

Chapter 2

Models Hierarchy

2.1 From Physical to Synthesis Models

Nowadays, engineering research always relies on the mathematical representation of the physical system under-investigation to ensure proper model-based optimization, control, and diagnosis task be performed, aiming at continuously improving performance, while still achieving cost-effectiveness targets.

Physical (i.e., white-box) models are obtained by suitably adapting well-known physical principles and knowledge to a plant or a process, in such a way as to define the governing equations of a specific phenomenon (Romijn et al. 2008). On the other hand, black-box models correspond to a purely mathematical description of the phenomenon that must be completely inferred from a suitable experimental data set (i.e., identification or training data set) and tested for generalization verification on further experimental data sets (i.e., test sets). Therefore, black-box models do not rely on physical content, thus resulting in lower computational burden since, as an example, no differential equations, neither ordinary nor partial, are to be solved. On the other hand, their accuracy necessarily relies on extended experimental campaigns. Regressions and neural networks are typical examples of black-box models, also known as synthesis models, since their mathematical representation is flexible enough to be applied for mapping any continuous functional relationship between outputs and inputs of a given process with a very low computational burden as compared to physical (i.e., white-box) models.

Between white- and black-box, gray-box models fall (Romijn et al. 2008). Such models are usually developed exploiting both physical content and experimental data availability, thus resulting into a middle level model category that exhibits a good compromise between computational and experimental burden. Typical examples of gray-box models are zero-dimensional or lumped models, in which a few or just one variable are assumed as state variables to characterize system behavior both in steady-state and transient conditions (Ramallo-González et al. 2013). Figure 2.1 shows the qualitative variation of required experimental burden as

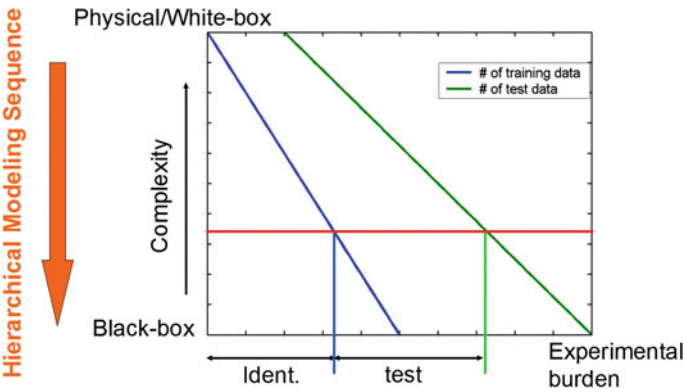


Fig. 2.1 Qualitative description of the impact of modeling approach on required experimental burden

a function of physical content. It is reasonable to expect that physical models require relatively few experimental data for their validation. On the other hand, black-box approaches entail performing a high number of experiments to be used for both identification and test.

The most suitable modeling approach has to be selected depending upon the specific application field, as shown on Table 2.1. As expected, high physical content is required to improve component design. Particularly in the fuel cell field, it is known that the main cell manufacturers utilize highly complex physical models to improve cell geometries and select the most performing materials (US Department of Energy 2004).

Regarding system sizing and optimal control strategies definition, black-box and gray-box models are both more suitable than physical, high computational intensive models, especially when destined to real-time tasks. Optimal balance of plant can be achieved adopting large-scale design optimization algorithms, which usually require several function evaluations (Rizzoni et al. 2005; Arsie et al. 1999). Therefore, the use of models with a good compromise between accuracy and computational burden is highly beneficial.

Table 2.1 Modeling approaches versus application fields

Modeling approach	Application fields		
	Component design	System sizing	Optimal control and diagnosis
Physical	X		
Steady gray/black-box		X	X
Dynamic gray/black-box		Possible	X
Hybrid modeling	Not applicable	Appropriate combination of different approaches	

Optimal control strategies are defined at both supervisory (i.e., high control level) and low control level (Arsie et al. 2010; Guezennec et al. 2003). The definition of the optimal working set-points, which competes to higher levels, does not necessarily require dynamic simulations. On the other hand, low-level control tasks are often accomplished via feedback strategies, thus requiring to take into account the main system dynamics (Pukrushpan et al. 2004). In both cases, suitable optimization analyses are required to define the best strategies, thus suggesting the combined use of steady and dynamic gray-/black-box models. Moreover, many plants, such as SOFC-based auxiliary power units (APUs), consist of devices with time constants that significantly differ from each other. Thus, proper combination of dynamic and steady gray-/black-box submodels (i.e., hybrid modeling) might allow to further reduce computational time.

Finally, model-based monitoring, feedback control, as well as model-based diagnosis, entail extending model applicability to real-time tasks, thus outlining once again the need of adopting hybrid approaches, preferably encouraging the use of very low computational intensive models, such as gray- and especially black-box ones.

The joint analysis of Fig. 2.1 and Table 2.1 indicates a significant conflicting need, which has to be carefully accounted for in the trade-off analysis on modeling approach: experimental burden. Such an issue can be addressed by recurring to a hierarchical approach. Particularly, the use of physical models can be optimized, in that once tested for validation with a reduced amount of experimental data, they can be used not only for single component optimal (see Table 2.1) but also as virtual-experiments generators. In such a way, the available reference data sets can be extended and then, following the hierarchical sequence, both gray- and black-box models can be identified and validated without further impact on experimental burden. Models hierarchy is of course also suitable to individuate the best balance between more and less physical models into a hybrid modeling architecture (see Table 2.1). In the following section, the hierarchical sequence proposed by the authors to suitably address model-based design, control, and diagnosis of SOFC systems is presented and discussed in detail.

2.1.1 Hierarchical Approach to SOFC Modeling

The hierarchical approach proposed in this book is illustrated in Fig. 2.2. The levels 1, 2, and 3 are representative of different physical contents. At the highest level (i.e., 1) is the real system, which of course may correspond either to an SOFC stack or to a fully operational SOFC system. Depending on which experimental set-up is currently available, the number of SOFC model-based development tasks, which might be conducted mainly exploiting real observations/measurements, will vary, thus indirectly but still effectively impacting on how to find the most suitable model development path.

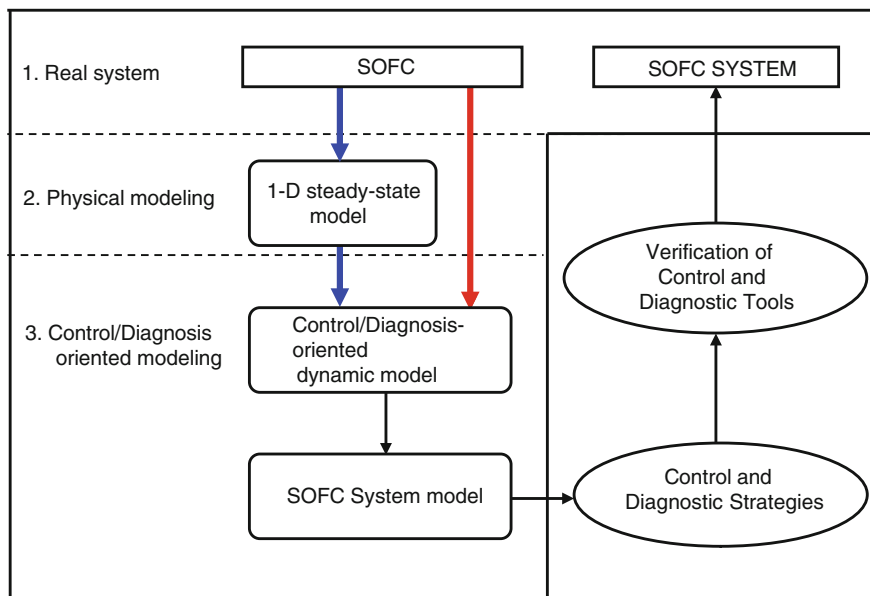


Fig. 2.2 Hierarchical approach for real-time modeling and model-based control and diagnosis of SOFC systems

Particularly, Fig. 2.2 indicates that two different paths (i.e., blue and red lines) can be followed to develop control- and diagnosis-oriented models (i.e., level 3 models). The former, which usually corresponds to limited availability of experiments or, as mentioned above, to less informative data sets as single SOFC stack characterization might be, first entails developing more physical models (i.e., level 2) prior to switch to level 3, where more computationally effective models are built. Such an articulated path (i.e., the blue one) is justified by the need for ensuring sufficiently extended data sets be available for identifying and validating less physical models, as shown on Fig. 2.2. On the other hand, whenever more experiments can be run on the real system, without reducing cost-effectiveness of the experimental campaign, the latter red path can be chosen. If this is the case, either gray-box or black-box or even hybrid models can be directly developed, i.e., without developing level 2 models, thus positively impacting on the development burden of advanced model-based control and diagnosis tools, which are the expected output of the hierarchical procedure shown on Fig. 2.2. Such a figure also highlights the importance of accounting for the opportunity of getting back to the physical plant for final validation of the developed model-based tools.

The next section deepens the methodological aspects associated to the development of the models hierarchy, starting from the description of SOFC one-dimensional modeling and then proceeding to treating synthesis models definition and development, according to the above discussed hierarchical approach.

2.2 Dimensional Modeling

The adoption of one-dimensional (1D) modeling approach for planar SOFCs allows meeting significantly conflicting needs, such as good accuracy and affordable computational burden. On one hand, the literature (Chan et al. 2001; Aguiar et al. 2005) clearly indicates how the correct estimation of current and temperature spatial distributions in the flow direction enhances the evaluation of effective cell performance. On the other hand, removing the need for solving the governing equations in the other dimensions contributes to greatly reducing computational time. Therefore, 1D modeling approach emerges as a very promising way to address SOFC-related optimization/design problems, such as balance of plant analyses and polarization models identification (Braun 2002).

Furthermore, the appreciable physical content characterizing 1D modeling ensures satisfactory flexibility to extend model validity to different cell geometries, materials, and fuels (fully or partially reformed petroleum fuels). The above positive features are particularly useful to provide “virtual” experimental data sets that suitably cover the typical SOFC operating domain. The latter aspect serves at accomplishing one of the main targets of this book, namely the exploitation of models hierarchy to develop real-time applicable model-based control and diagnostic tools.

2.2.1 The 1D Model

The proposed 1D model aims at describing spatial evolution of current, temperature and gas composition within a rectangular-planar SOFC, both in co- and counterflow configuration. Therefore, it consists of an integrated structure of submodels, mass, energy, and electrochemical balance, which are run in an iterative procedure. Particularly, spatial variations in the cell are modeled by discretizing the domain into computational elements along cell length. At each element, mass, energy, and electrochemical balances are solved.

The following hypotheses were assumed to model both hydrogen and methane reformat fed solid oxide fuel cells (Ormerod 2003; Braun 2002; Sorrentino et al. 2008):

- isopotential interconnect and electrodes (Braun 2002);
- completely stirred conditions are considered at the element level;
- air and fuel fed gases are treated separately as perfect gases;
- pressure drop within fuel and air channels is neglected, according to the indications provided in Burt et al. (2004);
- the flow velocity is constant over the channel cross section;
- the concentration of reactants is constant over the channel cross section;
- diffusion of reactants along the flow channel is negligible as convection prevails on transport;

- cell boundaries are adiabatic;
- radiative heat transfer between solid trilayer and metallic interconnects is assumed negligible.

In the following subsections, the basic working principle of SOFC is initially recalled, prior to describing with deep details the above-mentioned mass, energy, and electrochemical balances.

2.2.1.1 Mass Balance

Applying conservation of mass to a generic control volume Ω surrounding the entire cell shown in Fig. 2.3, the steady-state material balance for each specie m can be expressed as:

$$\int_{\Omega} \vec{\nabla} \cdot \vec{N}_m dV = 0 \quad m = [\text{H}_2, \text{CH}_4, \text{H}_2\text{O}, \text{CO}, \text{CO}_2, \text{N}_2, \text{O}_2] \quad (2.1)$$

Anode and cathode are discretized in N computational element in the flow direction, as shown on Fig. 2.3, where inlet, outlet and source (or sink) molar flows are represented for the i th computational element and the m_{an} th and m_{ca} th specie.

