

Prediction of electrochemical characteristics of practical-size solid oxide fuel cells based on database of unit cell performance

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Abstract

A novel numerical methodology for predicting the electrochemical characteristics of a practical-size solid oxide fuel cell (SOFC) is proposed. The core idea is to divide the practical-size cell into independent one-dimensional (1D) unit cells and to evaluate the characteristics of the practical-size cell as an aggregation of the performance of local unit cells. The proposed methodology consists of two steps. The first is to construct a database of the electrochemical performance of the unit cells under a comprehensive range of operating conditions. For this purpose, a 1D numerical simulation model is developed and validated by comparing the predicted values with experimental data. It is confirmed that not only the current–voltage characteristics but also the impedance characteristics are accurately reproduced by the developed unit cell model. The second is to reproduce the performance of the practical-size cell using the constructed database. The cell is considered as an assembly of unit cells and the electrochemical performance of each unit cell is determined by referring to the constructed database. Subsequently, the macroscopic characteristics of the entire cell are evaluated by using the derived theoretical expressions correlating the macroscopic characteristics with the local electrochemical performance. The predicted cell characteristics fairly agree with the experimental data found in the literature. Since the macroscopic characteristics of the practical-size cell is evaluated with simple arithmetic expressions, the computational cost is significantly reduced, which realizes an exhaustive parametric study of the practical-size cell to identify the optimal operation conditions.

Keywords: solid oxide fuel cell; numerical method; database; impedance; unit cell

1. Introduction

Solid oxide fuel cells (SOFCs) are one of the promising high-temperature energy conversion devices that can realize efficient energy conversion from chemical energy to electrical power, and their commercialization has begun in several countries [1]. In the research and development of SOFC systems, numerical simulation plays an important role in understanding not only the macroscopic behavior of the systems but also their internal states, such as temperature and reaction distributions within the cells and stacks. This is because a direct and detailed measurement of the physicochemical quantities inside the SOFC systems is practically difficult and also because parametric investigation using the real systems is costly.

Numerous studies on the numerical modeling of SOFCs can be found in the literature. They can be categorized into several types depending on the length scale of interest: atomic scale, electrode scale, cell scale, and stack scale. In the atomic-scale analysis, electrochemical reactions around the reaction sites in the electrodes, i.e., triple-phase boundaries (TPBs) and double-phase boundaries (DPBs) are modeled by taking into account elementary heterogeneous reactions. The conventional competitive adsorption model [2], [3], [4] considers adsorption and desorption of chemical species at the reaction sites in the electrodes and estimates the electrochemical reaction rates using surface coverages of adsorbed species, whereas the recently-developed species territory adsorption model [5], [6] considers selective adsorption and desorption of species on solid surfaces adjacent to the reaction sites. They offer valuable insights into the reaction kinetics in the electrodes so that the dependence of

their electrochemical activity on operating conditions, such as temperature, gas compositions, and overpotential, is predicted.

In the electrode-scale analysis, conservation equations of electrons, ions and gas species are solved in the porous electrodes, and the distributions of physicochemical quantities in the electrodes, such as electrochemical potential and gas partial pressures, are predicted in the length scale on the order of tens to hundreds of micrometers. Introducing mesoscale structures ($\sim 100\text{ }\mu\text{m}$) at the electrode-electrolyte interface in the cells have recently been attracting attention to expand the active reaction region [7], [8], and its effect on overall cell performance was quantitatively investigated on this length scale [9], [10], [11]. Recently, three-dimensional (3D) real microstructures of SOFC electrodes have become available by advanced tomography techniques, such as focused-ion beam scanning electron microscopy (FIB-SEM) [12], [13] and X-ray nano computed tomography (CT) [14], [15]. The obtained electrode microstructures were used in electrode-scale analysis using the finite volume method accompanied with the sub-grid-scale model [16], [17], the finite element method [18], [19], and the lattice Boltzmann method [20], [21]. Among the important findings from the analyses, it was revealed that electrochemical reactions mainly take place in the vicinity of the electrode–electrolyte interface with a thickness of $10\text{--}20\text{ }\mu\text{m}$ both in anode [22] and cathode [21]. Semi-analytical investigation on the reaction thickness was also performed to understand its dependence on operating conditions [23]. Unsteady-state analysis models were also developed to reproduce impedance spectra of composite anodes [24], [25] and mixed ion–electron conducting cathodes [26].

In the cell-scale analysis, the fuel and air channels are combined in the electrode models, which enables the analysis of various distributions on the cells on a larger length scale. The macroscopic performance of the cells with practical sizes (typically around $10\times 10\text{ cm}^2$) can be reproduced under realistic boundary conditions and operating conditions. Direct-internal-reforming SOFCs were often analyzed on this length scale to understand temperature distribution on the cell formed by combination of endothermic reforming reaction and exothermic electrochemical reaction [27], [28], [29]. Ammonia-fueled SOFCs were also analyzed for similar objectives [30] with growing interest on ammonia as a hydrogen carrier [31] and its utilization in SOFCs [32], [33].

In the stack-scale analysis, several layers of cell models are considered to reproduce much larger-scale distributions of temperature and gas concentration. Results will be useful for detecting hot spots and local fuel starvation within the stacks [34], [35]. Transient behavior of a short stack during heating-up and shutdown stages was analyzed to understand the temperature distribution and thermal stresses in the cells [36]. A short stack fueled with ammonia was analyzed to investigate the effect of aspect ratio of cells and position of an ammonia cracker on the temperature distribution on the cells [37]. Such analyses are typically performed in the development of commercial SOFC systems [38]. A more comprehensive review of modeling and simulation techniques for SOFCs across the length scale is also found elsewhere [39].

With increasing scale of numerical models, the computational cost inevitably soars up because strong coupling occurs among the governing equations for heat transfer, flow dynamics, and

electrochemistry. Therefore, it is unrealistic to perform the exhaustive parametric analysis of SOFCs on the entire cell/stack scales. Needless to say, the unsteady-state analysis of practical SOFC cells/stacks to predict their impedance response and also their-long term behavior, such as degradation, is almost impossible. Nevertheless, a strong demand exists for numerical models that can analyze practical SOFC cells/stacks to identify their optimal operating conditions and also to predict possible degradation behavior over long-time operation [40], [41]. In addition, such a large-scale analysis is useful in laboratory-scale investigations to estimate how newly synthesized electrode materials would perform when they are scaled up for use under practical operating conditions.

In this study, therefore, we propose a novel methodology of numerical analysis of practical-size SOFCs to predict their macroscopic performance with realistic computational cost. The numerical model assumes that the cell consists of independent one-dimensional (1D) unit cells, and the characteristics of the entire cell is evaluated as an aggregation of the performance of unit cells. For this purpose, a 1D unsteady-state numerical model of an SOFC unit cell is first developed, based on which a performance database is constructed by calculating the performance of a unit cell under a comprehensive range of operating conditions. Subsequently, theoretical expressions to correlate the macroscopic cell characteristics, such as cell current, power output, fuel utilization, and conversion efficiency, with the local unit cell performance are established to predict the macroscopic characteristics of the entire cell. The simulation results are compared with the experimental results found in the literature in terms of the current–voltage and impedance characteristics. In addition, by

using the proposed numerical methodology, we successfully carry out an exhaustive parametric study to investigate the dependence of the macroscopic cell characteristics on the operating conditions.

2. Numerical Model

2.1 Unit cell model

2.1.1 Calculation domain and assumptions

In this study, an unsteady-state numerical model of a 1D unit cell of SOFCs was first developed to reproduce its overpotential characteristics and impedance response. This model was used to construct a database of the unit cell performance for analysis of the practical-size SOFCs explained later. The unit cell consists of a porous Ni-YSZ (yttria-stabilized zirconia) anode, a dense YSZ electrolyte, and a porous LSCF (lanthanum strontium cobalt ferrite, $\text{La}_{0.6}\text{Sr}_{0.4}\text{Co}_{0.2}\text{Fe}_{0.8}\text{O}_{3-\delta}$) cathode. The electrode microstructure was considered homogeneous and represented by microstructural parameters, such as volume fraction, tortuosity factor, TPB density, and DBP density. The conservation of electrons, ions, and gas species was considered and coupled by electrochemical reactions as schematically shown in Fig. 1, where the charge-transfer process is represented as a resistor–capacitor parallel circuit. Noted that the values of the local resistors and capacitors can vary with the local temperature and gas composition among others; in this sense, the model we developed is different from the conventional transmission line model [42]. The governing equations were discretized using the finite-volume method and solved using an in-house Fortran program. An unsteady-state model for the

anode component was already developed and validated in our previous study [25], and the model was extended to the entire cell in this study.

