Development of a Quasi 2-D Modeling of Tubular Solid-Oxide Fuel Cell for Real-Time Control

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Abstract—This paper presents the modeling approach for a quasi-2-D tubular anode-supported solid-oxide fuel cell (SOFC) for real-time control implementation. The proposed system considers a multidomain electrochemical, fluidic, and thermal dynamic modeling and it is experimentally validated against a SOFC real world implementation. Implicit iterative algebraic equations have been introduced and implemented in C language in order to have fast real-time execution. The methodology for implementing such an iterative solver is discussed in details and the results demonstrate practical feasibilities in advancing real-time control of SOFC

Index Terms—Algorithm development, control, modeling, real-time, solid-oxide fuel cell (SOFC).

I. INTRODUCTION

SOLID-OXIDE fuel cells (SOFC) have been considered a successful commercial deployment for power applications since first deployed [1]. They have high energy efficiency, are considered environmental-friendly, and are praised to have a lot of potential as an energy conversion solution for distributed energy applications.

The SOFC electrode and electrolyte is made of solid ceramic materials capable to withstand very high temperature (typically 800°C–1000°C). The ceramic material properties and the cell cell operating conditions, such as electrode porosity, electrode thickness, reactant partial pressures, and cell temperature, have a tremendous impact on the SOFC operating performance. Because of such high temperature, it is very difficult to install electronics and monitor internal variables, therefore, the use of an accurate SOFC model for a model based fuel cell real-time controller can be very useful to achieve optimal operating conditions.

The challenges for achieving SOFC dynamic modeling with a model-based-control have been presented in the literature [1]. In order to consider physical quantities (temperature, current density) gradients in a model based control process, a real-time multidimensional model must be used. Although several SOFC or PEMFC models have been presented in the literature [2]–[13], they are not really sophisticated, because they are valid only for 0-D considerations. A model based SOFC controller has been designed in [14], but the developed model remains in 0-D. The importance of pressure and current gradient consideration in a control process has been mentioned in [4], but no further work has been developed. Multidimensional SOFC physical models have been studied in the literature [15]–[29]. But, those models are not suitable for real-time simulation, because of their mathematical complexity or being dependent of proprietary commercial software solutions. Model reduction methods such as local linearization [22], [23], or order-reduction [20] for control use have also been proposed, but those approaches are valid only about a linearized operating point. Neural network based fuel cell models for control purpose have been presented in [30], [31], showing interests for dynamic control, but eventually departing for real physical phenomenon that allows physical calibration with experimental data. In addition, some simplified SOFC models have also been used in the evaluation of SOFC power plant control [32], [33]. The authors of this paper thoroughly studied the state-of-art and found that, even the non-real-time multidimensional SOFC models have been commonly presented in the literature, the real-time oriented physical model considering current density distribution have not been explored so far.

The main objective of this paper is to present a dynamic quasi-2-D multiphysical SOFC (electrochemical, fluidic, and thermal) model that can be used directly for real-time applications. Therefore, the developed model can predict the multidimensional performance of SOFC while being executed under milliseconds time range. In addition, this paper presents a detailed implementation of algorithm with analysis of sampling time and CPU running time in order to validate it for the real-time control performance.

The iterative solver algorithm presented in this paper is original, it is a novel contribution in resolving the current density of a given control volume under different operation conditions in real-time. The proposed solver is not dependent of any platform, it is also agnostic to any proprietary commercial software and it can be implemented or retrofit to any embedded controller of SOFC systems.

II. SOLID-OXIDE FUEL CELL MODELING

This section presents a thermal dynamic, anode supported model for a high temperature tubular solid-oxide fuel cell.

A. Electrochemical Domain Modeling

The fuel cell output voltage is described by the following equation:

$$\eta_{\text{cell}} = E_{\text{EMF}} - \eta_{\text{act,C}} - \eta_{\text{act,A}} - \eta_{\text{ohm}}$$

(1)
where $E_{\text{EMF}}$ is the cell thermodynamic reversible voltage (V), $\eta_{\text{ohm}}$ is the cell ohmic losses (V), and $\eta_{\text{act, c}}, \eta_{\text{act, A}}$ are the cell activation losses (V) of the cathode and the anode side, respectively.

It should be noted that, the voltage losses due to the gas transport phenomena through electrodes, generally known as "concentration losses", are implicitly taken into account in the fluidic domain modeling by (23). Because the gas pressures used in (2)-(5) are the ones at catalyst sites of the reactants.

1) **EMF Voltage**: The cell reversible voltage is defined by the Nernst equation as a function of the Gibbs free energy change during the electrochemical reaction:

$$E_{\text{EMF}} = -\frac{\Delta G^0}{2F} + \frac{R \cdot T}{2F} \ln \left( \frac{P_{H_2} \cdot \sqrt{P_{O_2}}}{P_{H_2O}} \right)$$

where $\Delta G^0$ is the Gibbs free energy change from reactants to products (J/mol), $F = 96485.3$ is the Faraday constant (C/mol), $R = 8.314$ is the gas constant (J/(mol·K)), $T$ is the temperature (K) and $P_{H_2}, P_{O_2}, P_{H_2O}$ are the reacting gas pressures (atm) of hydrogen, oxygen, and vapor, respectively.

