subset \mathbb{R}$,

s.t.

$$\text{minimize} \quad J = \int_0^{t_f} fuel(p_{fc}(t))dt \tag{2}$$

$$\text{subject to} \quad p_{req}(t) = p_{fc}(t) + p_{bat}(t) \tag{3}$$

$$S\dot{O}C(t) = g(p_{bat}(t)) \tag{4}$$

$$SOC(0) = SOC(t_f) \tag{5}$$

$$R_{bat} \int_0^{t_f} i_{bat}^2(t)\, dt \le UB(const.) \tag{6}$$

where J represents the total fuel consumption through a driving pattern, and the instantaneous fuel consumption $fuel(\cdot)$ depends on the polarization curve given by equation (1) and the system configuration shown in Fig. 3 as well. Constraints on a battery are given by the state-of-charge (SOC) constraints (4) and (5), and a heat generation constraint (6). The upper bound on the heat generation imposes a limit on the battery current i_{bat}. Adjusting the upper bound and controlling the heat generation allows us to reduce the degradation of the battery. Conversely, permitting the amount of heat generation allows us to reduce the degradation of the PEMFC. Introducing an objective function

$$J' = \int_0^{t_f} \left[fuel\left(p_{fc}(t)\right) + \gamma\, p_{bat}^2(t)\right] dt, \tag{7}$$

in which J and the inequality (6) are integrated, allows us to derive a set of controllers that satisfy a necessary condition for the 1st step optimization problem. As shown in Fig. 4, the controllers are represented by a model that is parametrized by Θ and γ, where Θ represents a parameter related to the material property Θ_{mat} and the system configuration of fuel cell stack with the balance of plant (BOP), and γ is a control parameter that allows tuning of the power split between the fuel cell and the battery (Fig. 5).

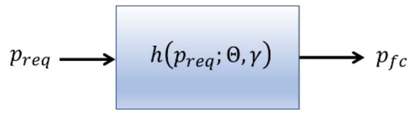

Fig. 4. Parametrized controller.

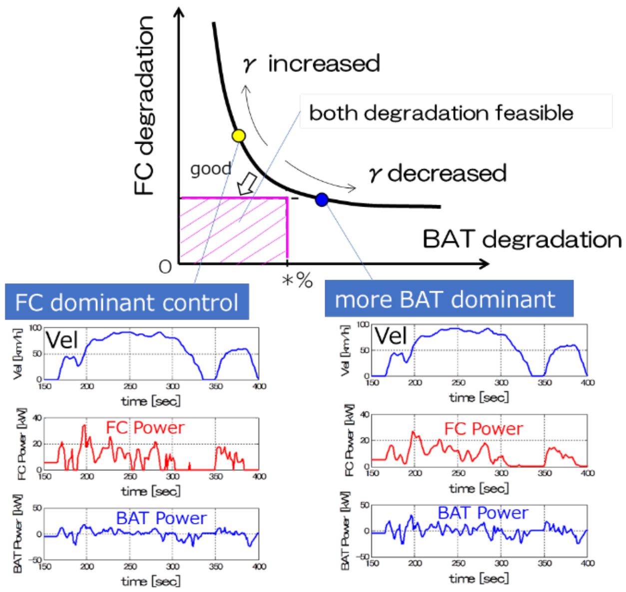

Fig. 5. Variation in the control strategy depending on γ.

4. COMPREHENSIVE MODEL AND OPTIMIZATION

By coupling the previously described fuel cell performance model, catalyst degradation model, hybrid system model, and optimal control model, a comprehensive model is developed, as shown in Fig. 6. The model uses the system requirements of the product, such as vehicle power performance and durability requirements, as inputs and outputs the total cost, including fuel cost, capital cost, and replacement and maintenance cost. This model predicts the total cost as a function of parameters Θ and γ as $\Phi(\Theta,\gamma)$, hence enabling estimation of the optimal values of Θ and γ with respect to the total cost. In the second step, we formulate the optimization problem

(Second step optimization)

$$\text{minimize} \quad \Phi(\Theta,\gamma). \tag{8}$$

This allows us to optimize hardware and software simultaneously. On the other hand, the above objective function can be made as small as possible by improving the material performance, but it is also necessary to properly identify the limit of material performance improvement and set a limit on it.