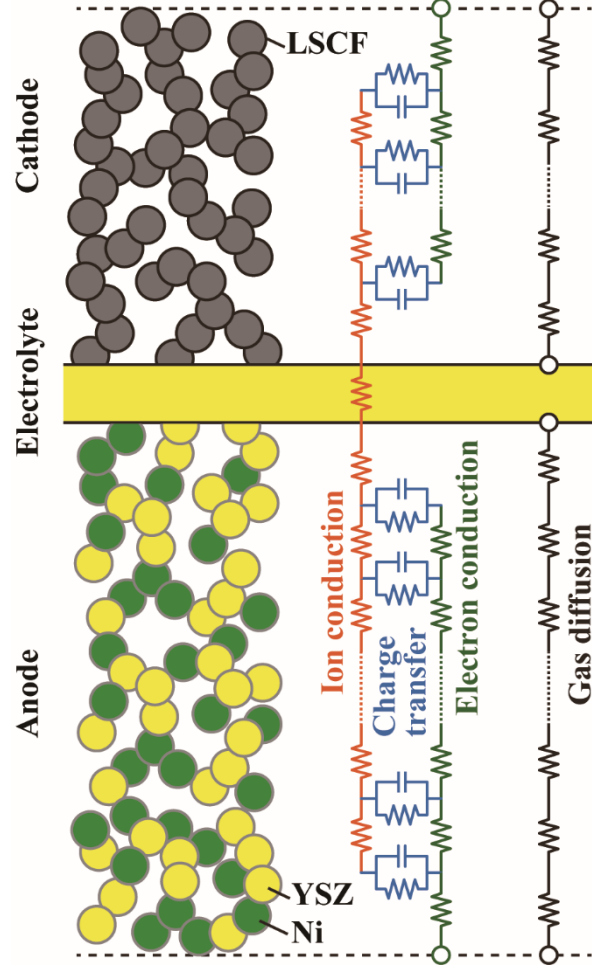


Fig. 1 Schematic image of 1D unit cell model.

2.1.2 Governing equations

The conservation of electrons and ions is described as follows in terms of the electrochemical potential of the electrons $\tilde{\mu}_{e^-}$ and ions $\tilde{\mu}_{O^{2-}}$. The charge/discharge current from the capacitors in the electrodes was considered.

$$c \frac{\partial}{\partial t} \left(\frac{\tilde{\mu}_{O^{2-}}}{2F} - \frac{\tilde{\mu}_{e^-}}{F} \right) - \frac{\partial}{\partial x} \left(\frac{\sigma_e^{\text{eff}}}{F} \frac{\partial \tilde{\mu}_{e^-}}{\partial x} \right) = -i_{ct} \quad (1)$$

$$-c \frac{\partial}{\partial t} \left(\frac{\tilde{\mu}_{O^{2-}}}{2F} - \frac{\tilde{\mu}_{e^-}}{F} \right) - \frac{\partial}{\partial x} \left(\frac{\sigma_{O^{2-}}^{\text{eff}}}{2F} \frac{\partial \tilde{\mu}_{O^{2-}}}{\partial x} \right) = i_{ct} \quad (2)$$

Here, c is the electrostatic capacitance, σ_e^{eff} and $\sigma_{O^{2-}}^{\text{eff}}$ are respectively the effective electron and ion conductivities, and i_{ct} is the charge-transfer current associated with the electrochemical reactions in the electrodes.

The conservation equation of gas species is described as

$$\frac{V_{\text{Pore}}}{RT} \frac{\partial P_i}{\partial t} + \frac{\partial N_i}{\partial x} = \dot{S}_i, \quad (3)$$

where V_{Pore} is the porosity of the electrodes, P_i is the gas partial pressure, N_i is the molar flux, and $\dot{S}_i$ is the sink/source term associated with the electrochemical reaction in the electrodes as follows.

$$\dot{S}_{H_2} = -\frac{i_{ct}}{2F}, \quad \dot{S}_{H_2O} = \frac{i_{ct}}{2F}, \quad \dot{S}_{O_2} = -\frac{i_{ct}}{4F}, \quad \dot{S}_{N_2} = 0 \quad (4)$$

The dusty-gas model [43], [44] was used to obtain the molar flux of gas species in porous electrodes.

$$\frac{N_i}{D_{i,K}^{\text{eff}}} + \sum_{j=1, j \neq i}^n \frac{X_j N_i - X_i N_j}{D_{ij}^{\text{eff}}} = -\frac{P_t}{RT} \frac{\partial X_i}{\partial x} - \frac{X_i}{RT} \left(1 + \frac{K P_t}{\mu D_{i,K}^{\text{eff}}} \right) \frac{\partial P_t}{\partial x} \quad (5)$$

Here, X_i is the molar fraction, $D_{i,K}^{\text{eff}}$ and D_{ij}^{eff} are respectively the effective Knudsen and molecular diffusivities, P_t is the total pressure, μ is the viscosity of the mixture gas, and K is the permeability of the porous electrodes.

The effective conductivities and gas diffusivities were evaluated by modifying the bulk transport coefficients using the volume fraction V_i and the tortuosity factor τ_i of the corresponding phases.

$$\Gamma_i^{\text{eff}} = \frac{V_i}{\tau_i} \Gamma_i \quad (\Gamma_i = \sigma_{e^-}, \sigma_{O^{2-}}, D_{ij}, D_{i,K}) \quad (6)$$

Empirical formulas were used for the bulk conductivities of the anode materials as follows [45], [46].

$$\sigma_{e^-, Ni} = 3.27 \times 10^6 - 1065T \quad (7)$$

$$\sigma_{\text{O}^{2-},\text{YSZ}} = 3.40 \times 10^4 \exp\left(-\frac{8.60 \times 10^4}{RT}\right) \quad (8)$$

The bulk conductivities of the cathode material were formulated by Matsuzaki et al. [21] using the experimental data obtained by Bouwmeester et al. [47].

$$\log_{10} \sigma_{\text{e}^-, \text{LSCF}} = -0.0222 \left(\log_{10} \frac{P_{\text{O}_2}}{10^5}\right)^2 - 0.0017 \log_{10} \frac{P_{\text{O}_2}}{10^5} + 4.8056 \quad (750^\circ\text{C}) \quad (9)$$

$$\log_{10} \sigma_{\text{e}^-, \text{LSCF}} = -0.0237 \left(\log_{10} \frac{P_{\text{O}_2}}{10^5}\right)^2 - 0.0034 \log_{10} \frac{P_{\text{O}_2}}{10^5} + 4.8126 \quad (800^\circ\text{C}) \quad (10)$$

$$\sigma_{\text{O}^{2-}, \text{LSCF}} = \frac{8F^2 \tilde{D}}{RTV_m} \frac{\partial \delta}{\partial \ln P_{\text{O}_2}} \quad (11)$$

$$\log_{10} \tilde{D} = -0.1884 \left(\log_{10} \frac{P_{\text{O}_2}}{10^5}\right)^2 - 0.3243 \log_{10} \frac{P_{\text{O}_2}}{10^5} - 9.4969 \quad (750^\circ\text{C}) \quad (12)$$

$$\log_{10} \tilde{D} = -0.1765 \left(\log_{10} \frac{P_{\text{O}_2}}{10^5}\right)^2 - 0.2724 \log_{10} \frac{P_{\text{O}_2}}{10^5} - 9.2256 \quad (800^\circ\text{C}) \quad (13)$$

Here, $\tilde{D}$ is the chemical diffusion coefficient, V_m is the molar volume, and δ is the oxygen nonstoichiometry of the LSCF [47].

The bulk molecular diffusivity [48] and Knudsen diffusivity [49] were evaluated as

$$D_{ij} = \frac{0.01013T^{1.75} \left(\frac{1}{10^3 M_i} + \frac{1}{10^3 M_j}\right)^{0.5}}{P_t \left[(\sum v_i \times 10^6)^{1/3} + (\sum v_j \times 10^6)^{1/3} \right]^2} \quad (14)$$

$$D_{i,K} = \frac{d_{\text{pore}}}{2} \frac{2}{3} \sqrt{\frac{8RT}{\pi M_i}}, \quad (15)$$

where M_i is the molar mass, $\sum v_i$ is the diffusion volume, and d_{pore} is the mean pore diameter.