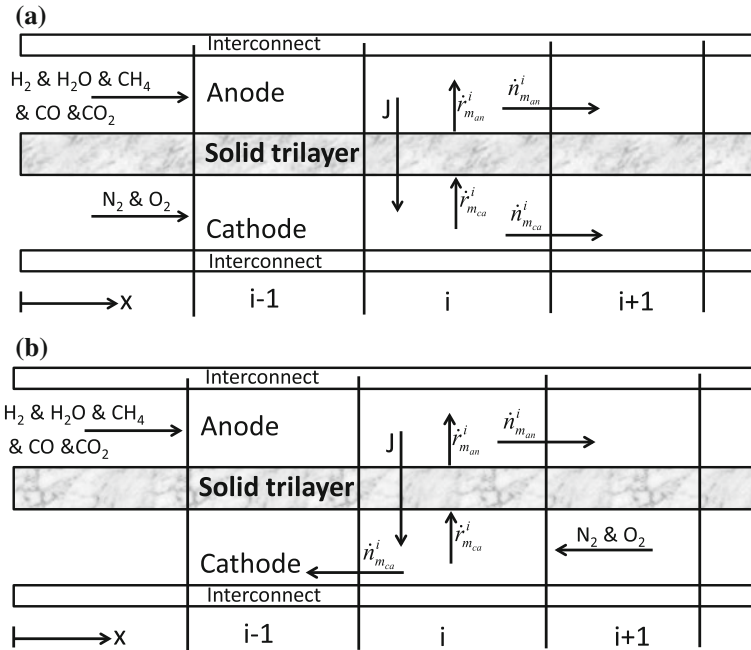


Fig. 2.3 Mass balance discretization for co-flow (a) and counter-flow (b) planar solid oxide fuel cell

Applying Eq. (2.1) to the discretized cell for all the species, the following mass balances are obtained for co- (see Fig. 2.3a) and counterflow configurations (see Fig. 2.3b):

$$0 = \dot{n}_{\text{H}_2}^{i-1} - \dot{n}_{\text{H}_2}^i + 3 \cdot \dot{r}_{\text{ref}}^i + \dot{r}_{\text{shift}}^i - \dot{r}_{\text{ox}}^i \quad (2.2a)$$

$$0 = \dot{n}_{\text{H}_2\text{O}}^{i-1} - \dot{n}_{\text{H}_2\text{O}}^i - \dot{r}_{\text{ref}}^i - \dot{r}_{\text{shift}}^i + \dot{r}_{\text{ox}}^i \quad (2.2b)$$

$$0 = \dot{n}_{\text{CH}_4}^{i-1} - \dot{n}_{\text{CH}_4}^i - \dot{r}_{\text{ref}}^i \quad (2.2c)$$

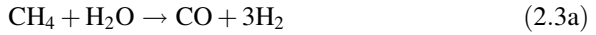
$$0 = \dot{n}_{\text{CO}}^{i-1} - \dot{n}_{\text{CO}}^i + \dot{r}_{\text{ref}}^i - \dot{r}_{\text{shift}}^i \quad (2.2d)$$

$$0 = \dot{n}_{\text{CO}_2}^{i-1} - \dot{n}_{\text{CO}_2}^i + \dot{r}_{\text{shift}}^i \quad (2.2e)$$

$$\begin{cases} 0 = \dot{n}_{\text{N}_2}^{i-1} - \dot{n}_{\text{N}_2}^i, & \text{co-flow} \\ 0 = \dot{n}_{\text{N}_2}^{i+1} - \dot{n}_{\text{N}_2}^i, & \text{counter-flow} \end{cases} \quad (2.2f)$$

$$\begin{cases} 0 = \dot{n}_{\text{O}_2}^{i-1} - \dot{n}_{\text{O}_2}^i - 0.5 \cdot \dot{r}_{\text{ox}}^i, & \text{co-flow} \\ 0 = \dot{n}_{\text{O}_2}^{i+1} - \dot{n}_{\text{O}_2}^i - 0.5 \cdot \dot{r}_{\text{ox}}^i, & \text{counter-flow} \end{cases} \quad (2.2g)$$

The quantities $\dot{r}_{\text{ref}}^i$, $\dot{r}_{\text{shift}}^i$ and $\dot{r}_{\text{ox}}^i$ appearing in Eq. (2.2a)–(2.2g) are the reaction rates (mol s^{-1}) of the methane reforming (see Eq. 2.3a), water–gas shift (see Eq. 2.3b) and electro-oxidation (see Eq. 2.3c) reaction, respectively:



The water gas shift reaction (Eq. 2.3b) is assumed to be in equilibrium, with equilibrium constant expressed as:

$$K_{\text{shift}}^i(p^i, T_s^i) = \exp\left(\frac{-\Delta G_{\text{shift}}(p^i, T_s^i)}{R \cdot T_s^i}\right) \quad (2.4)$$

K_{shift} can also be estimated as a function of molar fractions (Massardo and Lubelli 2000):

$$K_{\text{shift}}^i = \frac{x_{\text{H}_2}^i \cdot x_{\text{CO}_2}^i}{x_{\text{CO}}^i \cdot x_{\text{H}_2\text{O}}^i} = \frac{\left(\frac{\dot{n}_{\text{H}_2}^{i-1} + 3\dot{r}_{\text{ref}}^i + \dot{r}_{\text{shift}}^i - \dot{r}_{\text{ox}}^i}{\dot{n}_{\text{tot}}^{i-1} + 2\dot{r}_{\text{ref}}^i}\right) \cdot \left(\frac{\dot{n}_{\text{CO}_2}^{i-1} + \dot{r}_{\text{shift}}^i}{\dot{n}_{\text{tot}}^{i-1} + 2\dot{r}_{\text{ref}}^i}\right)}{\left(\frac{\dot{n}_{\text{CO}}^{i-1} + \dot{r}_{\text{ref}}^i - \dot{r}_{\text{shift}}^i}{\dot{n}_{\text{tot}}^{i-1} + 2\dot{r}_{\text{ref}}^i}\right) \cdot \left(\frac{\dot{n}_{\text{H}_2\text{O}}^{i-1} - \dot{r}_{\text{ref}}^i - \dot{r}_{\text{shift}}^i + \dot{r}_{\text{ox}}^i}{\dot{n}_{\text{tot}}^{i-1} + 2\dot{r}_{\text{ref}}^i}\right)} \quad (2.5)$$

The reaction rates $\dot{i}_{\text{ox}}^i$ and $\dot{i}_{\text{ref}}^i$ (see Eq. 2.2a–2.2g) are computed via Faraday's law (see Eq. 2.6) and the temperature and pressure dependent correlation (see Eq. 2.7) indicated by Achenbach and Riensche (1994), respectively:

$$\dot{i}_{\text{ox}}^i = \frac{J^i \cdot A^i}{F \cdot n_e} \quad (2.6)$$

$$\dot{i}_{\text{ref}}^i = 4274 \cdot p_{\text{CH}_4}^i \cdot A^i e^{-(82000/R/T_s^i)} \quad (2.7)$$

The last reaction rate $\dot{i}_{\text{shift}}^i$ is determined solving the system of Eqs. (2.4)–(2.7).

Boundary conditions of the systems of Eq. (2.2a)–(2.2g) are the inlet flows, estimated as a function of fuel utilization (Eq. 2.8) and excess air (Eq. 2.9a, 2.9b):

$$U_f = \begin{cases} \frac{\dot{n}_{\text{H}_2, \text{react}}}{\dot{n}_{\text{H}_2}^0} = \frac{\sum_{i=1}^N \dot{i}_{\text{ox}}^i}{\dot{n}_{\text{H}_2}^0} = \frac{\sum_{i=1}^N J^i \cdot A^i}{F \cdot n_e} \cdot \frac{1}{\dot{n}_{\text{H}_2}^0} & \text{pure H}_2 \text{ feed} \\ \frac{\dot{n}_{\text{H}_2, \text{react}}}{4\dot{n}_{\text{CH}_4}^{\text{pre, in}}} = \frac{\sum_{i=1}^N \dot{i}_{\text{ox}}^i}{4\dot{n}_{\text{CH}_4}^{\text{pre, in}}} = \frac{\sum_{i=1}^N J^i \cdot A^i}{F \cdot n_e} \cdot \frac{1}{4\dot{n}_{\text{CH}_4}^{\text{pre, in}}} & \text{reformat feed} \end{cases} \quad (2.8)$$

$$\lambda = \frac{\dot{n}_{\text{O}_2}^0}{\dot{n}_{\text{O}_2, \text{sto}}} = \frac{\dot{n}_{\text{O}_2}^0}{\frac{1}{2}\dot{n}_{\text{H}_2, \text{react}}} = \frac{\dot{n}_{\text{air}}^0}{4.76 \cdot \frac{1}{2}\dot{n}_{\text{H}_2, \text{react}}} \quad \text{co-flow} \quad (2.9a)$$

$$\lambda = \frac{\dot{n}_{\text{O}_2}^{N+1}}{\dot{n}_{\text{O}_2, \text{sto}}} = \frac{\dot{n}_{\text{O}_2}^{N+1}}{\frac{1}{2}\dot{n}_{\text{H}_2, \text{react}}} = \frac{\dot{n}_{\text{air}}^{N+1}}{4.76 \cdot \frac{1}{2}\dot{n}_{\text{H}_2, \text{react}}} \quad \text{counter-flow} \quad (2.9b)$$

It is worth noting that the denominator of Eq. (2.9a), (2.9b) for reformat feed equals 4 times the methane flow at pre-reformer inlet. This holds because, for each CH_4 molecule, four H_2 molecules can be obtained, as indicated by Eq. (2.3a)–(2.3c). The use of a pre-reforming stage, to partially pre-reform methane, is required to avoid the endothermic internal reforming reaction (see Eq. 2.3a) to cause excessive temperature drop at anode inlet. Moreover, it is evident that while Eq. (2.9a), (2.9b) allows directly evaluating the incoming air flows, to be fed as input to the system of Eqs. (2.2a)–(2.2g) and (2.8) must be suitably post-processed, in case of reformat feed, to precisely estimate the anode inlet flows. The following subsection treats in detail the numerical approach to be followed to perform such an estimation.

Estimation of Anode Inlet Flows

As shown in Fig. 2.4, an external pre-reformer is usually placed upstream the anode inlet. Therefore, the anode composition at anode inlet (i.e., pre-reformer outlet) will depend on the following parameters: pre-reformer conversion factor (i.e., REF) and SOFC inlet (i.e., pre-reformer outlet, see Fig. 2.4) temperature and pressure.

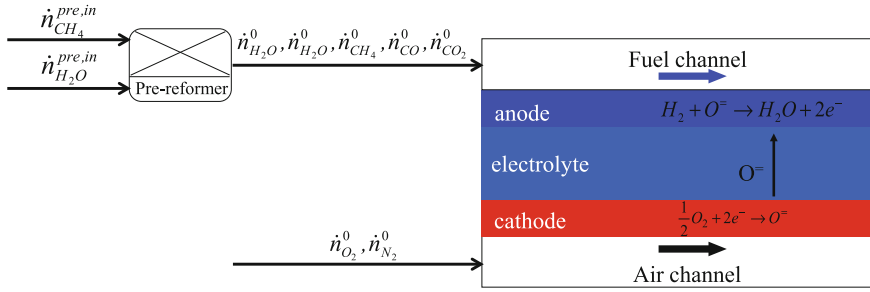


Fig. 2.4 Schematic representation of main variables involved in the procedure used to estimate anode inlet fuel composition (see Eqs. 2.10, 2.11a, 2.11b, 2.11c and 2.12)

Pre-reformer conversion factor is defined as the ratio between the methane flow entering the SOFC and the methane flow at pre-reformer inlet:

$$\text{REF} = \frac{\dot{n}_{\text{CH}_4}^0}{\dot{n}_{\text{CH}_4}^{\text{pre},\text{in}}} \quad (2.10)$$

where $\dot{n}_{\text{CH}_4}^{\text{pre},\text{in}}$ and $\dot{n}_{\text{CH}_4}^0$ are the methane flow entering the pre-reformer and the SOFC stack, respectively. Assuming a steam-pre-reformer is used, water has also to be fed, as shown on Fig. 2.4. Since in the pre-reformer both reforming (Eq. 2.3a) and water-gas-shift reaction (Eq. 2.3b) take place, the following balances hold for carbon, hydrogen, and oxygen, respectively:

$$\dot{n}_{\text{CH}_4}^0 + \dot{n}_{\text{CO}}^0 + \dot{n}_{\text{CO}_2}^0 - \dot{n}_{\text{CH}_4}^{\text{pre},\text{in}} = 0 \quad (2.11a)$$

$$4\dot{n}_{\text{CH}_4}^0 + 2\dot{n}_{\text{H}_2}^0 + 2\dot{n}_{\text{H}_2\text{O}}^0 - 4\dot{n}_{\text{CH}_4}^{\text{pre},\text{in}} - 2\dot{n}_{\text{H}_2\text{O}}^{\text{pre},\text{in}} = 0 \quad (2.11b)$$

$$\dot{n}_{\text{H}_2\text{O}}^0 + \dot{n}_{\text{CO}}^0 + 2\dot{n}_{\text{CO}_2}^0 - \dot{n}_{\text{H}_2\text{O}}^{\text{pre},\text{in}} = 0 \quad (2.11c)$$

In order to determine the five unknowns $\dot{n}_{\text{H}_2}^0$, $\dot{n}_{\text{H}_2\text{O}}^0$, $\dot{n}_{\text{CH}_4}^0$, $\dot{n}_{\text{CO}}^0$ and $\dot{n}_{\text{CO}_2}^0$ as a function of reformer conversion factor and anode inlet temperature and pressure, the system of Eqs. (2.10) and (2.11a, 2.11b, 2.11c) must be coupled to a fifth equation (i.e., Eq. 2.12), which is directly derived from the water-gas-shift reaction equilibrium constant (see Eq. 2.5). Such a fifth equation, holding valid at the SOFC inlet (i.e., pre-reformer outlet), can be simply expressed as:

$$K_{\text{shift}}(p^0, T_{\text{an}}^0) = \frac{\dot{n}_{\text{H}_2}^0 \cdot \dot{n}_{\text{CO}_2}^0}{\dot{n}_{\text{H}_2\text{O}}^0 \cdot \dot{n}_{\text{CO}}^0} \quad (2.12)$$

where K_{shift} is evaluated by means of Eq. (2.4).

2.2.1.2 Energy Balance

The energy balance is applied by dividing the computational element into three separate control volumes, namely solid trilayer and fuel (i.e., anode) and air (i.e., cathode) channels (see Fig. 2.5). The dominant effects described in the model are the convective heat transfer between solid trilayer and fuel and air streams, the energy transfer due to the reactants, and products flows and the conductive heat transfer through the solid trilayer.

The steady-state energy balance for an open system reads as:

$$\frac{dE}{dt} = \dot{E}_{in} - \dot{E}_{out} + \dot{Q} - \dot{W} = 0 \quad (2.13)$$

In the following subsections, the way Eq. (2.13) was particularized to each control volume is presented and discussed, along with basic theoretical principles through which each energy flow term shown on Fig. 2.5 was treated.