2) **Activation Losses**: The activation losses in the cell are expressed by the Butler–Volmer equation:

$$i = A_{el} \cdot j_0 \left( e^{\frac{\alpha \cdot \Delta G^0}{F \cdot T}} \cdot \gamma_{\text{act}} - e^{\frac{(1 - \alpha) \cdot \Delta G^0}{F \cdot T}} \cdot \gamma_{\text{act}} \right)$$

where $i$ is the cell electrical current (A), $A_{el}$ is the electrode area ($m^2$), $j_0$ is the exchange current density ($A/m^2$) at the cathode or the anode side, $\eta_{\text{act}}$ is the corresponding activation losses (V) at the cathode or the anode, $\alpha = 0.5$ is the symmetry factor, and $n_e = 4$ or 2 are the number of electrons involved in the half reactions of the cathode or the anode, respectively.

The cathode and the anode exchange current density equations for a typical SOFC are given by the following equations [34]:

$$j_{0, C} = \gamma_{C} \cdot P_{O_2}^{0.25} \cdot e^{-\frac{E_C}{RT}}$$

$$j_{0, A} = \gamma_{A} \cdot P_{H_2} \cdot P_{H_2O} \cdot e^{-\frac{E_A}{RT}}$$

where $P_{(\text{specie})}$ is the pressure (atm) of the corresponding specie, $E_C$ and $E_A$ are the activation energies (J/mol) at the cathode and the anode, respectively, $\gamma_{C}, \gamma_{A}$ are two empirical parameters ($A/m^2$) for the cathode and the anode, respectively, that should be adjusted from experimental tests.

3) **Ohmic Loss**: In SOFCs, the Yttria-Stabilized Zirconia (YSZ) membrane (electrolyte) electrical conductivity $\sigma_{YSZ}$ (S/m) can be calculated from [23]:

$$\sigma_{YSZ} = \sigma_0 \cdot e^{-\frac{E_{YSZ}}{RT}}$$

where $\sigma_0$ is the reference YSZ conductivity (S·K/m) and $E_{YSZ}$ is the YSZ membrane electrolyte activation energy (J/mol).

Thus, the ohmic losses can be obtained:

$$\eta_{\text{ohm}} = \frac{i \cdot \delta_{\text{mem}}}{A_{\text{mem}} \cdot \sigma_{YSZ}}$$

where $\delta_{\text{mem}}$ is the membrane thickness (m) and $A_{\text{mem}}$ is the membrane area ($m^2$).

### B. Fluidic Domain Modeling

The modeled SOFC cell has a tubular anode support structure.

The mixed-gas fuel ($H_2, H_2O, and Ar$) flows into the cell’s inner tube channel (anode) and the preheated air is supplied to the cell’s outer area (cathode). The presence of argon gas (Ar) is used to adjust the $H_2$ and $H_2O$ molar fraction supplied to the cell while conserving the constant inlet mixed-gas pressure and the molar flow rate.

1) **Anode Fuel Channel**: Assuming a segment of fuel channel as a fluidic control volume at the temperature $T_{ch}$ (K), the inlet-in-channel pressure $P_{in, ch}$ (Pa) of the inlet mixed-gas flow should be calculated at first according to the perfect gas law:

$$P_{in, ch} = \frac{T_{ch}}{T_{in}} P_{in}$$

where $P_{in}$ is the inlet gas pressure (Pa) before flowing into channel and $T_{in}$ is the inlet gas temperature (K).

From the fundamental law of mass conservation, the relations between the inlet gas and outlet gas flow rate can be obtained:

$$q_{H_2, in} = q_{in} \cdot X_{H_2, in}$$

$$q_{H_2O, in} = q_{in} \cdot X_{H_2O, in}$$

$$q_{Ar, in} = q_{in} \cdot X_{Ar, in}$$

$$q_{H_2, out} = q_{H_2, in} - \frac{i}{2F}$$

$$q_{H_2O, out} = q_{H_2O, in} + \frac{i}{2F}$$

$$q_{Ar, out} = q_{Ar, in}$$

$$q_{out} = q_{H_2, out} + q_{H_2O, out} + q_{Ar, out}$$

where $q_{in}$ and $q_{out}$ are the inlet and outlet mixed-gas molar flow rates (mol/s), respectively, $X_{(\text{specie})}$ in is the inlet molar fraction of one gas specie and $q_{(\text{specie})}, in, q_{(\text{specie})}, out$ are the corresponding species inlet and outlet molar flow rates (mol/s), respectively. The argon gas is not involved into the electrochemical reaction.

The mixed-gas pressure drop $\Delta P$ (Pa) through the channel tube can be modeled using the Darcy–Weisbach equation [35]:

$$\Delta P = \frac{32 \cdot \mu_{\text{gas}} \cdot L_{ch} \cdot k_{\text{gas}}}{D_{ch}^2}$$

where $\mu_{\text{gas}}$ is the mixed-gas viscosity (Pa·s), $k_{\text{gas}}$ is the mixed-gas velocity in the channel (m/s), $L_{ch}$ is the channel length (m), and $D_{ch}$ is the channel tube diameter (m).