The electrostatic capacitance of the anode was assumed to linearly depend on the volumetric density of the Ni-YSZ interfacial area $S_{\text{Ni-YSZ}}$ as [50]

$$c_{\text{ano}} = c_{\text{Ni-YSZ}} S_{\text{Ni-YSZ}}, \quad (16)$$

where $c_{\text{Ni-YSZ}}$ is the electrostatic capacitance per unit Ni-YSZ interfacial area as [25]

$$c_{\text{Ni-YSZ}} = 155 \exp\left(-\frac{3.61 \times 10^4}{RT}\right). \quad (17)$$

The electrostatic capacitance of the cathode was correlated with the oxygen nonstoichiometry δ of the LSCF [51].

$$C_{\text{cat}} = \frac{4F^2\delta}{V_m RT A_\delta} V_{\text{LSCF}} \quad (18)$$

Here, V_{LSCF} is the volume fraction of the LSCF phase, and A_δ is the thermodynamic factor defined as

$$A_\delta = -\frac{1}{2} \frac{\partial \ln P_{\text{O}_2}}{\partial \ln \delta}. \quad (19)$$

The permeability of the porous electrodes was evaluated as [22]

$$K = \frac{V_{\text{Pore}}}{6\tau_{\text{Pore}}(S/V)_{\text{Pore}}^2}, \quad (20)$$

where $(S/V)_{\text{Pore}}$ is the surface-to-volume ratio of the pore phase.

The electrochemical reactions were assumed to take place at the Ni-YSZ-Pore triple-phase boundaries in the anode, and at the LSCF-Pore double-phase boundaries in the cathode, which are described by the Butler–Volmer-type equations as follows [52], [21].

$$i_{\text{ct,ano}} = i_{0,\text{TPB,ano}} l_{\text{TPB,ano}} \left[\exp\left(\frac{2.0F}{RT} \eta_{\text{act,ano}}\right) - \exp\left(-\frac{F}{RT} \eta_{\text{act,ano}}\right) \right] \quad (21)$$

$$i_{\text{ct,cat}} = i_{0,\text{DPB,cat}} A_{\text{DPB,cat}} \left[\exp\left(\frac{1.2F}{RT} \eta_{\text{act,cat}}\right) - \exp\left(-\frac{F}{RT} \eta_{\text{act,cat}}\right) \right], \quad (22)$$

Here $i_{0,\text{TPB}}$ and $i_{0,\text{DPB}}$ are respectively the exchange-current density per unit TPB length and that per unit DPB area, l_{TPB} is the TPB density in the anode, A_{DPB} is the DPB density in the cathode, and η_{act} is the activation overpotential defined as follows.

$$\eta_{\text{act,ano}} = -\frac{1}{2F} (2\tilde{\mu}_{\text{e}^-} - \tilde{\mu}_{\text{O}^{2-}}) - \frac{RT}{2F} \left(\frac{\Delta G}{RT} + \ln \frac{P_{\text{H}_2\text{O}}^{\text{bulk}}}{P_{\text{H}_2}^{\text{bulk}}} \right) - \eta_{\text{con}} \quad (23)$$

$$\eta_{\text{act,cat}} = -\frac{1}{2F} (2\tilde{\mu}_{\text{e}^-} - \tilde{\mu}_{\text{O}^{2-}}) - \frac{RT}{4F} \ln P_{\text{O}_2}^{\text{bulk}} - \eta_{\text{con}} \quad (24)$$

Here, ΔG is the change in Gibbs free energy for the hydrogen oxidation reaction, P_i^{bulk} is the gas partial pressure at the electrode surfaces determined as the boundary condition, and η_{con} is the concentration overpotential evaluated as

$$\eta_{\text{con,ano}} = \frac{RT}{2F} \ln \frac{P_{\text{H}_2}^{\text{bulk}} P_{\text{H}_2\text{O}}}{P_{\text{H}_2} P_{\text{H}_2\text{O}}^{\text{bulk}}} \quad (25)$$

$$\eta_{\text{con,cat}} = \frac{RT}{4F} \ln \frac{P_{\text{O}_2}}{P_{\text{O}_2}^{\text{bulk}}}. \quad (26)$$

The exchange current density was evaluated using the following empirical formulas [53], [54]:

$$i_{0,\text{TPB,ano}} = 6.5 \times 10^{-3} P_{\text{H}_2}^{0.11} P_{\text{H}_2\text{O}}^{0.67} \exp\left(-\frac{8.49 \times 10^4}{RT}\right) \quad (27)$$

$$i_{0,\text{DPB,cat}} = 1.47 \times 10^6 P_{\text{O}_2}^{0.2} \exp\left(-\frac{8.59 \times 10^4}{RT}\right). \quad (28)$$

2.1.3 Boundary conditions

The boundary conditions are summarized in Table 1. For the impedance simulation, sinusoidal perturbation was applied to the electrochemical potential of electrons on the cathode surface at an amplitude of η_p and an angular velocity of $\omega = 2\pi f$. For the steady-state simulation, the amplitude was set as zero. V_t is the terminal voltage of the cell.

Table 1 Boundary conditions for unit cell simulation.

Parameter	Anode Surface	Cathode Surface
H ₂ partial pressure	$P_{\text{H}_2} = P_{\text{H}_2}^{\text{bulk}}$	—
H ₂ O partial pressure	$P_{\text{H}_2\text{O}} = P_{\text{H}_2\text{O}}^{\text{bulk}}$	—
O ₂ partial pressure	—	$P_{\text{O}_2} = P_{\text{O}_2}^{\text{bulk}}$
N ₂ partial pressure	—	$P_{\text{N}_2} = P_{\text{N}_2}^{\text{bulk}}$
Electrochemical potential of electrons	$\tilde{\mu}_{e^-} = 0$	$\tilde{\mu}_{e^-} = -F(V_t + \eta_p \sin \omega t)$
Electrochemical potential of oxide ions	$\frac{\partial \tilde{\mu}_{\text{O}^{2-}}}{\partial x} = 0$	$\frac{\partial \tilde{\mu}_{\text{O}^{2-}}}{\partial x} = 0$

2.1.4 Impedance simulation

First, the steady-state solution was obtained without the perturbation ($\eta_p = 0$). Subsequently, the unsteady-state simulation with the perturbation was conducted for several periods until the current response curve became identical between the neighboring periods. The amplitude of the perturbation was set as 5 mV. The time step used in this study was 1/64 of each period. The complex impedance of a unit cell and also that of its components, i.e., the anode, electrolyte, and cathode, were obtained as follows using the Fourier transform of the cell current and the overpotentials.

$$Z_{\text{cell}}(\omega) = \frac{\eta_p}{\tilde{i}_{\text{cell}}(\omega)} \quad (29)$$

$$Z_k(\omega) = \frac{\tilde{\eta}_k(\omega)}{\tilde{i}_{\text{cell}}(\omega)} \quad (30)$$

Here, $\tilde{\eta}_k$ is the overpotential in each cell component. Eq. (29) and (30) were explicitly expressed with the time evolution of the cell current and the overpotentials obtained in the simulation as

$$\tilde{Z}_{\text{cell}}(\omega) = \frac{\eta_p}{\frac{2}{\theta} \int_0^\theta i_{\text{cell}}(t) \sin(\omega t) dt + j \frac{2}{\theta} \int_0^\theta i_{\text{cell}}(t) \cos(\omega t) dt} \quad (31)$$

$$\tilde{Z}_k(\omega) = \frac{\frac{2}{\theta} \int_0^\theta \eta_k(t) \sin(\omega t) dt + j \frac{2}{\theta} \int_0^\theta \eta_k(t) \cos(\omega t) dt}{\frac{2}{\theta} \int_0^\theta i_{\text{cell}}(t) \sin(\omega t) dt + j \frac{2}{\theta} \int_0^\theta i_{\text{cell}}(t) \cos(\omega t) dt}, \quad (32)$$

where $\theta = 1/f$ is the period of the sinusoidal perturbation and j is the imaginary unit.