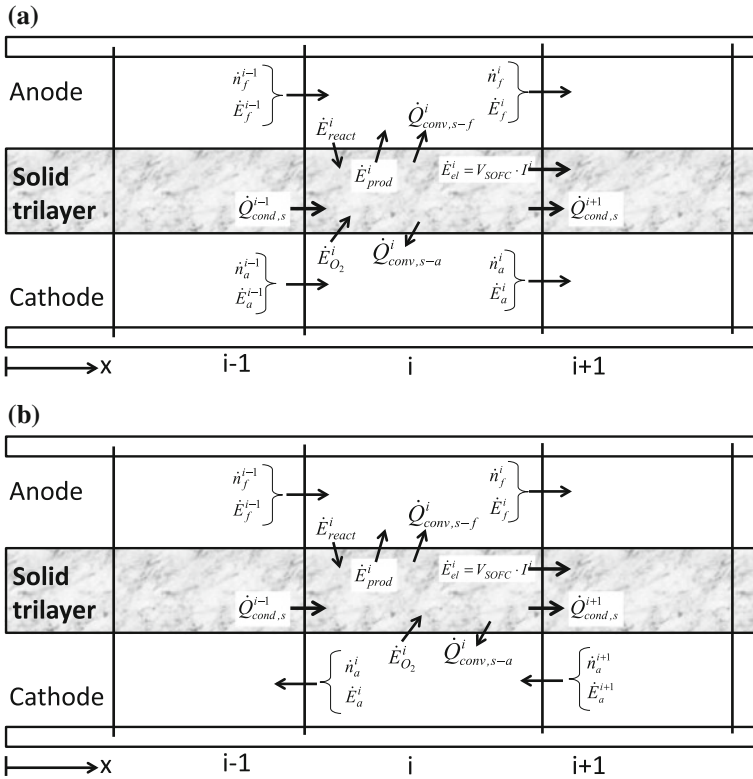


Fig. 2.5 Energy balance discretization for co-flow (a) and counter-flow (b) planar solid oxide fuel cell

Energy Balance for the Fuel Channel

As stated above, the energy balance for the fuel channel was obtained by assuming the only heat exchange mechanisms to correspond to: (i) the energy rates associated with species flow in and out of the i th computational element; (ii) convective heat exchange with the solid trilayer and (iii) the energy rates released by the reactions occurring at the anode surface, i.e., reforming, water-gas-shift and electro-oxidation. On the other hand, heat exchange with the surrounding environment is neglected in accordance to the adiabatic cell hypothesis introduced above. Therefore, since no useful work is delivered, the energy balance for the fuel channel can be written in the following compact form:

$$0 = \dot{E}_{f,\text{in}} - \dot{E}_{f,\text{out}} + \dot{Q}_{\text{conv},s-f} \quad (2.14)$$

where the energy rates entering and leaving the i th computational element (see Fig. 2.4) are evaluated as follows:

$$\dot{E}_{f,\text{in}} = \dot{E}_f^{i-1} + \dot{E}_{\text{prod}}^i \quad (2.15)$$

$$\dot{E}_{f,\text{out}} = \dot{E}_f^i + \dot{E}_{\text{react}}^i \quad (2.16)$$

Particularly, the energy rates associated with inlet and outlet flows and the electro-oxidation, reforming, and water-gas-shift reactions, are calculated as follows (Braun 2002):

$$\begin{aligned} \dot{E}_f^{i,i-1} = & \dot{n}_{\text{H}_2}^{i,i-1} \cdot h_{\text{H}_2} \left(T_f^{i,i-1} \right) + \dot{n}_{\text{CH}_4}^{i,i-1} \cdot h_{\text{CH}_4} \left(T_f^{i,i-1} \right) \\ & + \dot{n}_{\text{H}_2\text{O}}^{i,i-1} \cdot h_{\text{H}_2\text{O}} \left(T_f^{i,i-1} \right) + \dot{n}_{\text{CO}_2}^{i,i-1} \cdot h_{\text{CO}_2} \left(T_f^{i,i-1} \right) \\ & + \dot{n}_{\text{CO}}^{i,i-1} \cdot h_{\text{CO}} \left(T_f^{i,i-1} \right) \end{aligned} \quad (2.17)$$

$$\begin{aligned} \dot{E}_{\text{prod}}^i = & h_{\text{H}_2\text{O}}(T_s^i) \cdot \dot{r}_{\text{ox}}^i + \left[3 \cdot h_{\text{H}_2}(T_s^i) + h_{\text{CO}}(T_s^i) \right] \cdot \dot{r}_{\text{CH}_4}^i \\ & + \left[h_{\text{H}_2}(T_s^i) + h_{\text{CO}_2}(T_s^i) \right] \cdot \dot{r}_{\text{shift}}^i \end{aligned} \quad (2.18)$$

$$\begin{aligned} \dot{E}_{\text{react}}^i = & h_{\text{H}_2}(T_f^i) \cdot \dot{r}_{\text{ox}}^i + \left[h_{\text{CH}_4}(T_f^i) + h_{\text{H}_2\text{O}}(T_f^i) \right] \cdot \dot{r}_{\text{CH}_4}^i \\ & + \left[h_{\text{CO}}(T_f^i) + h_{\text{H}_2\text{O}}(T_f^i) \right] \cdot \dot{r}_{\text{shift}}^i \end{aligned} \quad (2.19)$$

On the other hand, the convective heat transfer between solid trilayer and fuel channel (see Fig. 2.5) is evaluated as:

$$\dot{Q}_{\text{conv},s-f} = \bar{h}_f^i \cdot A_s^i \cdot (T_s^i - T_f^i) \quad (2.20)$$

where $A_s^i = w_{\text{ch}} \cdot l_{\text{ch}} \cdot N^{-1}$ is the heat transfer area of the i th computational element. The convective heat transfer coefficient $\bar{h}_f^i$ is estimated, at each slice, as a function of fuel thermal conductivity (k_f), which in turn depends on both fuel composition and temperature:

$$\bar{h}_f^i = \frac{Nu \cdot k_f^i}{D_h} \quad (2.21)$$

$$k_f^i = \sum_{j=1}^n \frac{x_j^i \cdot k_j(T_f^i)}{\sum_{m=1}^n k_m(T_f^i) \cdot z_{jm}} \quad (2.22)$$

where the quantity z_{jm} is estimated as a function of the thermal conductivity and molar mass of both j th and m th species:

$$z_{jm} = \frac{\left[1 + (k_j/k_m)^{1/2} \cdot (M_m/M_j)^{1/4}\right]^2}{\left[8(1 + M_j/M_m)\right]^{1/2}} \quad (2.23)$$

Equation (2.21) also highlights the dependence of heat transfer coefficient on hydraulic diameter (Iwata et al. 2000) and Nusselt number (Braun 2002), here evaluated through the following relationships:

$$D_h = \frac{4A_{\text{ch}}}{2(h_{\text{ch}} + w_{\text{ch}})} = \frac{2w_{\text{ch}} \cdot h_{\text{ch}}}{(h_{\text{ch}} + w_{\text{ch}})} \quad (2.24)$$

$$\begin{aligned} \text{Nu} = & 7.541 \cdot 1 - (2.61 \cdot \beta + 4.97 \cdot \beta^2 - 5.119 \cdot \beta^3 \\ & + 2.702 \cdot \beta^4 + 0.548 \cdot \beta^5) \end{aligned} \quad (2.25)$$

where β is the ratio between channel height (h_{ch}) and channel width (w_{ch}).

Energy Balance for the Air Channel

In this case, the energy balance was written in such a way as to include, beyond the species flows entering and leaving the i th computational element, also the oxygen mass flow through the solid electrolyte (see Fig. 2.5). Thus, the following energy balance results for the air channel:

$$0 = \dot{E}_{a,\text{in}} - \dot{E}_{a,\text{out}} + \dot{Q}_{\text{conv},s-a} \quad (2.26)$$

$$\dot{E}_{a,\text{in}} = \dot{E}_a^{i-1} \quad \text{co-flow} \quad (2.27a)$$

$$\dot{E}_{a,\text{in}} = \dot{E}_a^{i+1} \quad \text{counter-flow} \quad (2.27b)$$

$$\dot{E}_{a,\text{out}} = \dot{E}_a^i + \dot{E}_{\text{O}_2}^i \quad (2.28)$$

where the energy rates associated with inlet and outlet flows are estimated as follows:

$$\dot{E}_a^{i-1,i+1} = \dot{n}_{\text{O}_2}^{i-1,i+1} \cdot h_{\text{O}_2}(T_a^{i-1,i+1}) + \dot{n}_{\text{N}_2} \cdot h_{\text{N}_2}(T_a^{i-1,i+1}) \quad (2.29)$$

$$\dot{E}_{\text{O}_2}^i = \frac{\dot{r}_{\text{ox}}^i}{2} h_{\text{O}_2}(T_a^i) \quad (2.30)$$

Finally, the heat exchange between air channel and solid trilayer ($\dot{Q}_{\text{conv},s-a}$) was modeled extending the approach outlined from Eqs. (2.20)–(2.25) to the species flowing in the air channel (i.e., oxygen and nitrogen).

Energy Balance for the Solid Trilayer

The last energy balance involves the control volume surrounding the entire solid trilayer and the interconnect (i.e., electrodes, electrolyte, and interconnect). Provided that radiative heat transfer can be safely neglected, the inclusion of the interconnect enables correct evaluation of heat transfer through the solid without the need of adding two further energy balances, i.e., fuel side- and air side-interconnect, as suggested by Braun (2002). Therefore, the energy rates to be included in the balance are related to the reactions occurring at electrodes surface, the heat exchange with fuel and air channels and the conductive heat transfer across the solid itself. Therefore, the following equation was obtained:

$$0 = \dot{E}_{\text{react}}^i - \dot{E}_{\text{prod}}^i + \dot{E}_{\text{O}_2}^i - \dot{Q}_{\text{conv},s-f}^i - \dot{Q}_{\text{conv},s-a}^i - \dot{E}_{el}^i + \Delta \dot{Q}_{\text{cond},s}^i \quad (2.31)$$

Among the seven terms appearing at the right-hand side of Eq. (2.31), only two of them were not introduced yet, namely the useful work released to the external load, evaluated via Eq. (2.32), and the conductive heat transfer. The last term was estimated (Braun 2002) as the difference between the heat coming from the $i - 1$ th slice and the heat leaving the i th computational element and heading for the $i + 1$ th slice (see Fig. 2.5 and Eq. 2.33):

$$\dot{E}_{\text{el}}^i = V_{\text{SOFC}} \cdot J^i \cdot A^i \quad (2.32)$$

$$\Delta Q_{\text{cond},s}^i = \frac{k_s}{\Delta X} \cdot A_{\text{front}} (T_s^{i-1} - T_s^i) - \frac{k_s}{\Delta X} \cdot A_{\text{front}} (T_s^i - T_s^{i+1}) \quad (2.33)$$

where ΔX equals the entire cell/channel length (l_{ch}) divided by the number of computational elements (N). The term V_{SOFC} at the right-hand side of Eq. (2.32) is evaluated through the electrochemical model described in Sect. 2.2.1.3. On the other hand, the term k_s at the right-hand side of Eq. (2.33) represents the solid thermal conductivity, which is usually higher in case of anode electrodes with a high percentage of Nickel cermets (Larrain et al. 2003). Furthermore, A_{front} is the solid frontal area, which is constant along the flow direction for rectangular planar SOFC designs. A_{front} is calculated as a function of electrodes, electrolyte, and interconnect thickness, thus lumping together the effects played by conduction heat transfer through solid trilayer and interconnect.

2.2.1.3 Electrochemical Balance

There are three major forms of polarization losses in fuel cells: activation, ohmic, and concentration losses. In some cases, a minor constant offset also contributes to the total polarization, which is the result of minor losses, such as internal current and leaks (e.g., fuel crossover, Chick et al. 2003). The sum of the different polarizations results in the voltage drop from Nernst potential (see Eq. 2.35) to effective operating value (0., V_{SOFC} , see Eq. 2.34). Since interconnect and electrodes are assumed isopotential, cell voltage is constant over the whole cell, and thus, the electrochemical balance can be written as follows:

$$0 = E_{\text{Nernst}}^i - V_{\text{Act}}^i - V_{\text{Ohm}}^i - V_{\text{Conc}}^i - V_{\text{SOFC}} \quad (2.34)$$

where the Nernst potential is estimated as:

$$E_{\text{Nernst}}^i = -\frac{\Delta G_{\text{ox}}^i(T_s^i)}{n_e F} - \frac{R_u T_s^i}{n_e F} \ln \left(\frac{p_{\text{H}_2\text{O}}^i}{p_{\text{H}_2}^i \sqrt{p_{\text{O}_2}^i}} \right) \quad (2.35)$$

Upon knowledge of SOFC voltage, the total power drawn out of a single cell can be evaluated as:

$$\dot{E}_{\text{el}} = V_{\text{SOFC}} \cdot I_{\text{SOFC}} = V_{\text{SOFC}} \cdot \sum_{i=1}^N (J^i \cdot A^i) \quad (2.36)$$

In the general fuel cell literature, the three main polarization losses (i.e., activation, ohmic, and concentration) are widely modeled by means of Eq. 2.37 [known as Tafel equation (Noren and Hoffman 2005)] through Eq. 2.39 (Braun 2002):

$$V_{\text{Act}}^i = \frac{R \cdot T_s^i}{\alpha(T_s^i) \cdot F} \cdot \sinh^{-1} \left(\frac{J^i}{2J_0(T_s^i)} \right) \quad (2.37)$$

$$V_{\text{ohm},k}^i = \frac{l_k}{\sigma_k(T_s^i)} \cdot J^i$$

$$V_{\text{ohm}}^i = \sum_k V_{\text{ohm},k}^i \quad k = [\text{an}, \text{ca}, \text{el}] \quad (2.38)$$

$$V_{\text{Conc}}^i = -\frac{RT_s^i}{2F} \cdot \left[\frac{1}{2} \ln \left(1 - \frac{J^i}{J_{\text{cs}}} \right) + \ln \left(1 - \frac{J^i}{J_{\text{as}}} \right) - \ln \left(1 + \frac{p_{\text{H}_2}^i \cdot J^i}{p_{\text{H}_2\text{O}}^i \cdot J_{\text{as}}} \right) \right] \quad (2.39)$$

Figure 2.6 shows the variation of activation losses as a function of current density and operating temperature. Activation polarization increases with a higher slope at low current densities (especially at low temperatures, as shown on Fig. 2.6) as compared to higher values, thus confirming that such a polarization is dominant at low loads (Larminie and Dicks 2003).

Figure 2.7 illustrates the effect of current density and temperature on SOFC ohmic losses. Even in this case temperature increase has a significantly positive effect on cell performance. Furthermore, Fig. 2.7 highlights the importance of operating fuel cells mostly at medium loads, mainly to avoid excessive ohmic resistance to occur. Using anode-supported (see Fig. 2.7b) instead of electrolyte-supported (Fig. 2.7a) cell structure allows reducing, such an overpotential, due to the higher conductivity of both electrodes as compared to electrolyte (see Table 2.2).