Assuming ideal gas conditions, the mixed-gas velocity in the channel can be obtained from the channel mixed-gas molar flow rate $q_{\text{gas}}$ (mol/s), the mixed-gas average molar mass $M_{\text{gas}}$ (kg/mol), the mixed-gas average density $\rho_{\text{gas}}$ (kg/m$^3$), and the channel diameter $D_{ch}$ (m):

$$k_{\text{gas}} = \frac{4 \cdot q_{\text{gas}} \cdot M_{\text{gas}}}{\pi \cdot \rho_{\text{gas}} \cdot D_{ch}^2}.$$
The hydrogen and vapor pressure in the channel can be also calculated:

\[
\begin{align*}
P_{H_2,ch} &= X_{H_2,ch} \cdot P_{ch} \\
P_{H_2O,ch} &= X_{H_2O,ch} \cdot P_{ch}
\end{align*}
\] (18)

2) Gas Diffusion Layers (GDL or Electrode): The \( H_2, H_2O, \) and \( O_2 \) molar flow rates (mol/s) through the gas diffusion layer can be calculated from the cell current \( i \) (A):

\[
\begin{align*}
q_{H_2,GDL} &= \frac{i}{2F} \\
q_{H_2O,GDL} &= -\frac{i}{2F} \\
q_{O_2,GDL} &= \frac{i}{4F}
\end{align*}
\] (20)

The individual gas pressure variation through the gas diffusion layer can be expressed from the modified Fick diffusion law:

\[
P_{ch} - P_{cata} = \frac{q_{sp,GDL} \cdot \delta_{GDL} \cdot R \cdot T}{D_{sp-GDL,eff} \cdot A_{GDL}}
\] (23)

where \( D_{sp-GDL,eff} \) is the gas effective diffusion coefficient to other gas through the porous gas diffusion layer (m\(^2\)/s), \( P_{cata} \) is the gas pressure in the catalyst sites (Pa), \( \delta_{GDL} \) is the gas diffusion layer thickness (m), and \( A_{GDL} \) is the gas diffusion layer area (m\(^2\)).

The effective gas diffusion coefficients can be obtained using the Slattery–Bird formula [35], [36] and the Bruggemann correction:

\[
D_{sp-GDL,eff} = D_{sp-GDL} \cdot \varepsilon^\tau
\] (24)

where \( D_{sp-GDL} \) is the binary gas diffusion coefficient (m\(^2\)/s) given in the references [35] and [36], between hydrogen and vapor in an argon environment (inert gas) at the anode side, and between oxygen and nitrogen at the cathode side. \( \varepsilon \) is the corresponding gas diffusion layer porosity, and \( \tau \) is corresponding gas diffusion layer tortuosity.

3) Cathode Air Side: Based on the cell configuration, the preheated air at cathode side is assumed to have a uniform gas pressure distribution equal to the cathode operating pressure. The \( O_2 \) molar fraction in the preheated air is assumed to be constant and equal to 20.9%.

C. Thermal Domain Dynamic Modeling

In the radial direction, the tubular SOFC cell is divided radially by four thermal control volumes: cathode gas diffusion layer, YSZ membrane electrolyte, anode gas diffusion layer, and anode gas channel. In the axial direction, the cell is divided into \( N \) identical thermal control volumes.

1) Solid Material: Cathode, Anode GDL, and Electrolyte: The dynamic energy conservation equation in one thermal control volume of solid material layers is given as follows:

\[
\rho_{CV} V_{CV} C_{CV} \frac{dT_{CV}}{dt} = Q_{cont} + Q_{fc} + Q_m + Q_{int}
\] (25)

where \( \rho_{CV} \) is the solid material control volume density (kg/m\(^3\)), \( V_{CV} \) is the volume (m\(^3\)), \( C_{CV} \) is the thermal capacity (J/(kg K)), \( T_{CV} \) is the control volume temperature (K), \( Q_{cont} \) is the conduction heat flow (J/s), \( Q_{fc} \) is the forced convection heat flow (J/s), \( Q_m \) is the convective mass energy flow (J/s), and \( Q_{int} \) is the internal heat sources in the corresponding control volume (J/s).

The conduction heat flow in the solid material control volume is due to the contact in both axial and radial directions between the adjacent thermal control volumes; which can be modeled by:

\[
Q_{cd} = \lambda_{CV} \sum \frac{A_{cont}}{\delta_{CV}} (T_{adj} - T_{CV})
\] (26)

where \( \lambda_{CV} \) is the layer thermal conductivity (W/(m K)), \( A_{cont} \) is the contact area with adjacent thermal control volume (m\(^2\)) in axial and radial directions, \( \delta_{CV} \) is the thickness (m), and \( T_{adj}, T_{CV} \) are, respectively, the temperature (K) of the adjacent and current thermal control volume.

The forced convection heat flow is due to the heat exchange between the forced gas flow through the fuel channel and the cell tube inner surface. The Newton cooling law is used here to describe this phenomenon:

\[
Q_{fc} = h_{fc} \cdot A_{inner} (T_{CV,ch} - T_{CV})
\] (27)

where \( h_{fc} \) is the forced convection coefficient (W/(m\(^2\) K)) in the tube channel, \( A_{inner} \) the tube inner area (m\(^2\)), and \( T_{CV,ch} \) the anode channel thermal control volume temperature (K).