2.2 Practical-size cell model

2.2.1 Assumptions and procedure

A novel methodology for predicting the performance of a practical-scale SOFC cell is

proposed in this study. The core idea is to express the characteristics of a practical-size cell as an aggregation of unit cell performance. For this purpose, the 1D numerical analysis described above was conducted under a comprehensive range of operating conditions to construct a performance database. The practical-size cell was assumed to consist of multiple 1D unit cells as shown in Fig. 2 by assuming that the transport of electrons, ions, and gas species in the in-plane direction was negligible. In the figure, r_i , i_i , and E_i are the area-specific resistance in $\Omega \text{ m}^2$, current density in A m^{-2} , and the electromotive force of the unit cells, respectively; $P_{\text{H}_2,i}$ is the hydrogen partial pressure at the anode surface; and i_{cell} is the current density of the entire cell in A m^{-2} . In the proposed methodology, the electrochemical performance of each unit cell was determined by referring to the database with the cell temperature, the gas partial pressures at the surface, and the terminal voltage being used as indexes. Subsequently, the macroscopic performance of the entire cell was evaluated by combining the characteristics of the local unit cells.

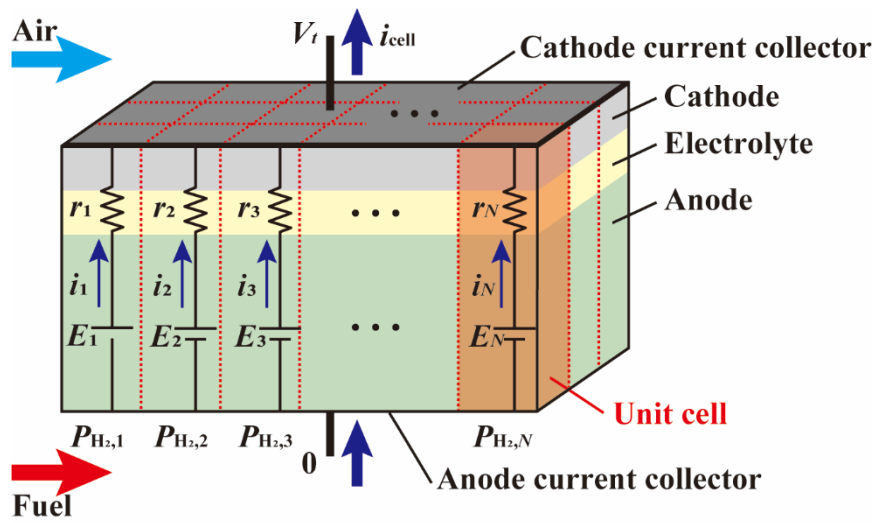


Fig. 2 Schematic image of practical-size SOFC cell model represented as an assembly of unit

cells.

Fig. 3 shows the schematic flowchart of the proposed methodology to predict the electrochemical performance of the practical-size SOFCs. The details are as follows. (i) The electrochemical performance of a unit cell was calculated using the 1D unit cell model we developed under a comprehensive range of operating conditions by varying the terminal voltage, cell temperature, and hydrogen concentration at the anode surface to construct a database. (ii) The cell temperature, terminal voltage, and supplied gas composition and flow rate were set as the operating conditions of the practical-size cell. (iii) The performance of the most upstream unit cell (the first unit cell) was determined by referring to the database using the temperature, cell terminal voltage, and supplied fuel composition. (iv) Hydrogen consumption and steam generation at the first unit cell were calculated using the generated current, and the fuel concentration on the second unit cell was obtained. (v) The performance of the second cell was similarly determined by referring to the database using the temperature, terminal voltage, and calculated fuel compositions. (vi) By repeating (iii)–(v), the performance of all the unit cells were determined one by one from upstream. (vii) The macroscopic performance of the entire cell was evaluated by aggregating the performance of the unit cells. Details of the data aggregation is explained in the next section.

Since in this study we aim to prove this novel numerical methodology for the simulation of practical-size SOFCs, several simplifications were applied. First, no complex thermo-fluid

dynamics simulation was performed within the cell; instead, a simple mass balance was considered in the flow channel under the assumption of a constant and homogeneous temperature. Second, the variation in the oxygen concentration on the cathode side was omitted. This assumption is acceptable because practical SOFCs are usually operated with excess oxygen (air) supply to carry away the heat generated from the electrochemical reaction. Under these simplifications, the dimensions of the database constructed in this study were reduced to three; the cell temperature, the cell terminal voltage, and the hydrogen concentration at the anode surface.

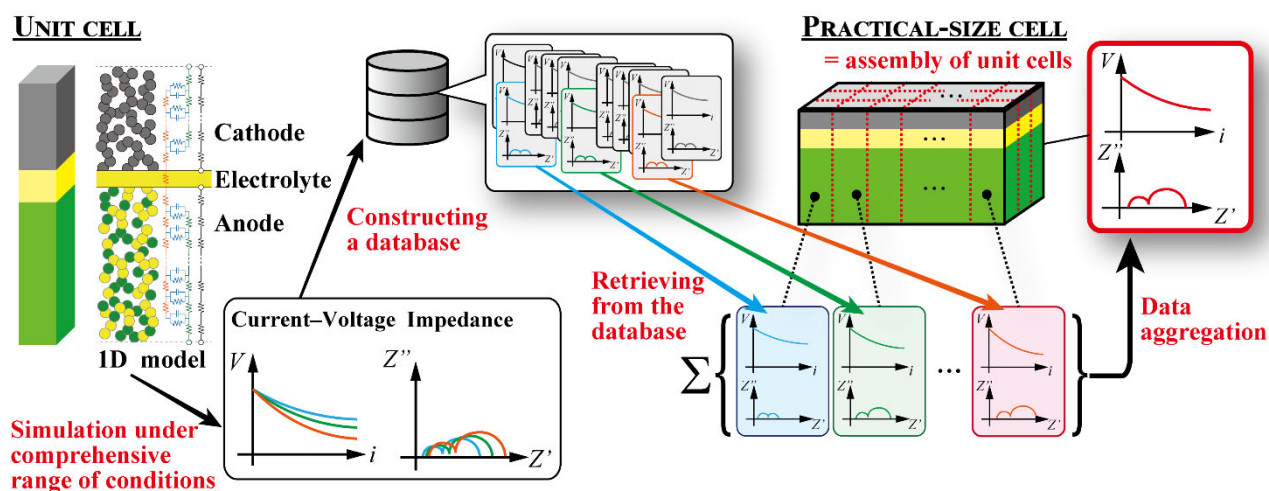


Fig. 3 Schematic flowchart of proposed methodology for predicting the electrochemical performance of practical-size SOFCs.

2.2.2 Expressions of macroscopic performance

The macroscopic characteristics of the practical-size cell were evaluated by aggregating the performance of the unit cells. Detailed expressions to correlate the macroscopic characteristics with

the local unit cell performance are explained below. First, the following equation holds in all the unit cells in Fig. 2:

$$V_t = E_i - r_i i_i. \quad (33)$$

Note that the terminal voltage is common to all the unit cells when the ideal current collectors are assumed on both electrode surfaces. By dividing eq. (33) by r_i and taking the sum of the local current density, i_i , with the apparent surface area of the unit cell, A_i , as a weight factor, the following expression can be obtained:

$$V_t = \frac{\sum \frac{A_i E_i}{r_i}}{\sum \frac{A_i}{r_i}} - \frac{\sum i_i A_i}{\sum \frac{A_i}{r_i}} = \frac{\sum \frac{A_i E_i}{r_i}}{\sum \frac{A_i}{r_i}} - \frac{\sum A_i}{\sum \frac{A_i}{r_i}} \frac{\sum i_i A_i}{\sum A_i}. \quad (34)$$

The performance of the entire cell can then be evaluated using the following formulas:

$$E_{\text{cell}} = \frac{\sum \frac{A_i E_i}{r_i}}{\sum \frac{A_i}{r_i}} \quad (35)$$

$$r_{\text{cell}} = \frac{\sum A_i}{\sum \frac{A_i}{r_i}} \quad (36)$$

$$i_{\text{cell}} = \frac{\sum i_i A_i}{\sum A_i}, \quad (37)$$

where E_{cell} , r_{cell} , and i_{cell} are the electromotive force, the area-specific resistance, and the current density of the entire cell, respectively. Similarly, the impedance of the entire cell can be obtained as

$$Z_{\text{cell}} = \frac{\sum A_i}{\sum \frac{A_i}{Z_i}}. \quad (38)$$

In addition, from the practical viewpoint, several performance measures were evaluated and discussed. Power density was defined simply as the product of terminal voltage and cell current density as

$$P_{\text{cell}} = V_t i_{\text{cell}}. \quad (39)$$

Energy conversion efficiency was evaluated as the ratio of the power output to the chemical enthalpy of the supplied fuel as

$$e = \frac{P_{\text{cell}} A_{\text{cell}}}{N_{\text{H}_2, \text{in}} \Delta H}, \quad (40)$$

where $A_{\text{cell}} = \sum A_i$ is the apparent surface area of the entire cell, $N_{\text{H}_2, \text{in}}$ is the molar flow rate of the supplied hydrogen in mol s^{-1} , and ΔH is the lower heating value of hydrogen at the standard state ($241.6 \text{ kJ mol}^{-1}$ at 0°C , 1 atm). Fuel utilization was evaluated as the ratio of the amount of fuel consumed to that of the fuel supplied as

$$U_f = \frac{i_{\text{cell}} A_{\text{cell}}}{2FN_{\text{H}_2, \text{in}}}. \quad (41)$$