Fig. 2.6 Activation losses dependence on current and temperature. The values shown in the figure were estimated via Eq. (2.37). Further details on the parameters utilized in Eq. (2.37) can be retrieved from Sorrentino et al. (2004)

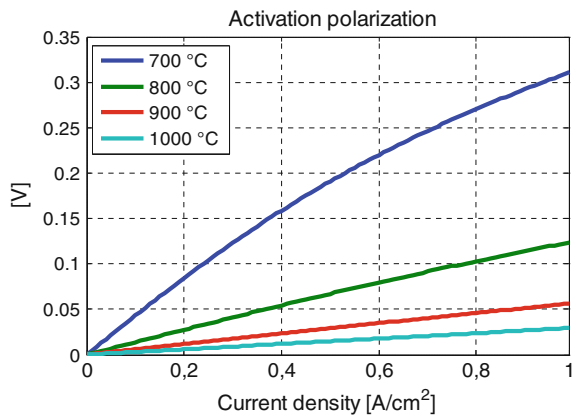


Fig. 2.7 Ohmic losses dependence on current and temperature for electrolyte- (a) and anode-supported (b) SOFC (see cell specifications in Table 2.2). The values shown in the figure were estimated via Eq. (2.38). Further details on the parameters utilized in Eq. (2.38) can be retrieved from Sorrentino et al. (2004)

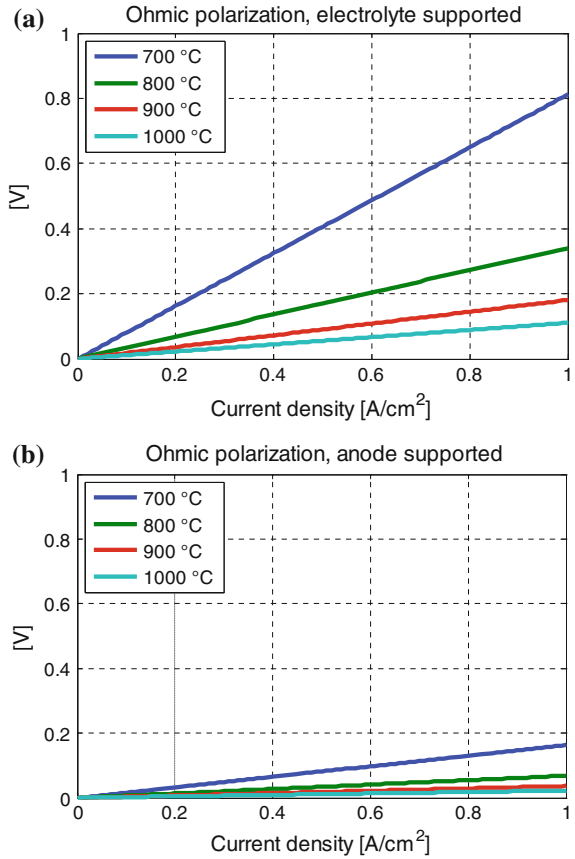


Figure 2.8 shows concentration polarization variation as a function of current density and temperature. Since both anode and cathode limiting current densities (see Eq. 2.39) depend on species diffusivity (Chick et al. 2003; Yang et al. 2013), the values shown in Fig. 2.8 were calculated assuming spatially averaged concentrations for the species involved in reformate-fed SOFC functioning (see Fig. 2.12). Concentration losses slightly increase with temperature, thus exhibiting an opposite behavior with respect to both activation and ohmic polarization (Yang et al. 2013). In any case, the comparative analysis of Figs. 2.6, 2.7, and 2.8 indicates that the negative temperature effect on concentration overpotential plays a very minor effect, thus not impacting on the general provision to make SOFC systems operate at the highest possible temperature. Furthermore, concentration polarization for anode-supported cell (see Fig. 2.8b) was shown to be higher than electrolyte-supported (see Fig. 2.8a), in accordance with the results presented and discussed in (Chan et al. 2001). Nevertheless, nowadays many stack manufacturers prefer adopting electrode-supported cells, due to the strong reduction in ohmic

Table 2.2 Input data and main cell specifications of the two model benchmarks (Ferguson et al. 1996; GENIUS 2013), both referring to a rectangular-planar SOFC

Cell type	Electrolyte-supported				Anode-supported
Validation benchmark	ES ₁	ES ₂	ES ₃	ES ₄	AS
Electroactive area (A) (cm ²)	100				100
Cell length (<i>l_{ch}</i>) (cm)	10				10
Channel width (<i>w_{ch}</i>) (mm)	3				1
Rib width (<i>w_{rib}</i>) (mm)	2.42				1
Channel height (<i>h_{ch}</i>) (mm)	1				1
Number of channels	18				50
Anode thickness (<i>l_{an}</i>) (μm)	50				1000
Cathode thickness (<i>l_{ca}</i>) (μm)	50				50
Electrolyte thickness (<i>l_{el}</i>) (μm)	150				30
Interconnect thickness (<i>l_{int}</i>) (μm)	2500				1100
Pressure (bar)	1				1
Inlet temperature (<i>T</i> ⁰) (°C)	900				[700 750]
Fuel utilization (<i>U_F</i>)	0.85				[0.5 0.6]
Excess air (λ)	7				5
Average current density (<i>J</i>) (A cm ⁻²)	0.3				[0.3 0.35]
ASR formula (Ω cm ²)	$ASR^i = \frac{l_{an}}{\sigma_{an}^i} + \frac{l_{ca}}{\sigma_{ca}^i} + \frac{l_{int}}{\sigma_{int}^i} + 3 \frac{l_{el}}{\sigma_{el}^i}$				$10^{-4} \cdot \exp\left[\frac{5 \cdot 10^4}{R} \cdot \left(\frac{1}{T_s^i} - \frac{1}{973}\right)\right]$
Anode conductivity (S cm ⁻¹)	$\sigma_{an}^i = \frac{9.5 \cdot 10^7}{T_s^i} \cdot \exp\left(-\frac{1150}{T_s^i}\right)$				–
Cathode conductivity (S cm ⁻¹)	$\sigma_{ca}^i = \frac{4.2 \cdot 10^7}{T_s^i} \cdot \exp\left(-\frac{1200}{T_s^i}\right)$				–
Electrolyte conductivity (S cm ⁻¹)	$\sigma_{el}^i = 3.34 \cdot 10^4 \cdot \exp\left(-\frac{10300}{T_s^i}\right)$				–
Interconnect conductivity (S cm ⁻¹)	$\sigma_{int}^i = \frac{9.3 \cdot 10^6}{T_s^i} \cdot \exp\left(-\frac{1100}{T_s^i}\right)$				–

(continued)

Table 2.2 (continued)

Cell type	Electrolyte-supported				Anode-supported
Thermal conductivity (k_s) (W m ⁻¹ K ⁻¹)	2				20
Fuel feed	Pure H ₂	Reformate fuel	Pure H ₂	Reformate fuel	Reformate fuel
Cell flow configuration	Co-flow		Counter-flow		Counter-flow
H ₂ O/CH ₄ fraction ($\dot{n}_{\text{H}_2\text{O}}^{\text{pre,in}} / \dot{n}_{\text{CH}_4}^{\text{pre,in}}$)	–	2.5	–	2.5	2
Inlet H ₂ composition	0.9	0.263	0.9	0.263	0.128
Inlet H ₂ O composition	0.1	0.493	0.1	0.493	0.560
Inlet CH ₄ composition	–	0.171	–	0.171	0.28
Inlet CO composition	–	0.029	–	0.029	0.0004
Inlet CO ₂ composition	–	0.044	–	0.044	0.032
Inlet O ₂ composition	0.21				
Inlet N ₂ composition	0.79				

losses and the very minor contribution of concentration losses on overall SOFC overpotential (Aguilar et al. 2004; Larrain et al. 2003).

It is finally worth remarking at the end of this section that, since SOFCs are mainly operated in the linear current-voltage profile region, some researchers (Andersson 2011) proposed to lump the total amount of polarization losses into one contribution, proportional to the area-specific resistance coefficient (ASR), thus resulting in the following simplified electrochemical balance:

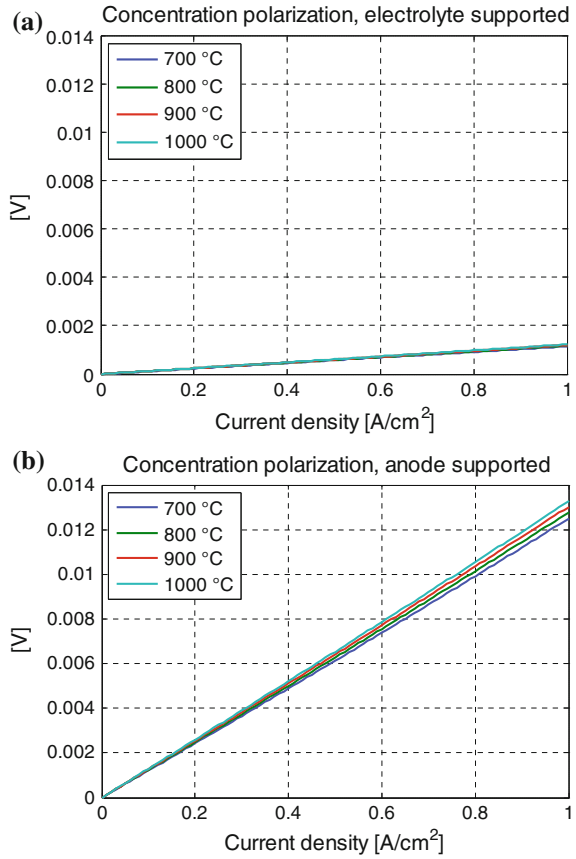
$$0 = E_{\text{Nernst}}^i - \text{ASR}^i \cdot J^i - V_{\text{SOFC}} \quad (2.40)$$

Standing the high reliability of Eq. (2.40), in this work the 1D model validation was performed by referring to ASR formulas proposed in the literature.

2.2.1.4 Load Balance

The last balance, to be satisfied to close the system of one-dimensional governing equations, is obtained by imposing that average current density along the cell channels corresponds to the applied load. This assumption well agrees with the

Fig. 2.8 Concentration losses dependence on current and temperature for electrolyte- (a) and anode-supported (b) SOFC (see cell specifications in Table 2.2). The values shown in the figure were estimated via Eq. (2.39). Further details on the parameters utilized in Eq. (2.39) can be retrieved from Sorrentino et al. (2004)



most common operation strategy adopted for fuel cells, namely to change current density to meet useful power demand, which in turn corresponds to galvanostatic operation of the stack. The mathematical counterpart of the above concept can be represented as:

$$0 = \frac{I_{\text{SOFC}}}{A} - \frac{1}{N} \sum_{i=1}^N J^i \quad (2.41)$$

where the term at the first denominator corresponds to the entire electroactive area of a single fuel cell.

2.2.1.5 Numerical Solution

The spatial variation of the main operating variables is evaluated by discretizing the SOFC in N computational elements and iteratively solving, for each element, the

governing equations. Particularly, energy, electrochemical, and current density balances are to be solved to estimate the distributions of current density, temperatures, and compositions along the cell channels. The numerical problem can thus be expressed as:

$$F(\Theta) = 0 \quad (2.42)$$

where Θ is a $5N + 1$ long vector of unknowns:

$$\begin{aligned} \Theta &= \{\theta^1, \theta^2, \dots, \theta^N, V_{\text{SOFC}}\} \\ \theta^i &= \{J^i, r_{\text{shift}}^i, T_f^i, T_a^i, T_s^i\} \end{aligned} \quad (2.43)$$

As explained in the previous sections, the system of governing equations is highly nonlinear, thus requiring to build-up a numerical iterative solution (Braun 2002; Haynes 1999; Sorrentino et al. 2004). Such a solution is here obtained as shown in Fig. 2.9, which highlights how the problem expressed by Eq. (2.42) is treated as a multi-objective optimization task, mathematically expressed as:

$$\min_{\Theta} |F(\Theta)| \quad (2.44)$$

Equation (2.44) ensures that the optimal Θ vector, obtained after successfully minimizing all of the f^i terms shown in Eq. (2.51), is as close as possible to those satisfying Eq. (2.42) exactly (Yang 2013). The vector F is calculated at each h iteration by concatenating the residuals associated to the electrochemical balance (i.e., res_{ele} , Eq. 2.45a, 2.45b), water-gas-shift equilibrium constant (i.e., $\text{res}_{\text{Kshift}}$, Eq. 2.46), energy balances (i.e., $\text{res}_{\text{energy},f}$, Eq. 2.47, $\text{res}_{\text{energy},a}$, Eq. 2.48, $\text{res}_{\text{energy},s}$, Eq. 2.49), and load balance (i.e., res_{load} , Eq. 2.50):