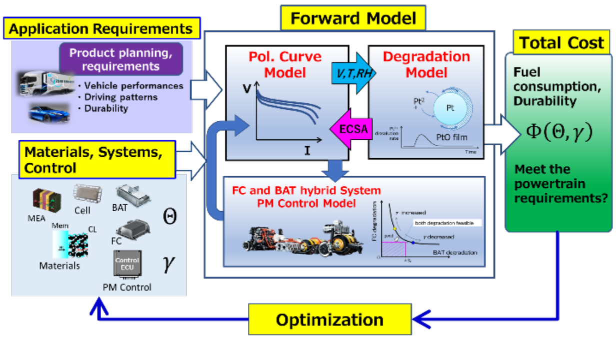

Fig. 6. Comprehensive model.

5. SETTING THE TARGET POLARIZATION CURVE

For fuel cells to be widely spread, they must have an advantage over the current power sources. To achieve this, it is necessary to improve the performance of fuel cells, as well as to evolve the system configuration and control methods in accordance with various applications. Using the comprehensive modeling and optimization methods described above, we set development targets for fuel cell performance from product goals of future fuel cell applications. Assuming applications such as railroads, ships, construction machinery, and agricultural tractors, including HDTs, a target value for the polarization curve was derived from the most demanding HDT product requirements.

We first obtain a set of polarization curves of PEMFCs for the HDTs that satisfy the durability requirement and maintain the driving performance of the HDTs, allowing the truck to run at a specified speed even on heavy-load roads at the end of life. The durability requirement is replaced by an inequality

$$Q_{FC}^{eol} \leq Q_{RD} \tag{9}$$

representing the relationship between the heat generation of PEMFCs on an end-of-life (EOL) polarization curve Q_{FC}^{eol} and the maximal cooling performance of a radiator Q_{RD}.

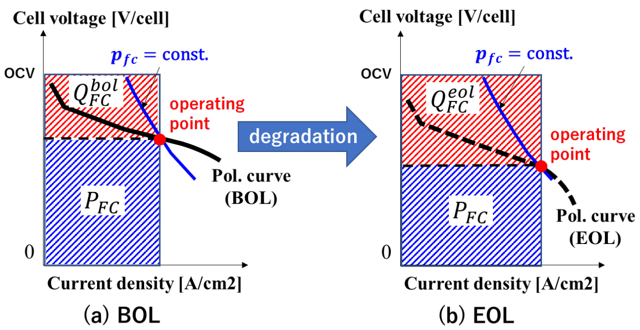

Fig. 7. Operating point and heat generation.

As can be seen in Fig. 7, the amount of heat generation depends on the power generation performance represented by the polarization curve and its deterioration due to degradation. Figures 8 and 9 show the calculation results. Fig. 7 shows a boundary plane in the material parameter space ($\Theta_{mat} = \{i_0 \quad R_\Omega \quad R_{MT}\}$); the durability requirement is satisfied in the space outside the boundary plane. The boundary plane suggests multiple strategies to meet these example requirements: a relatively small improvement in i_0 with a large improvement in R_Ω, or vice versa. The most promising strategy should be selected according to limitations in material development. Recently, we have derived development targets[4] of fuel cells using this method. Fig. 9 shows polarization curves representing development targets, which should be realized in approximately 2030 and 2040.