The expression of \( h_{fc} \) can be obtained as follows:

\[
h_{fc} = \frac{N_{u} \cdot \lambda_{gas}}{D_{ch}}
\] (28)

where \( N_{u} \) is the Nusselt number in circular tube and \( \lambda_{gas} \) is the mixed-gas average thermal conductivity (W/(m K)).

The convective mass energy flow is due to the gas species at different temperatures flowing into and out of the thermal control volume in both radial and axial directions. This flow can be expressed as:

\[
Q_m = \sum_{species} q_{sp} M_{sp} C_{sp} (T_{sp,flowin} - T_{CV})
\] (29)

where \( C_{sp} \) is the gas species thermal capacity (J/(kg K)).

The internal heat sources in the different solid material layers of SOFC are due to different phenomena: resistive losses, activation losses, and irreversible electrochemical process. These sources can be expressed as follow:

\[
\begin{align*}
\text{Cathode} : Q_{int} &= i \cdot \eta_{act,C} \\
\text{Anode} : Q_{int} &= i \cdot \eta_{act,A} - i \cdot \frac{T \cdot \Delta S^0}{2F} \\
\text{Electrolyte} : Q_{int} &= i \cdot \eta_{ohm}
\end{align*}
\] (30)

where \( \Delta S^0 \) is the entropy change (J/(mol K)) during the electrochemical reaction.

2) Anode Gas Channel: The energy conservation equation for the anode gas channel can be described as below:

\[
\rho_{gas} V_{CV,ch} C_{gas} \frac{dT_{CV,ch}}{dt} = Q_{fc} + Q_m
\] (33)
where \( C_{\text{gas}} \) is the mixed-gas average thermal capacity (J/(kg·K)), \( V_{\text{CV, ch}} \) is the channel tube thermal control volume (m\(^3\)), \( T_{\text{CV, ch}} \) is the channel temperature (K), \( Q_{\text{fc}} \) is the forced convection heat flow (J/s), and \( Q_{\text{m}} \) is the convective mass energy flow (J/s). The forced convection heat flow can be obtained from (27) with an opposite sign.

The convective mass energy flow in the anode tube channel should consider the mass flows in both radial and axial directions:

\[
Q_{\text{m}} = q_{\text{gas}} M_{\text{gas}} C_{\text{gas}} (T_{\text{prev, ch}} - T_{\text{CV, ch}}) + \sum_{\text{GDL}} q_{\text{sp}} M_{\text{sp}} C_{\text{sp}} (T_{\text{GDL, A}} - T_{\text{CV, ch}}) \quad (34)
\]

where the first term represents the convective mass energy flow of mixed-gas from previous axial channel control volume, the second term represents the radial convective mass energy flow to the anode GDL for electrochemical reaction.

3) Cathode Air Side: In the present SOFC model, based on the cell configurations, the air at cathode side of the cell is assumed to have a uniform and constant temperature distribution.

III. MODEL IMPLEMENTATION

A. Two Dimensional Considerations

A quasi-2-D model can be implemented with the physical equations presented in the previous section. Fig. 1 depicts the main features to be considered. The two main axial and radial dimensions are considered for this model. In the radial direction, four control volumes can be distinguished: 1) anode tubular channel; 2) anode GDL; 3) YSZ membrane electrolyte, and 4) cathode GDL. In axial direction, the tube is divided into \( N \) segments (control volumes) in order to investigate the axial distribution of current density, gas pressures, and so on. Each segment in axial direction has the same geometry and material properties.

B. Iterative Current Density Solver

The main simulation requirement for this quasi-2-D SOFC model is to determine the radical electrical current \( i_{\text{seg, n}} \) in each segment of the axial direction and the cell output voltage \( \eta_{\text{cell}} \). Two boundary conditions are known:

1) The electrical potentials \( \eta \) from (1) of each segment are the same:

\[
\eta_{\text{cell}} = \eta_{\text{seg, n}} \quad \text{for } n = 1 \text{ to } N. \quad (35)
\]

2) The total cell current \( i \) (known) is equal to the sum of the current in each segment:

\[
i = \sum_{n=1}^{N} i_{\text{seg, n}} \quad (36)
\]

where \( N \) is the segment number in axial direction, \( i_{\text{seg, n}} \) and \( \eta_{\text{seg, n}} \) are, respectively, current and voltage of each segment.

The current of each segment and cell potential (output voltage) cannot be calculated explicitly \( a \ p r i o r i \). Thus, an iterative method should be developed.

In addition, the activation loss \( \eta_{\text{act}} \) in the Butler–Volmer equation (equation (3)) shows as an implicit form. In order to calculate the cathode and anode activation losses, an iterative method should also be used.

The details of the solver algorithm are presented by the following flowcharts (see Figs. 2–Fig. 4).

The solver level 0 is the top level solver, from the known cell current \( i_{\text{real}} \), the solver uses an iterative method to compute both cell voltage (potential) and individual segment current. A second level solver (level 1) is included in the algorithm, in order to resolve each segment current from an estimated cell voltage.