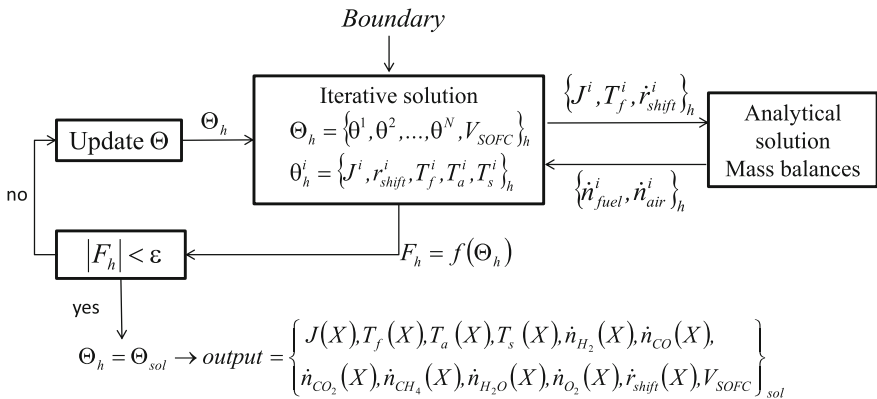


Fig. 2.9 Schematic representation of the procedure developed to solve, in a least square way, the system of governing equations expressed by Eqs. (2.45a, 2.45b)–(2.50). The variables $\dot{n}_{\text{fuel}}^i$ and $\dot{n}_{\text{air}}^i$ are nothing but vectors including the molar flows of anodic and cathodic species, respectively

$$\text{res}_{\text{ele}}^i = E_{\text{Nernst}}^i - V_{\text{ohm}}^i - V_{\text{conc}}^i - V_{\text{act}}^i - V_{\text{SOFC}} \quad (2.45a)$$

$$\text{res}_{\text{ele}}^i = E_{\text{Nernst}}^i - \text{ASR}^i \cdot J^i - V_{\text{SOFC}} \quad (2.45b)$$

$$\text{res}_{K\text{shift}}^i = \exp\left(\frac{-\Delta G_{\text{shift}}(T_s^i)}{R \cdot T_s^i}\right) - \frac{\dot{n}_{\text{H}_2}^i \cdot \dot{n}_{\text{CO}_2}^i}{\dot{n}_{\text{CO}}^i \cdot \dot{n}_{\text{H}_2\text{O}}^i} \quad (2.46)$$

$$\text{res}_{\text{energy},f}^i = \dot{E}_{f,\text{in}} - \dot{E}_{f,\text{out}} + \dot{Q}_{\text{conv},s-f} \quad (2.47)$$

$$\text{res}_{\text{energy},a}^i = \dot{E}_{a,\text{in}} - \dot{E}_{a,\text{out}} + \dot{Q}_{\text{conv},s-a} \quad (2.48)$$

$$\begin{aligned} \text{res}_{\text{energy},s}^i &= \dot{E}_{\text{react}}^i - \dot{E}_{\text{prod}}^i + \dot{E}_{\text{O}_2}^i - \dot{Q}_{\text{conv},s-f}^i - \dot{Q}_{\text{conv},s-a}^i - \dot{E}_{\text{el}}^i \\ &+ \Delta \dot{Q}_{\text{cond},s}^i \end{aligned} \quad (2.49)$$

$$\text{res}_{\text{load}} = \frac{I_{\text{SOFC}}}{A} - \frac{1}{N} \sum_{i=1}^N J^i \quad (2.50)$$

Thus, the following $5N + 1$ long vector F results at each h iteration:

$$\begin{aligned} F &= \{f^1, f^2, \dots, f^N, \text{res}_{\text{load}}\} \\ f^i &= \{\text{res}_{\text{ele}}^i, \text{res}_{K\text{shift}}^i, \text{res}_{\text{energy},f}^i, \text{res}_{\text{energy},a}^i, \text{res}_{\text{energy},s}^i\} \end{aligned} \quad (2.51)$$

It is worth noting here that the residuals (i.e., the res terms), introduced in Eqs. 2.45a, 2.45b–2.50, are nothing but the right-hand side of their respective governing equations, presented in the previous sections (e.g., res_{load} corresponds to the value of the right-hand side of Eq. 2.41).

Figure 2.9 highlights how the residual balances to be met, namely the mass balances expressed by Eq. 2.2a–2.2g, are not directly involved in the multi-objective minimization problem described above, in that no molar flows are fed as unknown parameters to the problem expressed by Eq. (2.44). This happens both because the water-gas-shift reaction rate is one of the unknowns (see Eq. 2.43) and, furthermore, the methane reforming and electro-oxidation reaction rates are respectively computed as a function of solid temperature (see Eq. 2.6) and current density (see Eq. 2.7), which are also present among the unknowns. Therefore, as shown in Fig. 2.9, at each iteration, beyond calculating the actual value of the vector F , the mass balances expressed by Eq. 2.2a–2.2g are solved analytically, thus yielding on output the molar flows distributions. Such molar distributions are then concatenated to the vector of unknowns (i.e., Eq. 2.43), thus resulting in the following comprehensive output vector yielded by the entire procedure schematically described in Fig. 2.9:

$$\text{Output} = \left\{ J(X), T_f(X), T_a(X), T_s(X), \dot{n}_{\text{H}_2}(X), \dot{n}_{\text{CO}}(X), \right. \\ \left. \dot{n}_{\text{CO}_2}(X), \dot{n}_{\text{CH}_4}(X), \dot{n}_{\text{H}_2\text{O}}(X), \dot{n}_{\text{O}_2}(X), \dot{r}_{\text{shift}}(X), V_{\text{SOFC}} \right\} \quad (2.52)$$

Figure 2.9 also highlights that the iterative procedure, to be developed to perform root-finding for the problem expressed by Eq. (2.44), can only be started upon knowledge of the vector of boundary conditions, which includes the following variables:

$$\text{Boundary} = \left\{ U_f, \lambda, \bar{J}, T^0, p, x_{f,m}^0, x_{a,m}^0 \right\} \quad (2.53)$$

Finally, it is worth shortly describing how the procedure illustrated in Fig. 2.9 operates. Once the boundary conditions expressed by Eq. (2.53) are known, the iterative procedure is started by providing as inputs the initial $5N + 1$ conditions for the vector of unknowns Θ to the multi-objective optimization problem, here solved by means of the well-known Levenberg–Marquardt minimization algorithm (Yang 2013). Then, at each h iteration the f_h^i values are determined as a function of the current Θ vector, depending on which the molar flow distributions also are analytically computed with (see “Analytical solution” block in Fig. 2.9). Afterwards, the vector F is checked in a least square way, namely if the norm $|F|$ is below a safe threshold, the actual values of the variables included in Eq. (2.43) are yielded on output as final solution of the system of governing equations. Otherwise, the procedure is repeated by updating the Θ vector by means of the Levenberg–Marquardt algorithm, until a final solution with a satisfactorily small norm $|F|$ is reached.

2.2.1.6 Model Validation

The model detailed above was tested for validation by referring to two different benchmarks. The first one (i.e., benchmark ES in Table 2.2, corresponding to a high temperature electrolyte-supported SOFC), which was already tested by the authors in a previous article (Sorrentino et al. 2008) for co-flow configuration only, was here further tested in counterflow configuration, thus resulting in four sub-benchmarks ES1 through ES4, as explained in Table 2.2. The second benchmark (i.e., benchmark AS in Table 2.2, corresponding to a low temperature anode-supported SOFC) was tested by authors’ institution, i.e., the University of Salerno (UNISA, Italy), the Technical Institute of Finland (VTT), and the University of Genoa (UNIGE, Italy), within the European Funded project GENIUS (GENIUS 2013). Both model benchmarks were solved assuming a simplified ASR formula, thus allowing to perform lumped modeling of polarization losses as a function of operating temperature (see Eq. 2.45b). Figure 2.10 provides the reader with a schematic explanation of the main geometrical data introduced in Table 2.2.

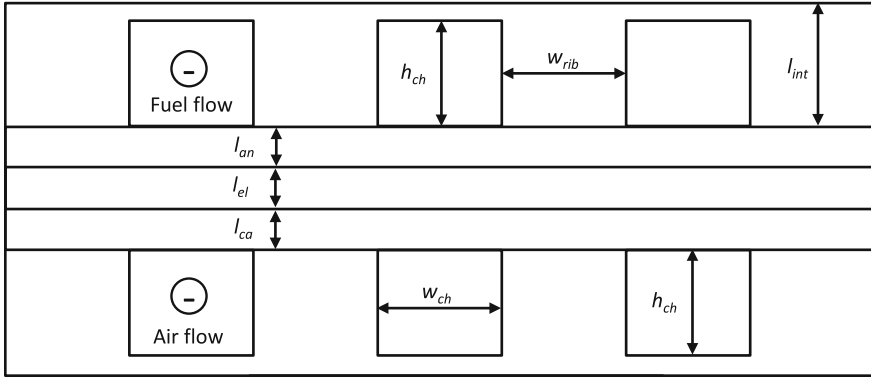


Fig. 2.10 Cross-sectional view of a single, planar, and co-flow SOFC consisting of three rectangular channels at both fuel and air side

The following two subsections present a deep discussion on the main outcomes of the above-introduced model benchmarking, performed by discretizing the cell into a number of computational elements N ranging between 10 and 50, depending on successful convergence of the root-finding problem shown in Fig. 2.9. As a consequence of different cell discretization, running time varied between 20 and 400 s on a 2.53 GHz Intel® Core™ Duo CPU. Afterwards, a parametric analysis is proposed in Sect. 2.2.1.7, whose aim is to show the potentialities, offered by the 1D model, to qualitatively analyze the effects played by main operating variables on SOFC performance and behavioral features.

ES Benchmark Results

The benchmarks ES₁ through ES₄ were modeled assuming that cell polarization losses can be estimated via the ASR formula proposed by the International Energy Agency (IEA) (Braun 2002; Ferguson 1996), which is also given in Table 2.2. The results obtained running the 1D SOFC model on the ES cases are summarized in Figs. 2.11, 2.12 and Table 2.3. It is worth noting here that in Fig. 2.11 only the solid-trilayer temperature profile is plotted, since the temperature of the other control volumes (i.e., fuel and air channels) do not differ significantly, as already observed in previous studies (Iwata et al. 2000).

In case of pure hydrogen feed (see subplots (a) and (c) in Figs. 2.11 and 2.12), the model results indicate that temperature monotonically increases in the direction of air-flow. Such a behavior is expected since SOFCs are air-cooled by supplying the cathode channels with extremely high excess of air with respect to stoichiometry. Therefore, the air-flow is subject to continuous heat adsorption going from

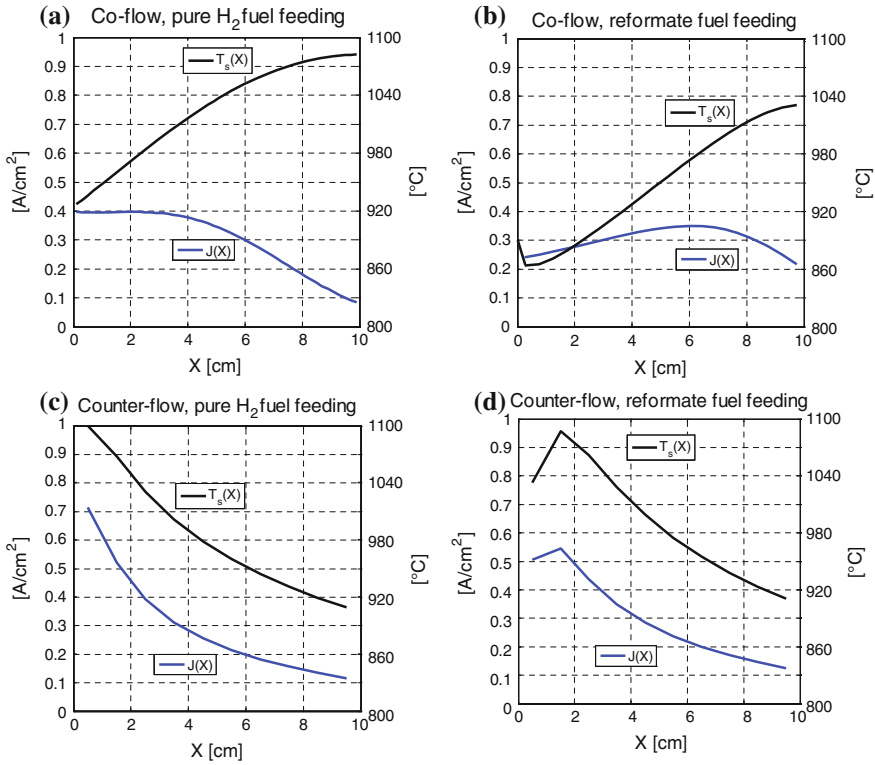


Fig. 2.11 Current and temperature distributions yielded on output by the 1D model executed on BA benchmarks (see Table 2.2)

cathode inlet to outlet. On the other hand, when reformat fuel is fed to the anode channels (see subplots (b) and (d) in Figs. 2.11 and 2.12), temperature distribution exhibits a sudden decrease in proximity of anode inlet. This happens because the residual methane, held by the inlet fuel flow after having undergone the external pre-reforming process (see Sect. 2.2.1.2.1), quickly gets internally reformed, as shown in Fig. 2.12b, d. Such an internal reforming process is endothermic, thus causing solid temperature to decrease until methane disappears, around one fifth of cell length. Afterwards, temperature trend is similar to that occurring in case of pure hydrogen feed.