3. Experimental

3.1 Cell fabrication

To validate the 1D unit cell model we developed, the predicted current–voltage and impedance characteristics were compared with those obtained from an experiment using an anode-supported button cell. The details of the fabrication of this cell are found elsewhere [55] and summarized as follows. First, 60 wt.% NiO powder (FUJIFILM Wako Pure Chemical Corp., Japan) and 40 wt.% YSZ powder (TZ-8Y, Tosoh Corp., Japan) were mixed by planetary ball milling in isopropanol with zirconia balls ($\phi 4.0 \text{ mm}$) at 300 rpm for 3 h. After evaporating the isopropanol, the resultant NiO-YSZ mixture powder was sieved with a $53 \mu\text{m}$ mesh to remove agglomerates. Then, the mixture

powder, ethanol as an organic solvent, and Triton X-100 (MP Biomedicals, LLC, U.S.A.) as a dispersant were mixed with zirconia balls (ϕ 4.0 mm) at 200 rpm for 24 h. After that, polyvinyl butyral (PVB, Mowital B60H, Kuraray Co., Ltd., Japan) as a binder and polyethylene glycol 400 (PEG 400, FUJIFILM Wako Pure Chemical Corp., Japan) and glycerin (Nacalai Tesque, Inc., Japan) as plasticizers were added and then mixed for another 24 h to form a homogenous anode slurry. To remove the dissolved gas in the slurry, the slurry was degassed under a pressure of about 0.15 atm for 10 min with magnetic stirring in a vacuum desiccator. The composition of the anode slurry is shown in Table 2.

The anode support layer was fabricated by tape-casting using the prepared anode slurry. The slurry was cast on a glass plate at a casting speed of 10 mm s⁻¹ and a blade gap of 2.0 mm. After fully drying the casted slurry at 20°C and 80%rh in a constant-temperature and constant-humidity chamber, a green tape was cut into a disk shape with a diameter of 30 mm. Finally, the disk was presintered at 1200°C for 2 h at heating and cooling rates of 200°C h⁻¹.

Table 2 Composition of NiO–YSZ anode slurry.

	Material	Weight %
Anode material	NiO	31.8
	YSZ	21.2
Solvent	Ethanol	33.8
Dispersant	Triton X-100	1.06
Binder	PVB	6.36
Plasticizer	PEG 400	2.89
	Glycerin	2.89

On top of the presintered anode disk, a YSZ electrolyte thin film was prepared by spin coating. A mixture of 10.0 wt.% YSZ powder, 0.8 wt.% PVB (Sigma-Aldrich Co., LLC, U.S.A.), and 89.2 wt.% ethanol was dropped on the anode disk and immediately spun at 3,000 rpm for 30 s; this was repeated 20 cycles. The coated anode disk was then cosintered at 1350°C for 5 h at heating and cooling rates of 120 and 200°C h⁻¹, respectively. Subsequently, a GDC (gadolinium-doped ceria) barrier layer was applied on top of the YSZ electrolyte by screen printing. A GDC ink composed of 50 wt.% GDC (GDC-10(AU), Shin-Etsu Astech Co., Ltd., Japan) and a 50 wt.% ink vehicle (VEH, Nexceris LLC, U.S.A.) were mixed by planetary ball milling at 600 rpm for 30 min. The prepared GDC ink was screen-printed on the surface of the YSZ electrolyte with a mask of 20 µm thickness and then sintered at 1250°C for 2 h.

Finally, an LSCF cathode was fabricated on the GDC barrier layer by screen printing. An LSCF ink composed of 67 wt.% LSCF powder (LSCF-6428-N, Kceracell Co., Ltd., South Korea) and a 33 wt.% ink vehicle was prepared by the same procedure as that for the GDC ink. The prepared ink was screen-printed on the surface of the GDC barrier layer with a circular mask of 60 µm thickness and 10 mm diameter, and then sintered at 950°C for 5 h.

3.2 Electrochemical characterization

The electrochemical performance of the fabricated cell was evaluated at 750°C and 800°C.

The prepared cell was held between two alumina tubes with Pyrex glass rings for gas sealing. The cell temperature was controlled by an electric furnace. 3% humidified hydrogen was supplied to the anode side, while synthetic dry air to the cathode side. Steam was added to the fuel using a bubbler. The flow rate of each gas was controlled by mass flow controllers. The total flow rate was 100 mL min⁻¹ for each electrode. A platinum mesh was used for current collection. A commercial silver ink (Nexceris, LLC, U.S.A.) was painted on the surface of each electrode to improve electrical connection. More details of the measurement system can be found elsewhere [56].

Prior to the electrochemical testing, NiO in the anode was reduced in a reducing atmosphere at 800°C for 2 h. Subsequently, the current–voltage and electrochemical impedance characteristics of the cell were measured using a Solartron Celltest System 1470E with a frequency response analyzer 1455A (Solartron Analytical, U.K.). In the impedance measurement, the amplitude of the perturbation current was 10 mA and its frequency range was from 10⁵ to 10⁻¹ Hz.

3.3 Microstructural analysis

After the electrochemical characterization, the electrode microstructure was analyzed by FIB-SEM. The cell was first impregnated with epoxy resin (EpoFix, Struers, Denmark) at 0.34 atm to enable an easier identification of the solid phases in the subsequent FIB-SEM imaging. The 3D microstructures of the anode and cathode were imaged using an NVision 40 (Carl Zeiss, Germany) FIB-SEM system. An in-lens secondary electron detector was used to distinguish the two solid

phases, i.e., Ni and YSZ in the anode, whereas a standard secondary electron detector located in the specimen chamber was used for cathode imaging. After the imaging, slice images were aligned, segmented into constituent phases, and reconstructed to 3D microstructures for quantification. In this study, the volume fraction, tortuosity factor, average particle/pore size, surface-to-volume ratio of the pore phase, TPB density, and DPB density were quantified and used for the numerical simulation. More details of the image processing procedures and quantification methods can be found elsewhere [22], [57].

4. Results and Discussion

4.1 Validation of unit cell model

To validate the 1D unit cell model we developed, the current–voltage and impedance characteristics were compared between the simulation and the experiment. The quantified electrode microstructural parameters used in the simulation are summarized in Table 3. The reconstructed structure sizes were $21.1 \times 13.0 \times 14.9 \text{ } \mu\text{m}^3$ and $15.1 \times 15.1 \times 22.3 \text{ } \mu\text{m}^3$ for the anode and cathode, respectively. The thicknesses of the anode, electrolyte, GDC barrier, and cathode layers were also measured from a 2D cross-sectional SEM image as 453, 8, 6, and 35 μm , respectively. In the numerical simulation, the thickness of the GDC barrier layer was included in the electrolyte thickness in the form of an equivalent YSZ thickness considering the ionic conductivity of the GDC phase [58] and the porosity of the barrier layer ($\sim 50\%$). In the numerical model, the tortuosity factor

of the pore phase was treated as a fitting parameter, and the value was tuned so that the simulation results agree with the experimental results.

Table 3 Microstructural parameters of electrodes of anode-supported button cell.

	Anode			Cathode	
	Ni	YSZ	Pore	LSCF	Pore
Volume fraction [–]	0.330	0.389	0.281	0.546	0.454
Tortuosity factor [–]	3.43	2.33	7.89	2.64	1.79
Average size [μm]	1.50	1.12	0.955	0.218	0.211
Surface-to-volume ratio [$\mu\text{m}^2 \mu\text{m}^{-3}$]	4.02	5.37	5.97	11.1	13.4
TPB density [$\mu\text{m} \mu\text{m}^{-3}$]		2.29			–
DPB density [$\mu\text{m}^2 \mu\text{m}^{-3}$]		–			6.07

Fig. 4 shows the current–voltage (i – V) and current–power (i – P) characteristics in the simulation and experiment at 750°C and 800°C. After calibrating the model at 750°C, the numerical results perfectly reproduce the i – V and i – P characteristics in the experiment. Fair agreement was also obtained at 800°C without further tuning the model parameters. The error in the high current densities can be attributed to the contribution of the gas diffusion in the porous anode. Although the DGM model was used in this analysis, the choice of the gas diffusion model for SOFC simulation is still an open question. The development and implementation of an accurate and robust gas diffusion model are required to further improve the accuracy of the unit cell model.