The solver level 1 is used to calculate the individual segment current from a given cell potential value. In order to calculate the anode and cathode activation losses from the implicit Butler–Volmer equation (3), a third level (level 2) iterative solver has been used.

The solver level 2 is used to calculate both anode and cathode activation losses using the same iterative algorithm.
Combining the three levels solver in a consistent way makes the cell voltage and individual current in each segment to be properly calculated from a known cell current value.

C. Real-Time Model Implementation

In order to allow a real-time computation for a SOFC model-based control, the authors also developed an ordinary differential equation (ODE) solver using mid-point Euler method for thermal dynamic equations in pure C language, which was implemented for a hardware-in-the-loop dSpace PowerPC processor and validated with a hardware experimentation.

IV. Real-Time Quasi-2-D SOFC Model Benchmark

The quasi-2-D SOFC has \( N \) configurable axial and four radial control volumes. Therefore, by assuming a large value of \( N \), one can improve the model quasi-2-D presentation accuracy, but at same time increase the model execution time. The choice of \( N \) must be a compromise of parameters such as controller processor performance, control time-step requirement, and model accuracy constraints.

From the model experimental benchmark tests, the quasi-2-D SOFC model execution times for different \( N \) values in 1-GHz and 250-MHz dSpace PowerPC processors are presented in this section.

In addition, in a model based real-time controller, the model input variables are commonly measured continuously by external sensors. Therefore, during the model benchmark tests, the external sensors I/O execution time is also considered for overall performance evaluation.

A. 1-GHz dSpace 1105-CPU Model Benchmark

The quasi-2-D model is implemented in a high performance 1-GHz CPU based dSpace system. During this benchmark, the external sensors have digital control Area network (CAN) bus messages in order to update model input variables at every time step. The CAN bus messages I/O time in dSpace 1105 system takes 50–70 \( \mu \)s and it is typically consistent with any CAN hardware of any other system. The benchmark results and the used model time steps are shown in Table I.

When \( N = 1 \), the model has only one axial control volume. Thus, the iterative current density solver is made inactive. In this case, the model execution time (497 \( \mu \)s) represents the time required for the ODE solver computation (four thermal control volumes), plus algebraic equations computation time and any processor housekeeping time.

A significant increase of model execution time is observed when it is compared \( N = 1 \) and \( N = 2 \) cases. This is because...
iterative current density solver algorithm begins execution. An interesting feature can be observed for this benchmark evaluation: the model execution timing has very small difference from \( N = 2 \) to \( N = 5 \). This occurs because the solver has two phases of execution, the initialization phase and the iterative computation phase. The solver initialization phase takes constant execution time at the beginning of each time step no matter the value of \( N \). On the other hand, the solver iterative computation phase execution time depends highly on \( N \) value: for higher number of control volumes, there are more iterations to solve. For a small value of \( N \), the solver initialization phase dominates its execution time. Thus, the small execution time difference can be observed from \( N = 2 \) to \( N = 5 \).

From \( N = 10 \), the model execution time increases quasi-linearly with \( N \) value. The experimental validation shows that the thermal transient time of the quasi-2-D model is about 2 s. For Euler method ODE solver stability issue, the model time step should be at least ten times smaller (around 200 ms). Thus, the model benchmark stops at \( N = 200 \), which presents a model execution time of 146.7 ms.

One can conclude from these results that, the model developed in this paper is capable to be executed with a 1-GHz real-time processor at the millisecond time step range. The fastest execution time step is about 600 \( \mu \)s, and the maximal axial control volumes number can reach to 200 with respect to the model ODE solver stability requirement.

### B. 250-MHz dSpace 1104-CPU Model Benchmark

The quasi-2-D model discussed in this paper has also been implemented in a low performance 250-MHz CPU based dSpace system for benchmark tests, where external sensors are connected to analog inputs of the controller. The model then uses values from analog to digital converters interrupts in order to update their input parameters. The analog module I/O time is around 140 \( \mu \)s in dSpace 1104 system. The benchmark results with associated sampling time for the model implementations are summarized in Table II.

The algorithm takes more time for execution, in this case for a 250-MHz CPU. Same model execution time behaviors have been observed, as described in the previous section. A significant increase of execution time between \( N = 1 \) and \( N = 2 \) occurs due to the iterative current density solver algorithm. And from \( N = 2 \) to \( N = 5 \), the execution times are always slightly higher due to the solver initialization phase.

For other \( N \) values, the model execution time increases quasi-linearly with \( N \). By considering the ODE solver stability issue, the maximal axial control volumes number at this time for a 250-MHz CPU is \( N = 50 \) with a model execution time of 146.3 ms.

It can be concluded from these benchmark tests that, the developed quasi-2-D model in this paper is ready to be used in real-time controllers with a time step level on the order of milliseconds. That means, a model based controller is capable to react in millisecond for process control, and depending on the processor speed, the model can have enough control volumes to predict the SOFC quasi-2-D behaviors, which is a breakthrough achievement, since this would enable not only controlling SOFC but also diagnosis and self-healing in real-time, given that SOFC have slow dynamics when compared to these results.