The analysis of current distributions is shown in Figs. 2.11 and 2.12 highlights that they are strongly dependent on both temperature and hydrogen composition. Indeed, current always decreases when hydrogen composition becomes very low. However, in case of co-flow configuration the current profile is more flat as

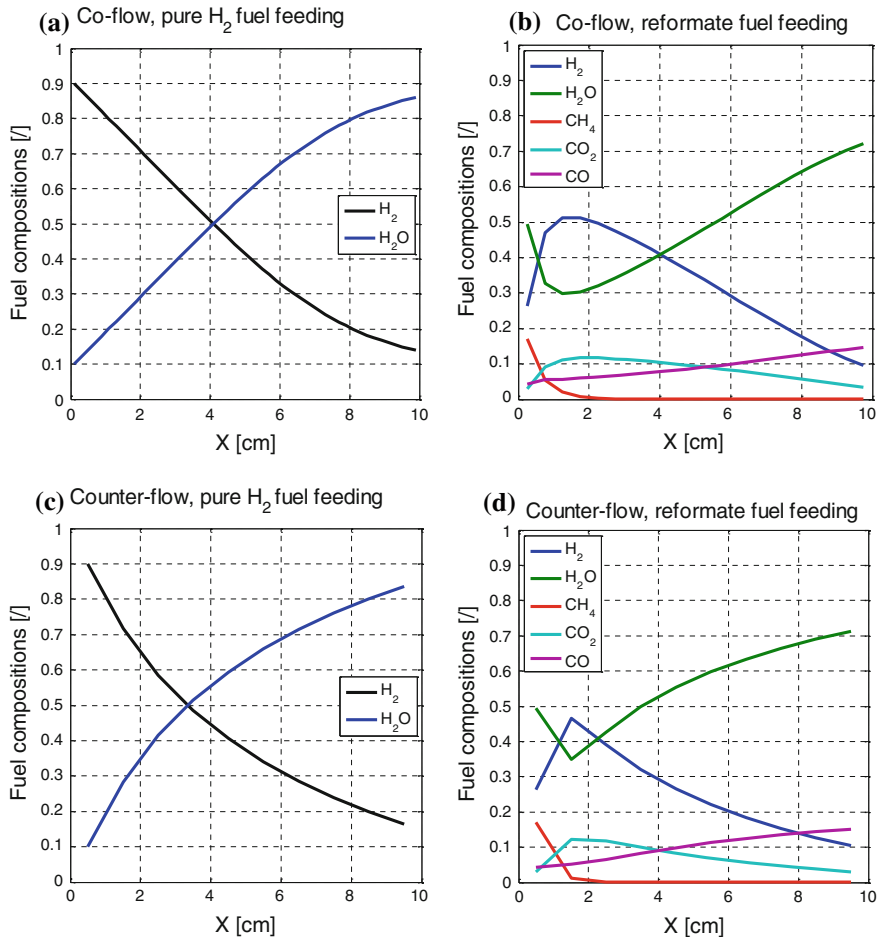


Fig. 2.12 Fuel compositions distributions yielded on output by the 1D model executed on the ES benchmarks (see Table 2.2)

compared to counterflow cases. Such a behavior can be justified considering that, as explained in the previous paragraph, counterflow temperature distribution reaches the maximum values nearby anode inlet, whereas the opposite happens in co-flow cases. As it is well known (Braun 2002; U.S. Department of Energy 2004), temperature increase always causes polarization losses to decrease. Therefore, counterflow current profiles start (at $X = 0$) from very high values at anode inlet, due to the beneficial effects of temperature increase and high hydrogen concentration. On the other hand, in co-flow configuration current profile starts with a flat shape in

Table 2.3 Comparison of 1D SOFC model results with literature data

Variable	Benchmark	1D SOFC model	Literature data ranges (min max) (Braun 2002; Ferguson et al. 1996)
Voltage (V)	ES ₁ (co-flow, pure H ₂)	0.713	[0.702 0.722]
	ES ₂ (co-flow, methane reformat)	0.656	[0.633 0.650]
	ES ₃ (counter-flow, pure H ₂)	0.715	[0.709 0.730]
	ES ₄ (counter-flow, methane reformat)	0.693	[0.680 0.693]
Maximum current density (A cm ²)	ES ₁ (co-flow, pure H ₂)	0.397	[0.373 0.396]
	ES ₂ (co-flow, methane reformat)	0.350	[0.3040 0.367]
	ES ₃ (counter-flow, pure H ₂)	0.715	[0.711 0.897]
	ES ₄ (counter-flow, methane reformat)	0.544	[0.533 0.655]
Minimum current density (A cm ²)	ES ₁ (co-flow, pure H ₂)	0.085	[0.102 0.137]
	ES ₂ (co-flow, methane reformat)	0.218	[0.175 0.251]
	ES ₃ (counter-flow, pure H ₂)	0.116	[0.108 0.124]
	ES ₄ (counter-flow, methane reformat)	0.125	[0.099 0.133]
Maximum solid temperature (°C)	ES ₁ (co-flow, pure H ₂)	1082	[1048 1098]
	ES ₂ (co-flow, methane reformat)	1031	[1020 1034]
	ES ₃ (counter-flow, pure H ₂)	1099	[1062 1084]
	ES ₄ (counter-flow, methane reformat)	1087	[1062 1089]
Minimum solid temperature (°C)	ES ₁ (co-flow, pure H ₂)	927	[924 930]
	ES ₂ (co-flow, methane reformat)	864	[845 862]
	ES ₃ (counter-flow, pure H ₂)	909	[904 913]
	ES ₄ (counter-flow, methane reformat)	911	[906 915]

case of pure hydrogen feeding, while, when reformat fuel is used, current is even lower than maximum values at anode inlet. Lower currents at anode inlet, in case of co-flow configuration, are determined by the high polarization losses caused by low temperature values in those locations. The difference between pure hydrogen and reformat fuel feeding is due again to the reforming process occurring nearby cathode inlet, which causes temperature to be further low at those locations. It is of

course straightforward that minimum current values occur near anode outlet, since hydrogen gets almost completely depleted and, thus, concentration overpotential induced by fuel starvation becomes dominant.

Regarding fuel compositions shown in Fig. 2.12, one significant difference emerges from the comparative analysis of co- and counterflow configurations, namely the different slope with which hydrogen composition decreases. Indeed, counterflow hydrogen composition decreases with a larger slope at the beginning, as it can be easily noted by looking at the much earlier intersection occurring among H_2 and H_2O distributions as compared to co-flow configuration. Particularly, in case of pure hydrogen feeding the intersection corresponds to the ordinate value of 0.5, which is reached after 4 and 3.2 cm for co- (Fig. 2.12a) and counterflow (Fig. 2.12c), respectively. On the other hand, in case of reformat fuel, the intersection of interest is the second one, since the first one occurs because hydrogen/water concentration initially increases/decreases due to the reforming reaction, which mostly occurs nearby the anode inlet. In this case, the intersection corresponds to an ordinate value of 0.4, which is reached by hydrogen and water concentrations after 4 and 2.2 cm in case of co- (Fig. 2.12b) and counterflow (Fig. 2.12d), respectively. This behavior is strictly linked to what was explained in the previous paragraphs about temperature and current. Particularly, the higher the temperature the lower polarization losses will be, thus the electrochemical reaction mostly occurs nearby anode inlet in counterflow, which in turn results in faster H_2 depletion at those channel locations.

The reliability of the 1D SOFC model here presented and, as a consequence, the validity of the considerations made above, is confirmed by the very good agreement emerging from the results comparison described in Table 2.3. Particularly, 1D SOFC model outputs always fall within or very close to the data ranges provided in the literature for the IEA benchmark. Furthermore, the comparison between pure hydrogen and reformat fuel voltages indicates that the latter feeding always results in lower SOFC voltage, due to the lower average temperature as compared to the hydrogen feed (see Fig. 2.11). This does not mean that adopting a reformat fuel results in less efficient SOFC operation, due to the different lower heating values of the working fuels, methane, and hydrogen, respectively. Indeed, efficiencies in the two cases are evaluated as follows:

$$\eta_{H_2} = \frac{V_{SOFC} \cdot \bar{J} \cdot A}{n_{H_2}^0 \cdot LHV_{H_2}} \quad (2.54)$$

$$\eta_{CH_4} = \frac{V_{SOFC} \cdot \bar{J} \cdot A}{n_{CH_4}^{pre,in} \cdot LHV_{CH_4}} \quad (2.55)$$

Substituting Eq. (2.8) in Eqs. (2.54) and (2.55), the efficiencies in cases ES_1 and ES_3 (i.e., pure hydrogen, see Table 2.2) and cases ES_2 and ES_4 (i.e., reformat fuel) are, respectively:

$$\begin{aligned}\eta_{H_2} &= \frac{V_{SOFC} \cdot \bar{J} \cdot A}{\frac{\bar{J} \cdot A}{2F \cdot U_f} \cdot LHV_{H_2}} = \frac{2F}{LHV_{H_2}} \cdot V_{SOFC} \cdot U_f = 0.8 \cdot 0.713 \cdot 0.85 \\ &= 0.485 \text{ co-flow} = 0.8 \cdot 0.715 \cdot 0.85 = 0.486 \text{ counter-flow}\end{aligned}\quad (2.56)$$

$$\begin{aligned}\eta_{CH_4} &= \frac{V_{SOFC} \cdot \bar{J} \cdot A}{\frac{\bar{J} \cdot A}{8F \cdot U_f} \cdot LHV_{CH_4}} = \frac{8F}{LHV_{CH_4}} \cdot V_{SOFC} \cdot U_f = 0.96 \cdot 0.656 \cdot 0.85 \\ &= 0.535 \text{ co-flow} = 0.96 \cdot 0.693 \cdot 0.85 = 0.565 \text{ counter-flow}\end{aligned}\quad (2.57)$$

It is worth noting that Eqs. (2.56) and (2.57) enable fast and easy estimation of SOFC gross efficiency, which is mainly dependent on voltage (easily measurable on real systems) and fuel utilization values.

AS Benchmark Results

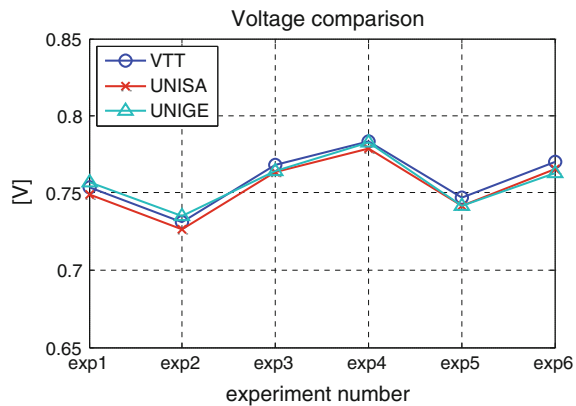
As mentioned above, the second benchmark was specifically created, within the EU project GENIUS (2013), aiming at performing a comparative analysis between variables estimated via three different 1D static models. The results of such a comparative analysis, shown in Figs. 2.13, 2.14 and 2.15, were considered worthy to be included in this book, not only to further assess the reliability of the 1D model proposed by the authors, but also to examine the performance of a planar SOFC with geometry and operating temperatures significantly different than ES benchmark (see Table 2.2). Particularly, the anode-supported cell (i.e., the one modeled in benchmark AS) is quite representative of what is currently addressed by stack manufacturers as the most suitable configuration to meet the conflicting requirements of lifetime, performance and cost, with the final aim of enhancing SOFC commercial deployment (Blum et al. 2013; Topsoe Fuel Cell 2013; Sofcpower 2013).

Figure 2.13 highlights the very good agreement achieved by the involved institutions¹ on SOFC voltage estimation, with values ranges bounded within 8.8 mV. On the other hand, Figs. 2.14 and 2.15 allow appreciating the fact that all models predicted similar temperature and current spatial distributions, also with similar shapes, especially when comparing VTT and UNISA data.

The comparative analysis of current and temperature profiles, predicted in the ES (specifically ES₄) and AS benchmarks (i.e., Fig. 2.11 with Figs. 2.14 and 2.15), clearly outlines that, despite being both operated in counterflow, the AS profiles are much smoother than ES₄. This can be explained considering that in the AS benchmark a higher thermal conductivity was assumed with respect to ES₄ (see Table 2.2). Such an assumption, which could represent a case in which a higher percentage of Nickel cermet is present in the anode material, makes the effect of

¹UNISA model corresponds to the 1D SOFC model label of Table 2.3.

Fig. 2.13 Comparison of single cell voltages estimated by the three 1D SOFC models on the AS benchmark. Exp 1 through exp 6 corresponds to the specification provided in the plot titles shown on Fig. 2.14 (Reprinted with permission of original authors —GENIUS 2013)



thermal conduction through the solid (see Eq. 2.33) more relevant, which in turn results in the more even temperature distributions shown on Fig. 2.15, as compared to Fig. 2.11d. As deeply discussed in Sect. 2.2.1.6.1, the flatter temperature profile of Fig. 2.15 causes also the current profile to smooth out (see Fig. 2.14), due to strict dependence of current density on temperature through polarization losses.

2.2.1.7 Steady-State Parametric Analysis

This section presents an analysis and discusses related outcomes on the effects played by main operating variables, namely fuel utilization, excess air, and temperature, on SOFC performance in steady conditions. For this purpose, the cell geometry and polarization losses model used for the AS benchmark (see Table 2.2) were referred to when performing a dedicated 1-D model-based numerical analysis.

The analysis was carried-out for both pure H_2 and methane reformat feeds, by separately varying the operating variables around the nominal values listed in Table 2.4. Hereinafter, atmospheric operation is assumed (i.e., operating pressure was set to 1 bar). It is finally worth mentioning that only results obtained in co-flow configuration are shown hereinafter for sake of conciseness, as a consequence of the fact that the impact played by main operating variables on cell performance is substantially the same as in the counterflow configuration.