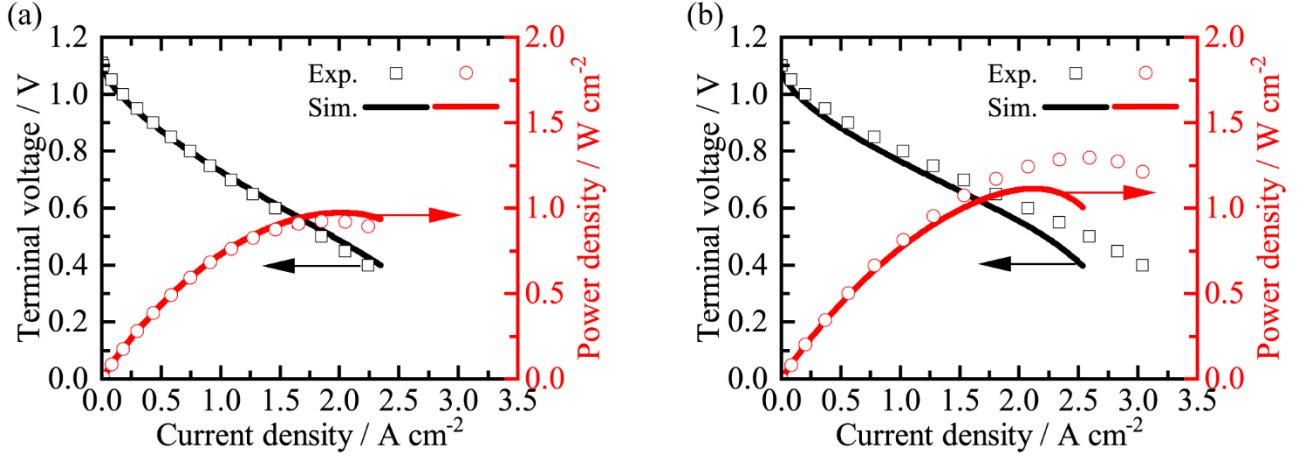


Fig. 4 i - V and i - P characteristics of anode-supported button cell in the experiment and simulation.

(a) 750°C and (b) 800°C. $H_2:H_2O = 97:3$ for the anode and $O_2:N_2 = 21:79$ for the cathode.

Fig. 5 shows the impedance characteristics in the simulation and the experiment at the open-circuit voltage at 750°C and 800°C. Almost perfect agreement was obtained in the Nyquist plot at 750°C. Two major arcs are observed in the impedance arc; the higher frequency arc can be associated with the electrochemical reaction, and the lower frequency arc with the gas diffusion mainly in the anode. Although the characteristic frequency of the lower frequency arc in the Bode plot is slightly shifted, the extent of deviation is within an acceptable range considering that the x -axis is in the logarithmic scale. Fair agreement was also obtained at 800°C without further tuning the model parameters. From the results shown in Fig. 4 and 5, the validity of the developed 1D unit cell model has been confirmed.

It should be emphasized that the developed model successfully reproduces the impedance characteristics of the entire cell; most of the works in the literature only reproduced those of an

electrode [59], [60], [61],[62]. In addition, the proposed model is thoroughly based on the physicochemical phenomena within the cell, which allows the inhomogeneous distributions of electrochemical potentials and gas compositions, and hence, those of the electrochemical and transport properties of the electrode materials. This is a distinct superiority to conventional circuit-based models, such as the transmission line model [42], which usually assume uniform material properties within the cell. In this study, the developed unit cell model is only part of the proposed methodology for predicting the performance of the practical-size SOFCs, as schematically shown in Fig. 3; however, the unit cell model itself is expected to be useful for the analysis of laboratory-scale SOFCs, such as button cells, to understand the reaction and transport phenomena occurring within the cells.

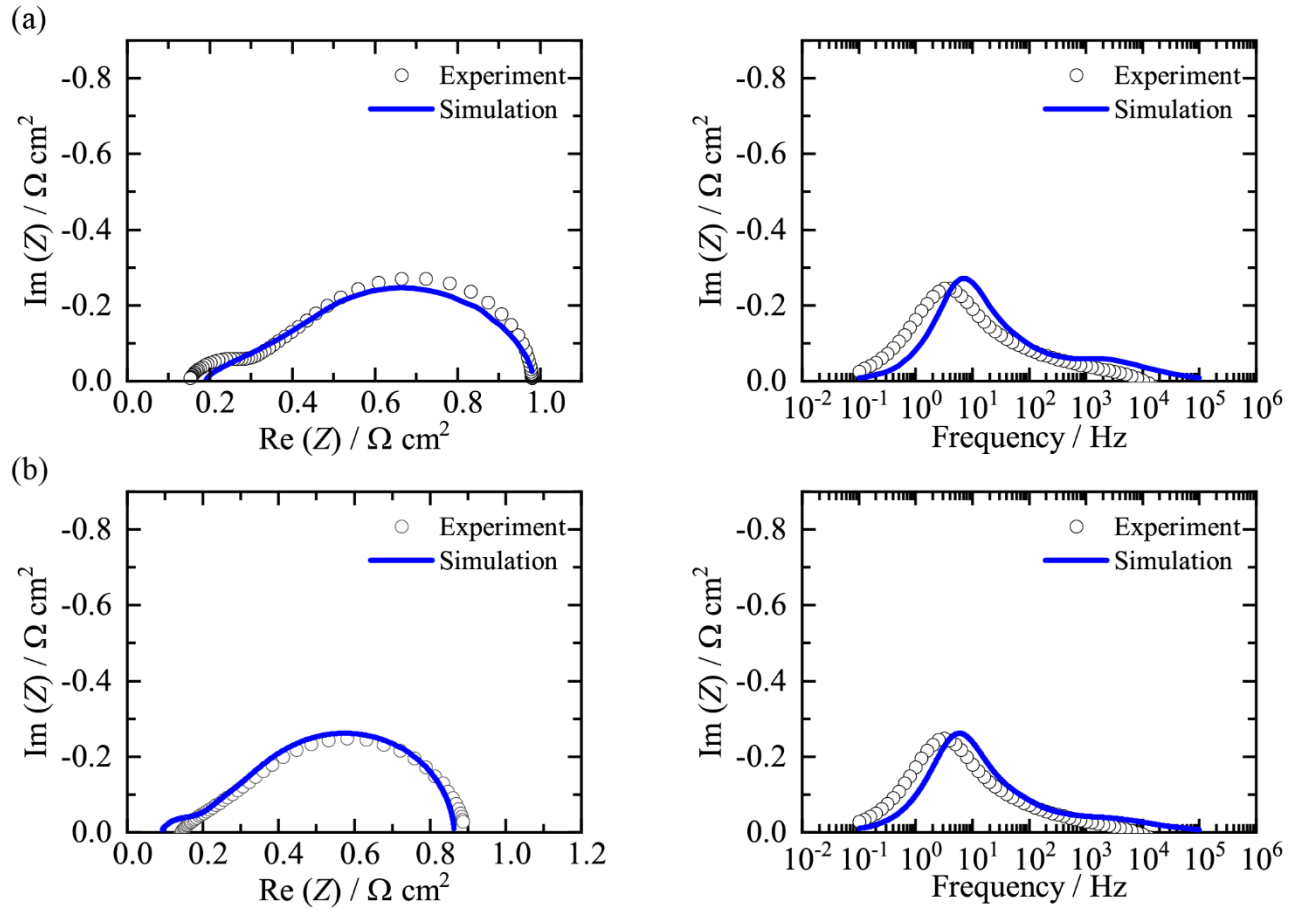


Fig. 5 Impedance spectra obtained by experiment and simulation at open-circuit voltage. (a) 750°C and (b) 800°C. $\text{H}_2:\text{H}_2\text{O} = 97:3$ for anode and $\text{O}_2:\text{N}_2 = 21:79$ for cathode.