#### C. Benchmark Results Comparison With Other Real-Time Model in the Literature

Similar real-time benchmark results for a real-time oriented SOFC model have been found in [25]. A comparison is given in Table III.

The model benchmark in [25] has been implemented with a 3-GHz CPU. By taking into account the CPU clock difference, it can be concluded that, the presented model with the original solver algorithm can achieve slightly higher performance than the model in [25] which uses commercial software solver (FEMLAB and Matlab/Simulink). However, it is important to consider that the model in [25] uses the assumption of uniform current density distribution in the SOFC, and by making such assumption, the current density is no longer needed to be calculated. By taking this consideration into account, the method proposed by the authors and described in this paper clearly improves the system performance.

One should emphasize that the proposed solver algorithm in this paper can be easily implemented with any real-time coding language. Thus, the proposed solution does not need any proprietary solutions, and it is completely independent of commercial software solvers.

### V. MODEL EXPERIMENTAL VALIDATION AND DISCUSSION

#### A. Experimental Conditions

The real-time oriented model presented in the aforementioned sections is validated with a prototype SOFC. The cell parameters and its operating conditions are listed in the Table IV.

It should be noted that, the inlet gas of the experimental test bench is a mixed gas flow from three gases: \( \text{H}_2 \), \( \text{H}_2\text{O} \), and \( \text{Ar} \). During experimental tests, the dry gas flows (\( \text{H}_2 \) and \( \text{Ar} \)) are controlled by two mass flow controllers. The water is injected from a controlled water pump and mixed with the dry gas in a

### TABLE II

<table>
<thead>
<tr>
<th>( N ) value (segment)</th>
<th>Model CPU execution time</th>
<th>model time step used</th>
<th>CPU occupation with sensor I/O (analog)</th>
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<tbody>
<tr>
<td>1</td>
<td>2.31 ms</td>
<td>2.5 ms</td>
<td>97.96%</td>
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<td>2</td>
<td>8.53 ms</td>
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<td>10</td>
<td>21.5 ms</td>
<td>25 ms</td>
<td>86.61%</td>
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<td>20</td>
<td>48.2 ms</td>
<td>50 ms</td>
<td>96.70%</td>
</tr>
<tr>
<td>50</td>
<td>146.3 ms</td>
<td>150 ms</td>
<td>97.65%</td>
</tr>
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### TABLE III

<table>
<thead>
<tr>
<th>( N ) value (segment)</th>
<th>this proposed model 1 GHz CPU</th>
<th>this proposed model (3 GHz estimated)</th>
<th>model in [25] 3 GHz CPU</th>
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<tr>
<td>10</td>
<td>4.78 ms</td>
<td>1.59 ms</td>
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<td>20</td>
<td>10.7 ms</td>
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<td>50</td>
<td>31.1 ms</td>
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TABLE IV

<table>
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<th>Symbol</th>
<th>Parameter Description</th>
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<td>mm</td>
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<td>(D_{outer})</td>
<td>Cell tube outer diameter</td>
<td>9.8</td>
<td>mm</td>
</tr>
<tr>
<td>(\delta_{C,GDL})</td>
<td>Cathode GDL thickness</td>
<td>30</td>
<td>(\mu m)</td>
</tr>
<tr>
<td>(\delta_{E,GDL})</td>
<td>Anode GDL thickness</td>
<td>1000</td>
<td>(\mu m)</td>
</tr>
<tr>
<td>(\delta_{mem})</td>
<td>Membrane thickness</td>
<td>20</td>
<td>(\mu m)</td>
</tr>
<tr>
<td>(L_{cell})</td>
<td>Cell length</td>
<td>25</td>
<td>mm</td>
</tr>
<tr>
<td>(e_{c})</td>
<td>Cathode GDL porosity</td>
<td>0.35</td>
<td></td>
</tr>
<tr>
<td>(e_{a})</td>
<td>Anode GDL porosity</td>
<td>0.4</td>
<td></td>
</tr>
<tr>
<td>(\tau_{c})</td>
<td>Cathode GDL tortuosity</td>
<td>4.0</td>
<td></td>
</tr>
<tr>
<td>(\tau_{a})</td>
<td>Anode GDL tortuosity</td>
<td>2.3</td>
<td></td>
</tr>
<tr>
<td>(q_{inlet})</td>
<td>Inlet mixed-gas fuel flow rate</td>
<td>400</td>
<td>scm</td>
</tr>
<tr>
<td>(P_{cathode})</td>
<td>Cathode operating pressure</td>
<td>0.83</td>
<td>atm</td>
</tr>
<tr>
<td>(P_{anode})</td>
<td>Anode inlet gas pressure</td>
<td>0.83</td>
<td>atm</td>
</tr>
<tr>
<td>(T_{C})</td>
<td>Cathode activation energy</td>
<td>7.0 (\times) 10^3</td>
<td>J/m^2</td>
</tr>
<tr>
<td>(T_{A})</td>
<td>Anode activation energy</td>
<td>19.8 (\times) 10^4</td>
<td>J/m^2</td>
</tr>
<tr>
<td>(E_{C})</td>
<td>Cathode activation energy</td>
<td>120</td>
<td>kJ/mol</td>
</tr>
<tr>
<td>(E_{A})</td>
<td>Anode activation energy</td>
<td>100</td>
<td>kJ/mol</td>
</tr>
<tr>
<td>(E_{YSZ})</td>
<td>YSZ activation energy</td>
<td>80</td>
<td>kJ/mol</td>
</tr>
<tr>
<td>(\rho_{YSZ})</td>
<td>Reference YSZ elec. conductivity</td>
<td>3.6 (\times) 10^5</td>
<td>S/Km</td>
</tr>
<tr>
<td>(\lambda_{C,GDL})</td>
<td>Cathode thermal conductivity</td>
<td>18.2</td>
<td>W/(m-K)</td>
</tr>
<tr>
<td>(\lambda_{mem})</td>
<td>Membrane thermal conductivity</td>
<td>505</td>
<td>J/(kg-K)</td>
</tr>
<tr>
<td>(\lambda_{E,GDL})</td>
<td>Anode thermal conductivity</td>
<td>10.1</td>
<td>W/(m-K)</td>
</tr>
<tr>
<td>(C_{mem})</td>
<td>Membrane thermal capacity</td>
<td>538</td>
<td>J/(kg-K)</td>
</tr>
<tr>
<td>(C_{C,GDL})</td>
<td>Cathode thermal capacity</td>
<td>10.3</td>
<td>W/(m-K)</td>
</tr>
<tr>
<td>(C_{E,GDL})</td>
<td>Anode thermal capacity</td>
<td>534</td>
<td>J/(kg-K)</td>
</tr>
</tbody>
</table>