Figure 2.16 shows the cause-effect diagram associated to temperature increase. At high current loads, cell voltage increases, due to the beneficial impact of temperature rise on both activation and ohmic polarization (Braun 2002; Haynes 1999). On the other hand, at low loads the reduction in Nernst potential slightly prevails on losses decrease. The above cause-effect relationships are consistent with the parametric analysis carried-out on temperature influence, as shown in Fig. 2.17. Temperature increase throughout the cell length was simply obtained by increasing inlet temperature. The comparison between the Fig. 2.17a, b highlights that the

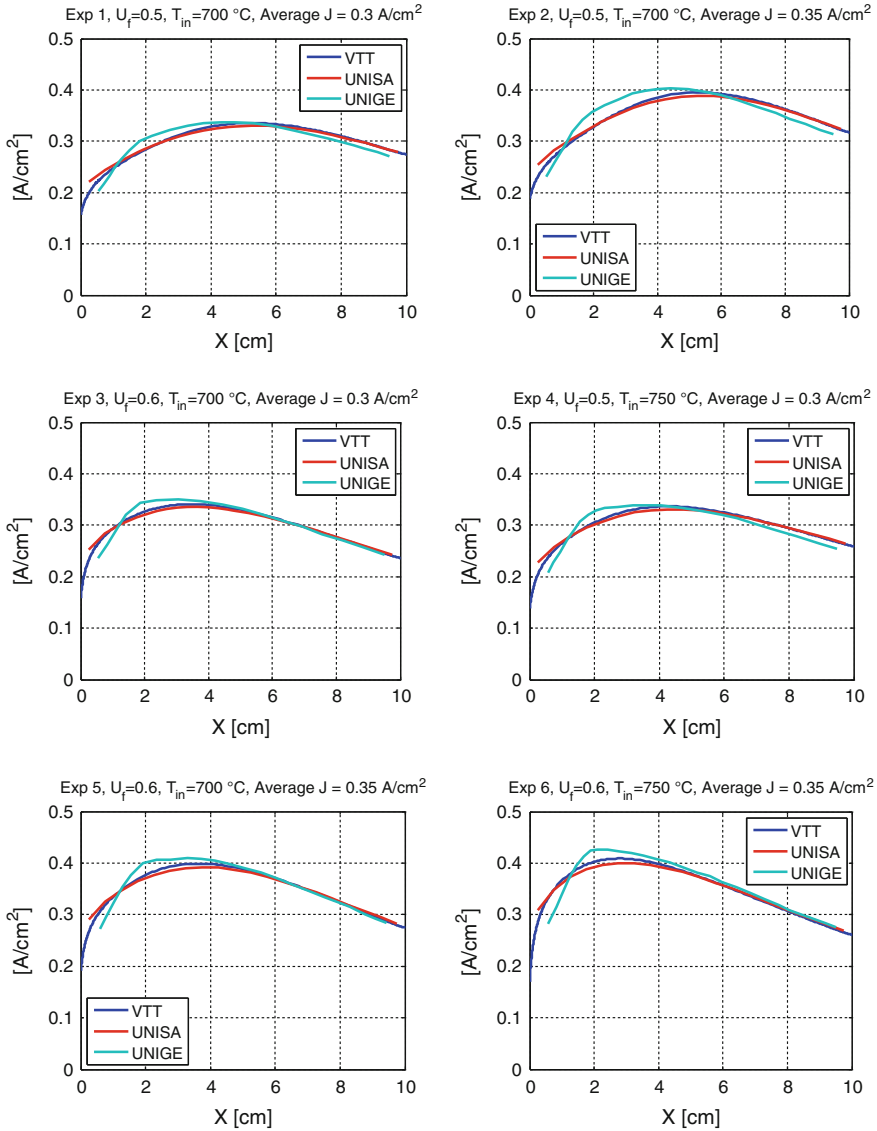


Fig. 2.14 Comparison of current density profiles yielded on output by the three models involved in the AS benchmark (Reprinted with permission of original authors—GENIUS 2013)

slope of the voltage curves obtained for methane reformat feed is higher than pure H_2 feed.

Figure 2.18 shows the cause-effect diagram associated to fuel utilization variation. Fuel utilization influence on cell voltage is twofold. Whenever fuel utilization

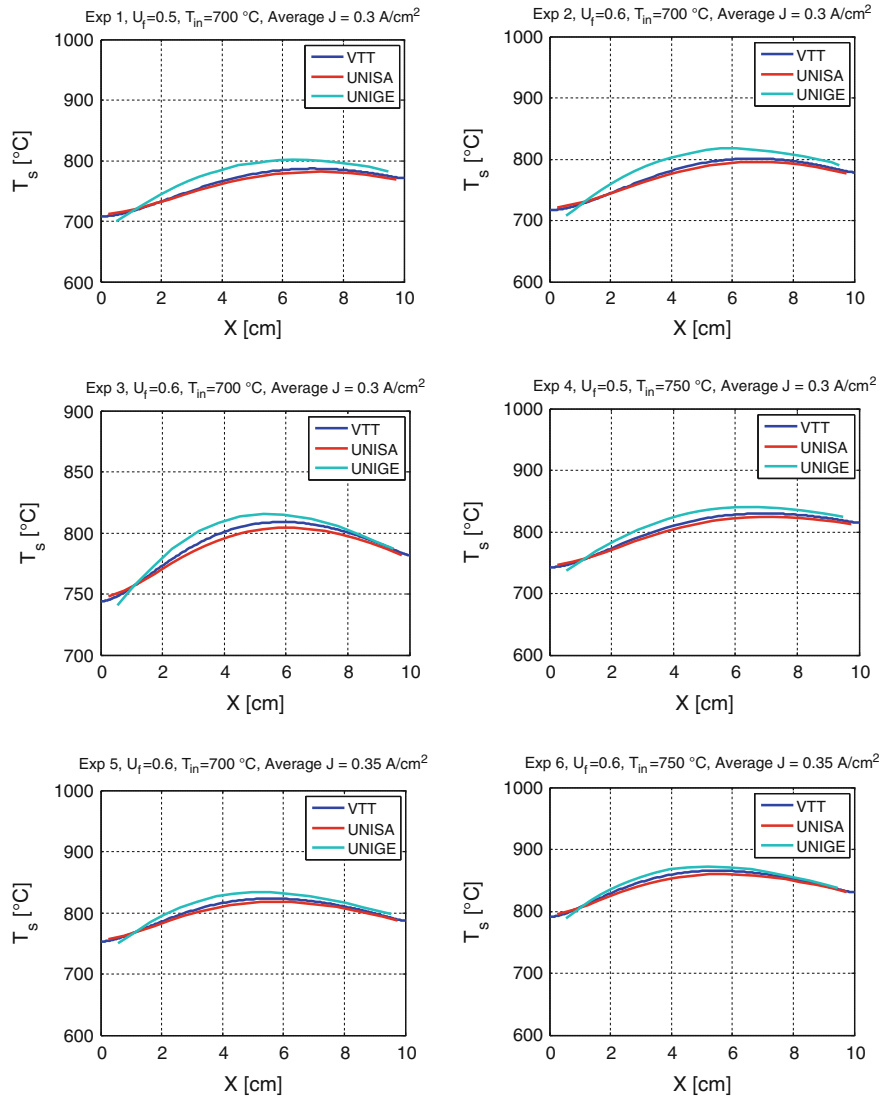


Fig. 2.15 Comparison of solid temperature profiles yielded on output by the three models involved in the AS benchmark (Reprinted with permission of original authors—GENIUS 2013)

Table 2.4 Nominal operating conditions assumed in the parametric analysis

Parameter	Value
U_f (l)	0.65
λ (l)	7
T_{in} (°C)	750

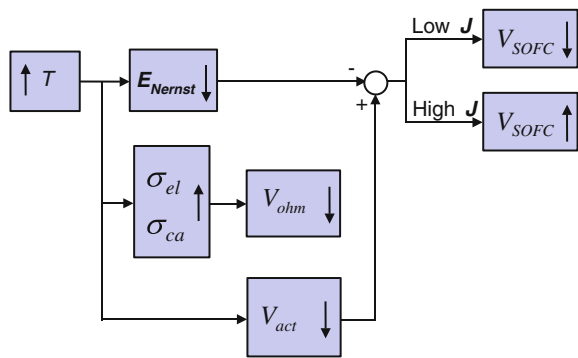


Fig. 2.16 Cause-effect diagram showing the overall effect of temperature increase on cell voltage

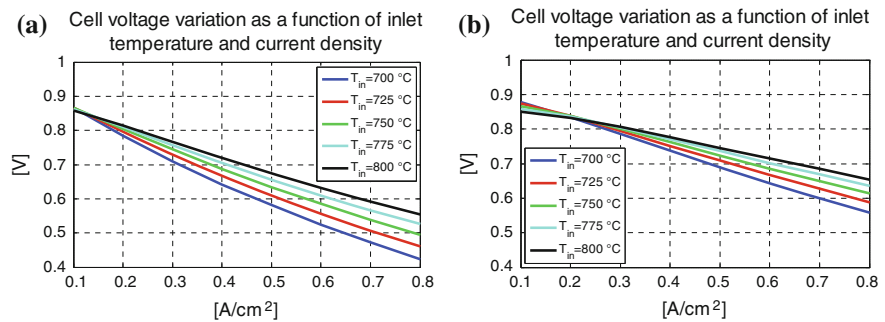


Fig. 2.17 Impact of temperature increase on SOFC voltage for **a** methane reformat and **b** pure H_2 feed

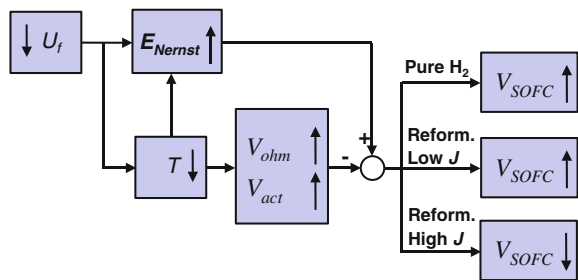


Fig. 2.18 Cause-effect diagram showing the overall effect of fuel utilization variation on cell voltage

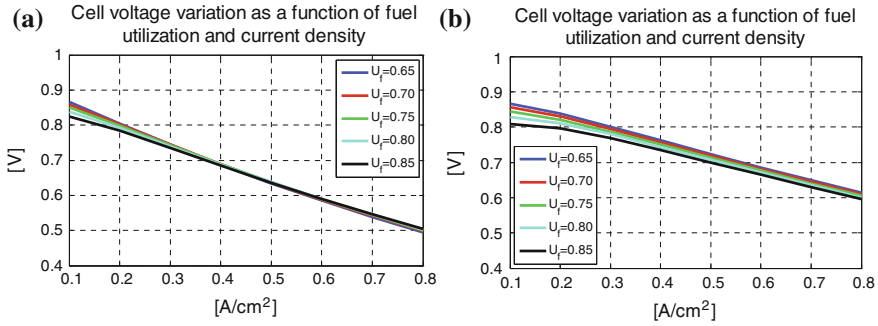
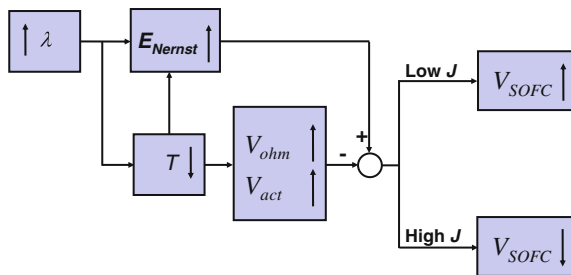


Fig. 2.19 Impact of fuel utilization variation on SOFC voltage for **a** methane reformat and **b** pure H_2 feed

reduces, reactant partial pressure in the fuel channel increases, thus resulting in higher Nernst potential throughout the cell. On the other hand, a higher amount of fuel results in temperature decrease because of two reasons: more heat adsorbed by flowing gases and, for reformat feed, more heat required for internally reforming the residual amount of methane. In Fig. 2.19 the results obtained when varying fuel utilization are shown. For pure H_2 feed (see Fig. 2.19b), a voltage gain is observed throughout the investigated load range of current, although it decreases when current density increase. In case of methane reformat feed, instead, U_f effect is positive at low loads, then slightly negative at medium-high current densities (see Fig. 2.19a). Therefore, the indications provided in the cause-effect diagram were shown to be consistent.

In Fig. 2.20, the cause-effect diagram describing the excess air effect is shown. Such an operating variable, similarly to what was discussed previously for the temperature effect, influences cell performance in two ways. A high excess of air positively affects Nernst potential, due to the higher reactants partial pressure at the cathode side. On the other hand, a high amount of air overcools the cell, thus causing activation and ohmic polarization to increase. The dominance of one effect

Fig. 2.20 Cause-effect diagram showing the overall effect of excess air variation on cell voltage



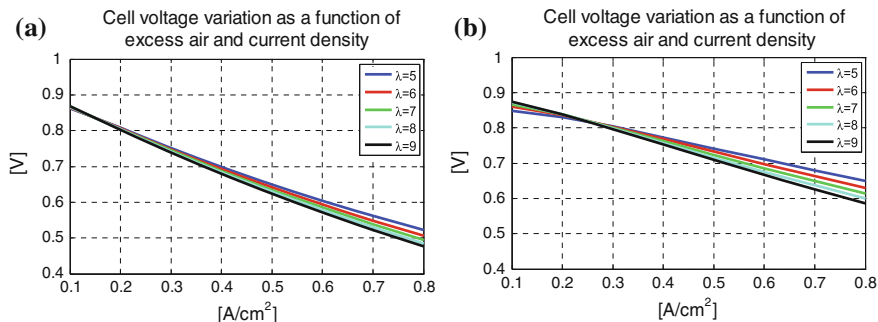


Fig. 2.21 Impact of excess air variation on SOFC voltage for **a** methane reformat and **b** pure H_2 feed

on the other results in the occurrence of two separate effect zones, as confirmed by the parametric analysis performed on λ , whose results are shown on Fig. 2.21. The comparison between methane reformat (see Fig. 2.21a) and pure H_2 (Fig. 2.21b) feed evidences how in the former case λ effect on cell voltage is less evident and, moreover, the switch from the first to the second effect zone corresponds to a different current density value.

2.3 Lumped (Gray-Box) Modeling

As deeply discussed in Chap. 1 and Sect. 2.1, the availability of fast and accurate dynamic models is nowadays considered highly strategic, especially to enhance the development of reliable and effective control and diagnostic strategies for SOFC systems. In this section, lumped modeling is proposed as a suitable approach to achieve a satisfactory compromise between computational time, experimental burden, and accuracy. The hierarchical sequence shown in Fig. 2.2 was fruitfully exploited to derive a control-oriented model of SOFC dynamic performance. Particularly, such a model was proven effective to study and the SOFC dynamic response to load change, thus deriving useful information towards the definition of real-world applicable management strategies for SOFC-based energy systems.