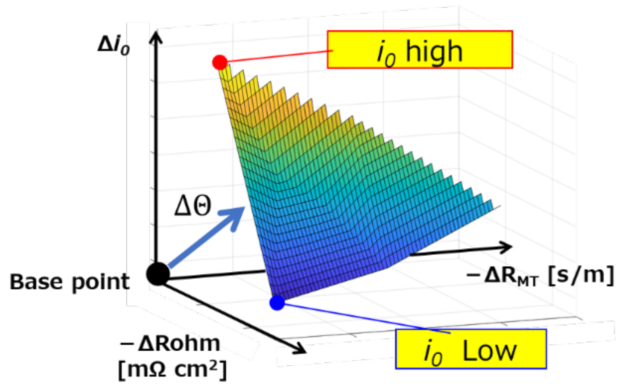

Fig. 8. Target values of material properties.

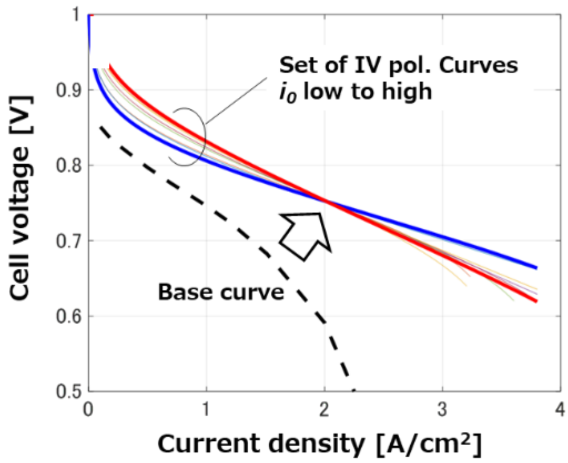

Fig. 9. Derived target polarization curves.

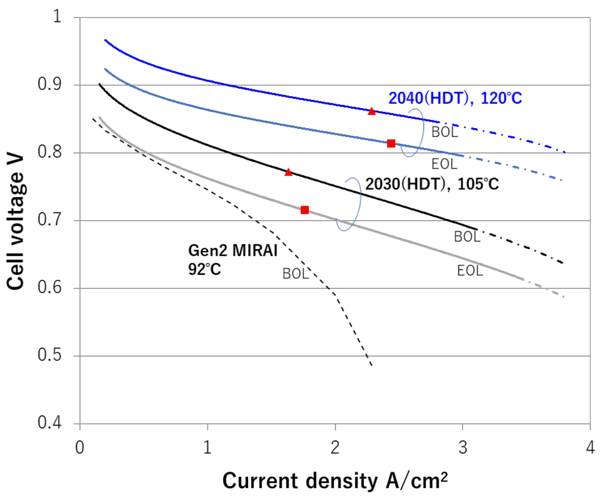

Fig. 9. Polarization curves representing development targets.

6. CONCLUSIONS

This paper described a modeling and optimization method for deriving fuel cell materials, systems, and control methods from fuel cell application requirements. This method was used to set the fuel cell roadmap for HDTs and the target polarization curves for 203X and 204X by the New Energy and Industrial Technology Development Organization (NEDO) [4].

ACKNOWLEDGMENT

We would like to thank the NEDO Roadmap Study Committee and working group members for their cooperation in setting performance targets for future fuel cells.

REFERENCES

(1) D. A. Cullen, et al., "New roads and challenges for fuel cells in heavy-duty transportation", *NATURE ENERGY.* 6, pp. 462-474, 2021.

(2) Weber, A. Z., et al., "A Critical Review of Modeling Transport Phenomena in Polymer-Electrolyte Fuel Cells." Journal of The Electrochemical Society 161(12): F1254-F1299, 2014.

(3) R. M. Darling and J. P. Meyers, "Kinetic Model of Platinum Dissolution in PEMFCs," *Journal of The Electrochemical Society*, 150, (11), pp. A1523-A1527, 2003.

(4) New Energy and Industrial Technology Development Organization, "NEDO Fuel Cell Technology Development Roadmap" - Fuel Cell Roadmap for HDV, (Explanatory Document, in Japanese), 2022. available from https://www.nedo.go.jp/content/100944011.pdf