heated vaporizer cylinder with a pressure controller. Due to the presence of argon gas, the test bench allows the molar fraction of \(H_2\) and \(H_2O\) to vary at the same time (with a total fraction smaller than 1.0), without changing the inlet molar flow rate and the inlet pressure.

B. Model Segment Independency Analysis

The SOFC model has a configurable axial segment number \(N\) as needed for the simulation. Therefore, a segment independency (scaling) test has to be conducted with the specific modeling parameter set shown in Table IV. The model results can be considered as “segment independent” if the changes observed in the model results are less than a pre-defined acceptable error, when increasing the segment number gradually.

The SOFC model output voltage for increasing number of segments \((N\) from 2 to 25) and under different current and \(H_2/H_2O\) molar fraction values are presented in Fig. 5. The results show a slight numeric variation (less than 5% but higher than 1%) when the number of segments are small. One can observe that for \(N = 13\), the numeric value variation is less than 0.05 %, and for \(N = 17\), this variation becomes less than 0.01 %. Thus, the model could be considered as “segment independent” for more than \(N = 15\) to 20 in this case.

In order to verify the model segment independency, the SOFC model axial current density distributions for three different number of segments \(N = 15, 20,\) and 25 are shown in the Fig. 6. Two different cases with a high and a low \(H_2\) fraction are illustrated. It can be seen from the figure that, with a value of \(N\) larger than 15, the current density distributions are no longer affected by the change of number of segments in the model (the relative error between different values of \(N\) is less than 0.03 %).

Based on the previous analysis results, the axial segments number \(N = 20\) is chosen for the SOFC model experimental validation with the parameters in Table IV.

It should also be noted that, the previous results of the segment independency test are only valid for the specific parameter set shown in table IV. The segment independency of the model relies heavily on the model input parameters, such as cell geometry (small or large cell) and properties. Thus, if the proposed SOFC model is used to model another SOFC of different scale, this segment independency test must be conducted again to determine the new value of \(N\).

C. Results and Discussions

The experimental and simulated single cell polarization curve at 850°C under 35.53% \(H_2\) molar fraction and 19.74% \(H_2O\) molar fraction conditions are shown in Fig. 7. The model predicted values have a very good accuracy (less than 5% relative error) compared to the measured data for the entire fuel cell operating range.

The axial current density distribution when the cell current is equal to 3 A is illustrated in Fig. 8. The current densities decrease along the direction of the cell channel flow. That is because the fuel is taken progressively along the channels leading to the diminutions of the fuel pressure (\(H_2\) pressure) in the gas flow direction. The maximum current densities difference is about 5% between inlet and outlet of the cell.
The axial and radial temperature distribution at 3 A in steady-state is shown in Fig. 9. In the radial direction, the temperatures of gas in the anode channel, anode GDL, YSZ electrolyte, and cathode GDL for each axial control volume are presented. It can be seen from the figure that, the gas in the anode channel is heated progressively alone in the channel. At the outlet, the anode gas temperature in the tube reaches the SOFC anode operating temperature. From the figure, it can also be seen that the SOFC body temperature at inlet is slightly higher than the one at outlet. This is because the current density is higher at inlet (see Fig. 7), which leads to a higher heat generation rate from electrochemical reactions.

The cell electrode temperature transient for a current step of 3 A is shown in Fig. 10. It can be concluded that, during the cell operation, the temperature difference between the cell electrode and external environment is less than 1°C. The single cell temperature can reach steady-state in few seconds.