4.2 Validation of practical-size cell model

By using the validated 1D unit cell model, we predicted the electrochemical performance of a practical-size cell. The experimental values of the current–voltage and impedance characteristics reported by Comminges et al. [63] were used for the validation of the proposed methodology. Since microstructural parameters of the electrodes used in their study were not reported, parameters found in another report [64], in which a similar cell provided by SOLIDpower S.p.A. (Italy) was analyzed in three dimensions by FIB-SEM, were alternatively used in this study. The reported microstructural

parameters are summarized in Table 4. The cell consists of a Ni-YSZ anode, a YSZ electrolyte, an LSCF-GDC cathode function layer, and an LSCF cathode current collection layer, whose thicknesses are 240, 9, 15, and 35 μm , respectively. Note that the GDC phase in the cathode function layer was assumed to act only as a catalyst for the electrochemical reaction by forming TPBs; hence, it does not contribute to the electron and ion conduction in the cathode. In the experimental work by Comminges et al. [63], a short stack consisting of five cells was used in the experiment and the electrochemical performance of each cell was measured. In this study, the performance of the cell located at the middle of the short stack was used for comparison. Since the cathode material in ref. [63] was not LSCF but an LSCF–GDC composite in the function layer, the electrochemical reaction model described by the following Butler–Volmer-type equation was alternatively used [65] instead of eq. (22) and (28).

$$i_{ct,cat} = i_{0,TPB,cat} l_{TPB,cat} \left[\exp\left(\frac{2F}{RT} \eta_{act,cat}\right) - \exp\left(-\frac{2F}{RT} \eta_{act,cat}\right) \right] \quad (42)$$

$$i_{0,TPB,cat} = 3.23 \times 10^{-2} P_{O_2}^{0.2} \exp\left(-\frac{8.59 \times 10^4}{RT}\right) \quad (43)$$

Table 4 Microstructural parameters of electrodes in practical-size cell in ref. [64].

	Anode			Cathode				
	Ni	YSZ	Pore	Function layer		Collection layer		
				LSCF	GDC	Pore	LSCF	Pore
Volume fraction [–]	0.28	0.44	0.28	0.33	0.26	0.41	0.59	0.41
Tortuosity factor [–]	15.0	2.27	7.99	4.85	21.9	2.32	2.11	2.45
Average size [μm]	1.12	0.92	1.01	1.17	0.92	1.01	0.92	1.01
Surface-to-volume ratio [$\mu\text{m}^2 \mu\text{m}^{-3}$]	5.01	5.24	6.64	4.94	5.61	4.50	3.74	6.24
TPB density [$\mu\text{m} \mu\text{m}^{-3}$]		3.63			3.36			–

To reproduce the results in the experiment, a performance database was first constructed by 1D unit cell simulation using the microstructural parameters in Table 4. The temperature was set at 800°C. The hydrogen concentration in the fuel was from 5% to 95% with 5% interval, and also 97%. The terminal voltage was at 1.0, 0.9, 0.8 and 0.7 V. Subsequently, the electrochemical characteristics of the entire cell were predicted using the proposed methodology. The inlet fuel composition was 3% humidified hydrogen and the cell temperature was assumed to be uniform at 800°C.

Fig. 6 shows the i - V and i - P characteristics in the simulation and experiment. Although there is a small deviation in the high current density range, good agreement is obtained. Fig. 7 shows the impedance characteristics in the simulation and experiment. Similarly, fair agreement was achieved in both the Nyquist and Bode plots. Although there is an error in the relative location of the impedance arcs in the Nyquist plot, the size of the entire arc is well reproduced by the simulation. The error in the relative location of the arc may be due to the ohmic resistance of the separators in the short stack and the contact resistance between the stack components, which were not taken into account in the numerical model. When taking a closer look at the size of the entire impedance arc predicted by numerical simulation, it is slightly larger than that obtained in the experiment, which is possibly because the temperature of the cell in the experiment was higher than that set for an electric furnace. The temperature in the middle of the short stack is expected to be higher than 800°C because of the exothermic electrochemical reaction in the stack. Overall, we confirmed that the

proposed methodology can reproduce the trends in the experiment within an acceptable range of errors. Further validation with a comprehensive dataset of experimental and microstructure data will be performed in our future study.

To the best of our knowledge, this is the first study in which the impedance spectra of a practical-size SOFC having a non-uniform distribution of the gas compositions on the electrode surface are reproduced by numerical simulation. This was realized because the proposed methodology can significantly reduce the computational time for the analysis. The same methodology can be applied to the numerical analysis of SOFC stacks consisting of multiple practical-size cells, and this will also be our future study.

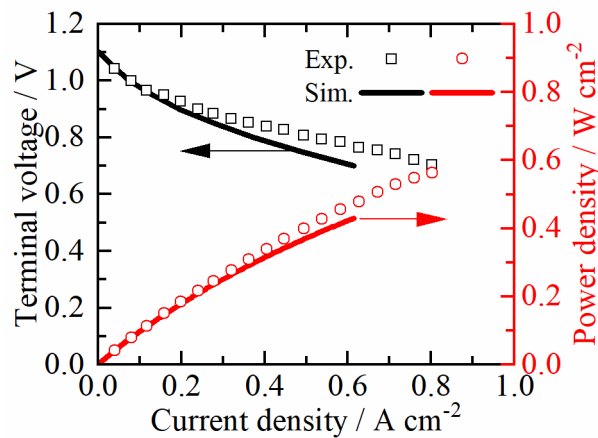


Fig. 6 i - V and i - P characteristics of practical-size cell obtained by simulation and experiment [63]

at 800°C.

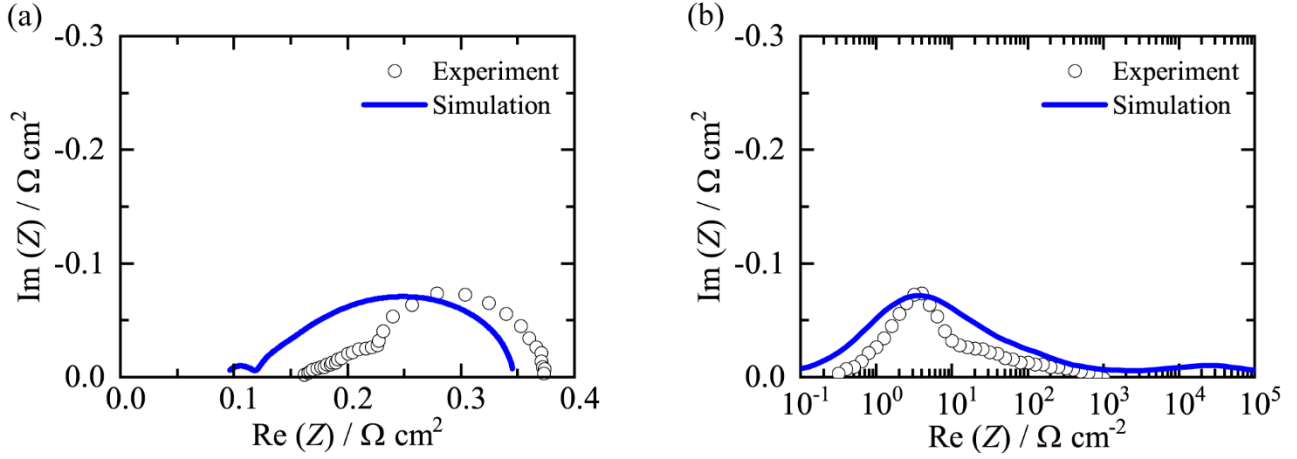


Fig. 7 Impedance characteristics of practical-size cell obtained by simulation and experiment [63] at 800°C and 0.8 V. (a) Nyquist and (b) Bode plots.

4.3 Prediction of practical-size cell performance

On the basis of the proposed methodology, the macroscopic performance of a practical-size cell was predicted under various operating conditions determined by the terminal voltage and fuel utilization. The terminal voltage was set at 0.9, 0.8, 0.7, and 0.6 V, and the fuel utilization was up to 90%. The size of the cell was assumed to be 10×10 cm². The inlet composition was 3% humidified hydrogen on the anode side and dry air on the cathode side. The cell temperature was assumed to be constant and uniform at 800°C. The microstructural parameters in Table 3 were used for the electrodes. To construct the unit cell performance database, 1D numerical simulation was performed at the terminal voltage of 0.9, 0.8, 0.7, and 0.6 V, with the hydrogen concentration from 5% to 95% with 5% interval and also 97% at 800°C.