The cell polarization curve with a lower H$_2$ molar fraction (24.67%) and a higher H$_2$O molar fraction (59.22%) at 850°C is given in Fig. 11. Because of the lower fuel pressure, the cell polarization curve is lower compared to that of Fig. 7. Under similar 3 A cell current conditions, the axial cell current densities distribution is shown in Fig. 12. It can be clearly observed in Fig. 8 and Fig. 12 that, under lower H$_2$ pressure, the cell current densities in fuel flow direction have a more significant gradient than those under higher H$_2$ pressure. The difference at the beginning and the end of cell can reach up to 8%.

The radial and axial distribution of temperature in anode gas tube channel, gas diffusion layers (electrodes), and YSZ electrolyte is illustrated in Fig. 13 for a current value of 1.5 A.
Under a lower fuel cell current, the axial temperature gradient in SOFC body is less significant compared to Fig. 9. In radial direction, the temperature of cathode GDL is lower than that of anode GDL and YSZ electrolyte, because the SOFC cathode is exposed to the heated air at constant temperature of 850°C around the prototype SOFC.

The H₂ and H₂O pressures variations in the radial (electrode) and axial (flow) direction for the cell current equal to 1.5 and 3 A are shown in Figs. 14 and Fig. 15. In this test, the H₂O pressure is higher than the H₂ pressure in the cell. It can be seen from the figure that, the gas pressures at electrode-electrolyte interface is slightly lower than the ones in the gas channel. This pressure difference at radial direction is due to the gas transport phenomena through the electrode as described by (23). Under higher current (thus higher gas flow rates), the gas pressure difference between the channel and electrode-electrolyte interface are more important. It can be also seen that (because of the electrochemical reaction), the H₂ (reactant) pressure decreases continuously along the channel in the axial direction and the H₂O (product) pressure increase at the same time. Under higher cell current, these pressures variations are more significant.

The cell polarization results for a higher H₂ molar fraction (59.22%) at 850°C is given in Fig. 16. The H₂O molar fraction at this time is fixed to 19.74%. The simulation results have a slight difference at higher cell current compared to the experimental ones. This error is certainly due to the simplification of the gas mass transport model in the gas diffusion layer. Indeed, the Fick Law for binary gas diffusion is used to describe the gas diffusion phenomenon (equation (23)), but with the presence of argon gas, the multigas diffusion law, such as the Stefan–Maxwell diffusion should be more accurate. Another reason for such behavior is related to the empirical parameters, like the electrode porosity and the tortuosity, when not properly identified. These empirical parameters have also an important impact on the gas diffusion coefficient as shown in (24).

The cell anode gas pressure variations for a current step of 1.5 and 3 A are illustrated Fig. 17. In this case, the H₂ inlet pressure is higher than the H₂O inlet pressure. A higher current leads to a more significant H₂ pressure decrease and H₂O pressure increase in the channel. The figure shows that, even with a
relatively high H₂ inlet pressure, the difference between the H₂ inlet and outlet pressure could reach to nearly 10% at a current of 3 A.

The cell polarization curve at 800°C is shown in Fig. 18, with 35.53% H₂ molar fraction and 19.74% H₂O molar fraction operating conditions and eventually, the model results show a very good agreement with the measured data.

VI. CONCLUSION

A comprehensive quasi-2-D dynamic tubular solid-oxide fuel cell model has been presented in this paper. The model included electrochemical, fluidic, and thermal features and the dynamic equations in thermal domain.

In order to calculate the current density distribution from implicit algebraic equations, an iterative solver has been built in the model. The iterative methods and corresponding algorithms were given and discussed in details in the paper. The algorithm can predict the axial and radial distributions of model variables, such as current density, temperature, and gas pressure, during the cell operation under different conditions. The proposed generic solver algorithm can be easily applied to any size of the flow channel at SOFC cell or stack level, and can be easily implemented by any real-time coding language.

The proposed model has been validated with a SOFC prototype cell and the results showed a very good agreement between simulations and experimentations. It can be noted from the results that, in the cases with a low H₂ molar fraction, the current density and fuel gas pressure differences between the inlet and the outlet of the small prototype cell in experimental validations could reach to about 10%. A low H₂ molar fraction is common in the SOFC applications that are supplied by reformed gas. This observation shows the interest of using a multidimensional SOFC model for the control purpose in these cases. With such a model, the local performance of the SOFC can be monitored and improved.

A complete real-time model benchmark test has also been performed. The real-time capabilities of the model for different segment numbers (N) compared with two processors (at1-GHz and a 250-MHz clock rates) were evaluated and carefully discussed. Based on different N values and processor clocks, the model shows to be capable for execution in real-time in millisecond control loop range. Such short execution time of the presented quasi-2-D model allow controllers to make fast control decisions and actions even to compensate parameter variations and external disturbances, by predicting actual SOFC performance with a real-time model simulation.

The proposed real-time based model controller shows great interests in practice cases, since it enables not only controlling SOFC but also diagnosis and self-healing management in real-time, given that a SOFC has slower dynamic response when compared to the capabilities of the proposed solver.

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Dedication: The authors dedicate this paper to the memory of their friend and coauthor, Dr. B Blunier, formerly an Associate Professor with the Université de Technologie de Belfort–Montbéliard, who passed away in February 23, 2012.

REFERENCES