Fig. 8 shows the relationships between the energy conversion efficiency and the output power

density at several terminal voltages. The inlet fuel flow rate was varied to adjust the fuel utilization. Note that the dotted lines in the graph indicate the isolines that connect the operating points with the same fuel utilization. The results indicate the following: (i) when fuel utilization is increased at a constant terminal voltage by decreasing the inlet flow rate, the conversion efficiency can be improved by sacrificing the output power density. (ii) At the same fuel utilization, the output power density can be increased by lowering the terminal voltage, which however decreases the conversion efficiency. (iii) When the terminal voltage is low (0.6 V in this analysis), the line is flattened in the low flow rate region; hence, high conversion efficiency cannot be achieved.

These findings mentioned above are rather intuitive; however, it should be emphasized that such a parametric study is practically difficult in conventional numerical simulation approaches owing to their heavy computation load. In comparison, the computation time required for the numerical analysis of a practical-size cell using eq. (35) – (38) is within ten seconds because there are no iterative processes involved; instead, the local performance of the unit cells is successively determined from the upstream of the cell by referring to the database, and the overall cell characteristics are evaluated as their simple weighed averages. Of course, some amount of time is required to construct the unit cell performance database, the computational load is relatively low because each 1D unit cell simulation is decoupled from the thermo-fluid simulation. This advantage on the computation load will become more significant when exhaustive parametric studies, such as those that provide results shown in Fig. 8, are performed on practical-size cells.

Additionally, the derived expressions of the macroscopic performance of a practical-size cell in eq. (35) – (38) are expected to be useful for evaluating the state-of-the-art electrode materials in the development stage. Once the electrode/cell performance is evaluated in a button-cell configuration under a comprehensive range of operating conditions, the macroscopic performance of the electrode/cell in a practical scale can be easily predicted by aggregating the experimental data.

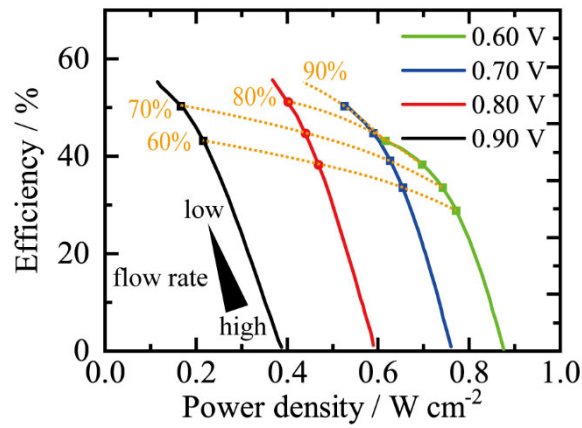


Fig. 8 Macroscopic characteristics of practical-size cell. Each solid line represents the relationship between energy conversion efficiency and output power density at a constant terminal voltage. The dotted lines are the isolines connecting points having the same fuel utilization.

5. Conclusions

A novel numerical methodology for predicting the macroscopic characteristics of practical-size SOFCs has been proposed and verified. The core idea is to express the characteristics of a practical-size cell as an aggregation of the performance of unit cells. The proposed methodology

consists of two steps. The first is to construct a database of the electrochemical performance of a 1D unit cell under a comprehensive range of operating conditions. For this purpose, a 1D numerical simulation model has been developed and validated by comparing the simulation results with the corresponding experimental data obtained from an anode-supported button cell. It has been confirmed that not only the current–voltage characteristics but also the impedance characteristics are accurately reproduced by the developed unit cell model. The second is to reproduce the practical-size cell characteristics using the constructed database. The cell is divided into several unit cells and their electrochemical performance is determined by referring to the constructed database. The macroscopic characteristics of the entire cell are estimated by using the derived theoretical expressions correlating the macroscopic cell characteristics with the local electrochemical performance. The predicted cell characteristics fairly agree with the experimental data in the literature. It should be emphasized that the impedance spectra of a practical-size cell having a non-uniform distribution of the gas compositions on the electrode surface are reasonably reproduced by numerical simulation for the first time.

The proposed method is used to perform a comprehensive parametric study of a practical-size SOFC single cell to predict its macroscopic characteristics and its dependence on the operating conditions. The correlation among the conversion efficiency, power density, and fuel utilization of the cell is analyzed. Such an exhaustive parametric study can only be executed with the proposed numerical methodology considering the realistic computational resources.

Note that this is a proof-of-concept study; therefore, rather strict assumptions were applied: a homogeneous cell temperature and constant oxygen concentration on the cathode surface. These limit the dimensions of the database. A more accurate prediction of the practical-size cell/stack performance may require the analysis of flow dynamics and heat transfer within the cell/stack to evaluate local gas composition and temperature, which will be our future study.

Acknowledgments

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Nomenclature

A_{cell}	apparent surface area of the entire cell	$[\text{m}^2]$
A_{DPB}	double-phase boundary density	$[\text{m}^{-1}]$
A_i	apparent surface area of a unit cell	$[\text{m}^2]$
A_δ	thermodynamic factor	$[-]$
c	electrostatic capacitance	$[\text{F m}^{-3}]$
$c_{\text{Ni-YSZ}}$	electrostatic capacitance per unit Ni-YSZ interfacial area	$[\text{F m}^{-2}]$
$\tilde{D}$	chemical diffusion coefficient	$[\text{m}^2 \text{s}^{-1}]$
D_{ij}	molecular diffusivity	$[\text{m}^2 \text{s}^{-1}]$
$D_{i,K}$	Knudsen diffusivity	$[\text{m}^2 \text{s}^{-1}]$
d_{pore}	mean pore diameter	$[\text{m}]$
E_{cell}	electromotive force of the entire cell	$[\text{V}]$
E_i	electromotive force of a unit cell	$[\text{V}]$
F	Faraday constant	$[\text{C mol}^{-1}]$
f	frequency	$[\text{s}^{-1}]$
ΔG	Gibbs free energy	$[\text{J mol}^{-1}]$
ΔH	lower heating value of hydrogen	$[\text{J mol}^{-1}]$
i_{cell}	area-specific current density of the entire cell	$[\text{A m}^{-2}]$
i_{ct}	charge-transfer current density	$[\text{A m}^{-3}]$

i_i	area-specific current density of a unit cell	$[\text{A m}^{-2}]$
$i_{0,\text{TPB}}$	exchange current per unit TPB length	$[\text{A m}^{-1}]$
$i_{0,\text{DPB}}$	exchange current per unit DPB area	$[\text{A m}^{-2}]$
j	imaginary unit	$[-]$
K	permeability	$[\text{m}^2]$
l_{TPB}	TPB density	$[\text{m}^{-2}]$
M_i	molar mass	$[\text{kg mol}^{-1}]$
$N_{\text{H}_2,\text{in}}$	inlet molar flow rate of hydrogen	$[\text{mol m}^{-2} \text{ s}^{-1}]$
N_i	molar flux	$[\text{mol m}^{-2} \text{ s}^{-1}]$
P_{cell}	output power density	$[\text{W m}^{-2}]$
P_i	partial pressure	$[\text{Pa}]$
P_t	total pressure	$[\text{Pa}]$
R	gas constant	$[\text{J mol}^{-1} \text{ K}^{-1}]$
r_{cell}	area-specific resistance of the entire cell	$[\Omega \text{ m}^2]$
r_i	area-specific resistance of a unit cell	$[\Omega \text{ m}^2]$
$(S/V)_{\text{pore}}$	surface-to-volume ratio of pore phase	$[\text{m}^{-1}]$
$\dot{s}_i$	sink/source term	$[\text{mol m}^{-3} \text{ s}^{-1}]$
T	temperature	$[\text{K}]$
U_f	fuel utilization	$[-]$

V_{LSCF}	volume fraction of LSCF phase	[-]
V_m	molar volume	[m ³ mol ⁻¹]
V_{Pore}	porosity	[-]
V_t	terminal voltage	[V]
$\sum v_i$	diffusion volume	[m ³]
X_i	molar fraction	[-]
Z_{cell}	area-specific impedance of the entire cell	[Ω m ²]
Z_i	area-specific impedance of a unit cell	[Ω m ²]

Greek symbols

δ	oxygen nonstoichiometry	[-]
η_{act}	activation overpotential	[V]
η_{con}	concentration overpotential	[V]
η_p	overpotential amplitude	[V]
θ	period	[s]
μ	viscosity	[Pa s]
$\tilde{\mu}$	electrochemical potential	[J mol ⁻¹]
σ	conductivity	[S m ⁻¹]
τ_{Pore}	tortuosity factor of pore phase	[-]
ω	angular velocity	[s ⁻¹]

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