Furthermore, the lumped modeling approach was extended to the other main ancillary components, which an SOFC system consists of. Particularly, Fig. 2.22 highlights how achieving proper SOFC functioning entails surrounding the stack with several devices, the most significant ones being the air pre-heater, fuel pre-reformer, postburner, and air compressor. The following subsections present in detail the lumped submodels developed to enable dynamic simulation of an entire SOFC system. A larger attention was of course paid to the SOFC stack, for which not only the basic equations are presented and tested in simulation, but also

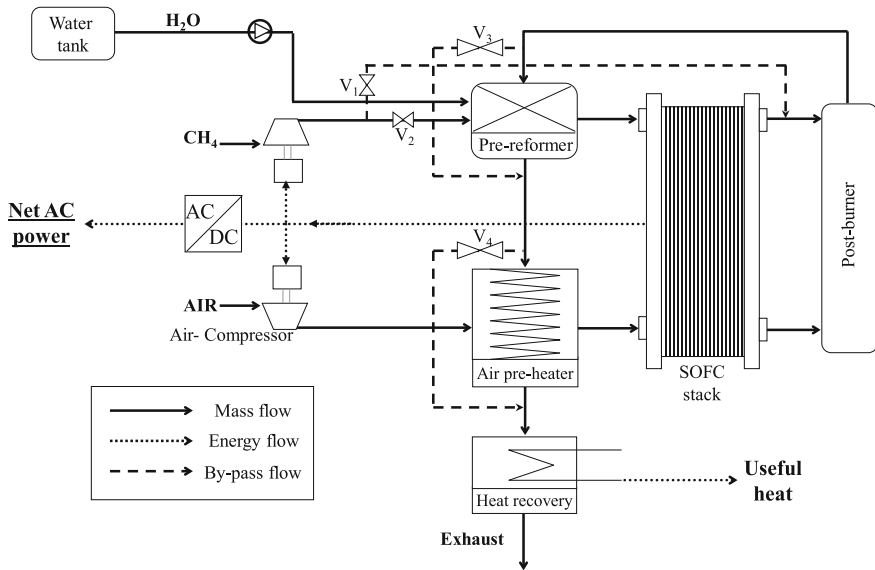


Fig. 2.22 Typical layout (adapted from Sorrentino and Pianese 2009) of an SOFC APU, showing the most significant ancillary devices along with principal energy and mass flows

experimental verification was carried-out to further confirm the high potential offered by lumped modeling approach for control and diagnostic purposes.

2.3.1 Lumped Model of Planar SOFC

The control-oriented model here described was conceived in such a way as to enable fast and accurate prediction of cell/stack dynamic response to any change in operating conditions. The model was developed assuming specific simplifying assumptions, listed below, whose validity is supported by previous studies:

- no heat exchange with the surroundings takes place, therefore adiabatic conditions are assumed (Braun 2002);
- gases sensible heat is neglected;
- pressure drop is assumed negligible (Burt et al. 2004);
- both electrochemistry and mass transfer are assumed as instantaneous processes, thus, thermal dynamics is the dominant phenomenon during transients (Achenbach 1995);
- the temperature of the solid trilayer is assumed as representative of the entire control volume (i.e., lumped modeling approach) (Iwata et al. 2000);
- a rectangular, planar, anode-supported, and co-flow SOFC is considered;

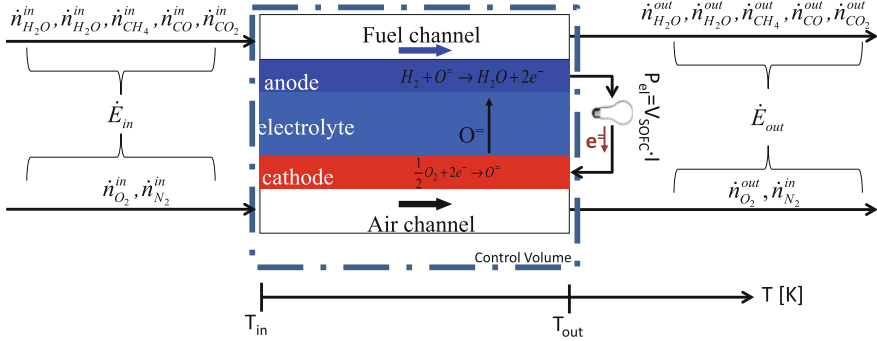


Fig. 2.23 Control volume (i.e., the one fully included within the *dotted-dashed* border) with reference to which the state-space model expressed by Eq. (2.58) was derived. Heat exchange with the surroundings was neglected as a consequence of adiabatic hypothesis, thus it was not included in the above illustration

- single SOFC dynamics is considered as representative of the entire stack behavior;
- T_{out} (see Fig. 2.23) is assumed as the state variable.

The above assumptions allow describing the dynamic behavior of an SOFC cell as a first-order system, with the outlet temperature being the only state variable. Particularly, the application of the first principle of Thermodynamics to the control volume shown in Fig. 2.23 results in the following state-space model:

$$\begin{cases} \dot{x} = \frac{dT_{out}}{dt} = f(x, u) = \frac{1}{K_{cell}} [\dot{E}_{in}(T_{in}) - \dot{E}_{out}(T_{out}) - \bar{J} \cdot V_{SOFC}(\bar{J}, T_{out}, U_f, \lambda) \cdot A] \\ y = V_{SOFC} = g(x, u) \end{cases} \quad (2.58)$$

where K_{cell} is the cell thermal capacity and $x = T_{out}$, $y = V_{SOFC}$ and $u = \{\bar{J}, T_{out}, U_f, \lambda\}$ are the state, output, and input variables, respectively. Particularly, K_{cell} is the key model parameter to be determined when specifically aiming at simulating transient SOFC response. The authors themselves previously discussed (Sorrentino et al. 2008) how the lumped capacity approach adopted to describe SOFC thermal dynamics (i.e., Eq. 2.58), would suggest to identify such a parameter against transient experiments. Nevertheless, geometrical-based estimation of K_{cell} also can be reliable.

The following subsection provides the reader with further details on how are estimated the energy flows leaving the control volume shown in Fig. 2.23 (i.e., $\dot{E}_{out}$ in Eq. 2.58).

It is also worth mentioning here that the state-space model output, i.e., V_{SOFC} in Eq. 2.58, is here computed by means of black-box submodels, which are developed according to the hierarchical sequence shown in Fig. 2.2. Later on in the chapter,

specifically in Sects. 2.3.1.2 and 2.4.2, the two possible paths that can be potentially exploited to derive such a black-box relationship will be described and discussed in detail.

2.3.1.1 Estimation of Outlet Energy Flows

As shown in Fig. 2.23, the most general case here considered corresponds to a reformat fuel feeding resulting from methane pre-reforming. If this is the case, the outlet anode composition must be estimated to correctly evaluate the $\dot{E}_{\text{out}}$ term in Eq. (2.58). Here, a similar approach to the one proposed in Sect. 2.2.1.1 to estimate pre-reformer outlet composition was followed. Particularly, outlet molar flows can be estimated assuming that methane gets completely reformed inside the anode channels. Such a hypothesis well fits with experimental evidence and it was further demonstrated, in this work itself, through the analysis of estimated fuel composition along the gas channels (see Fig. 2.12).

The above hypothesis led to write the following system of four equations (C, H, and O balances plus the equilibrium constant evaluated for the water-gas-shift reaction) with four unknowns, namely all the terms having “out” as superscript:

$$\dot{n}_{\text{CH}_4}^{\text{in}} + \dot{n}_{\text{CO}}^{\text{in}} + \dot{n}_{\text{CO}_2}^{\text{in}} - \dot{n}_{\text{CO}}^{\text{out}} + \dot{n}_{\text{CO}_2}^{\text{out}} = 0 \quad (2.59a)$$

$$4\dot{n}_{\text{CH}_4}^{\text{in}} + 2\dot{n}_{\text{H}_2}^{\text{in}} + 2\dot{n}_{\text{H}_2\text{O}}^{\text{in}} - 2\dot{n}_{\text{H}_2}^{\text{out}} - 2\dot{n}_{\text{H}_2\text{O}}^{\text{out}} = 0 \quad (2.59b)$$

$$\dot{n}_{\text{H}_2\text{O}}^{\text{in}} + \dot{n}_{\text{CO}}^{\text{in}} + 2\dot{n}_{\text{CO}_2}^{\text{in}} + 2\dot{n}_{\text{O}_2, \text{cons}} - \dot{n}_{\text{H}_2\text{O}}^{\text{out}} - \dot{n}_{\text{CO}}^{\text{out}} - 2\dot{n}_{\text{CO}_2}^{\text{out}} = 0 \quad (2.59c)$$

$$K_{\text{shift}}(p, T_{\text{out}}) = \frac{\dot{n}_{\text{H}_2}^{\text{out}} \cdot \dot{n}_{\text{CO}_2}^{\text{out}}}{\dot{n}_{\text{H}_2\text{O}}^{\text{out}} \cdot \dot{n}_{\text{CO}}^{\text{out}}} \quad (2.59d)$$

where K_{shift} is evaluated by means of Eq. (2.4). As it emerges from the comparison between Eqs. (2.59a)–(2.59d) and (2.11a)–(2.11c) and (2.12), the major difference lies in the absence of the methane molar flow (i.e., $\dot{n}_{\text{CH}_4}^{\text{out}} = 0$) at the control volume outlet (shown on Fig. 2.23). A further difference corresponds to the fact that the oxygen molar flow, which crosses the electrolyte from cathode to anode to enable the hydrogen electro-oxidation (see Fig. 2.23), must be considered as a further inlet flow (i.e., $\dot{n}_{\text{O}_2, \text{cons}}$). Such oxygen consumption is accounted for when writing the oxygen balance, here expressed by Eq. 2.59c.

2.3.1.2 Analysis of Transient Response

The physical meaning of the lumped, control-oriented model presented above was tested by simulating the response of V_{SOFC} to step changes in load (i.e., average current density $\bar{J}$) and excess air λ . The interest for analyzing these particular

responses is justified by the use of $\bar{J}$ and λ as control variables for matching the power requests and limiting temperature rise across the cell, respectively (Aguilar et al. 2004).

Below are defined the dynamic performance metrics used to study and discuss SOFC thermal response to step changes:

- $V_{\text{drop}} = V_{\text{SOFC}}(t_{\infty}) - \min[V_{\text{SOFC}}(t)]$: voltage undershoot intensity [mV];
- $\Delta V = V_{\text{SOFC}}(t_{\infty}) - V_{\text{SOFC}}(t_0)$: voltage difference between second (t_{∞}) and first (t_0) stationary point [mV];
- τ_V : voltage relaxation time [s];

Voltage relaxation time, which is a very significant variable to be accounted for when performing optimal design and balance of plant analysis for SOFC systems (Selimovic et al. 2005), is defined as the time needed for V_{SOFC} to recover up to 90 % of the voltage drop occurring after load or excess air step variation (Achenbach 1995):

$$V_{\text{rec}} = 0.9 \cdot V_{\text{drop}} + \min[V_{\text{SOFC}}(t)] \quad (2.60a)$$

$$\tau_V = t|_{V_{\text{SOFC}}=V_{\text{rec}}} - t_0 \quad (2.60b)$$

The cell geometry considered in this analysis is almost identical to the ES one specified in Table 2.2. In this specific analysis, anode, cathode and electrolyte thicknesses were assumed equal to 600, 50 and 10 μm , respectively, thus allowing to switch from an electrolyte- to a more up-to-date anode-supported cell. Upon knowledge of geometrical data and cell material (i.e., ceramic), the following geometrically derived value of cell capacity was assumed in the transient analysis of SOFC performance:

$$K_{\text{cell}} = \rho_{\text{cer}} \cdot \text{VOL}_{\text{cell}} \cdot c_{\text{cer}} = 6600 \left[\frac{\text{kg}}{\text{m}^3} \right] \cdot 2.08 \cdot 10^{-5} [\text{m}^3] \cdot 400 \left[\frac{\text{J}}{\text{kg} \cdot \text{K}} \right] = 55 \left[\frac{\text{J}}{\text{K}} \right] \quad (2.61)$$

As for the estimation of V_{SOFC} , the following multiple linear regression (MLR) was used for a methane-fed, un-pressurized, planar, co-flow SOFC:

$$\begin{aligned} V_{\text{SOFC}} = g(x, u) = & 0.18 - 0.08U_f - 1.25\bar{J} + 0.0041\lambda \frac{T_{\text{out}}}{1000} \\ & + 0.86J \frac{T_{\text{out}}}{1000} + 0.71T_{\text{in}} \end{aligned} \quad (2.62)$$

Equation (2.62) was obtained adopting the hierarchical approach described in Sect. 2.1. Particularly, the blue-line path shown in Fig. 2.2 was applied as schematically described in Fig. 2.24: the 1D model presented in Sect. 2.2 was deployed to generate a set of virtual steady-state experiments, through which it was possible to well capture, as shown on the lower right corner of the figure, the

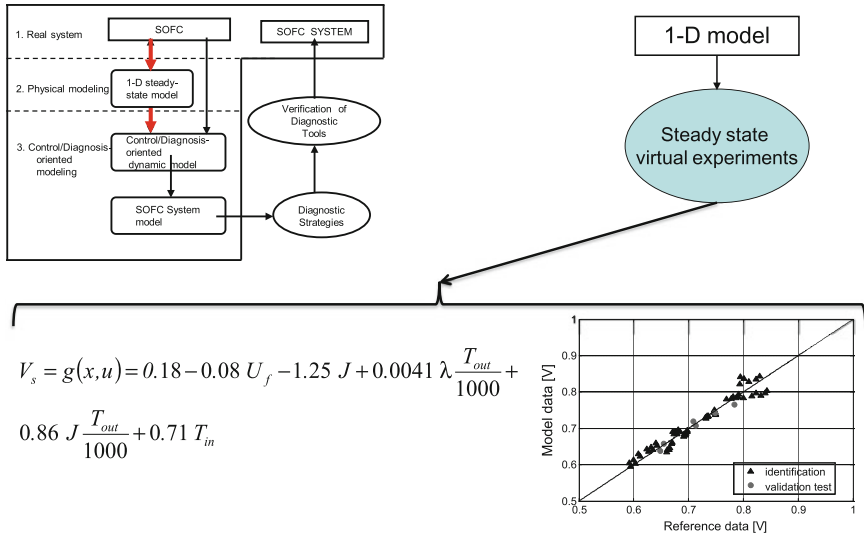


Fig. 2.24 Schematic description of hierarchical approach deployment for the development of the MLR correlation expressed by Eq. (2.62)

dependence of voltage on current density, inlet temperature, and fuel and air utilization (see Sect. 2.2.1.7).

Despite being a steady-state voltage submodel, the correlation expressed by Eq. (2.62) well adapts to the lumped, control-oriented model features. Indeed, voltage transient variation mainly depends on temperature, whose dynamics is assumed being the dominant one as in this work as in other relevant contributions devoted to SOFC dynamic behavior (Achenbach 1995; Haynes 2002). Therefore, the fact that Eq. (2.62) directly links voltage to inlet temperature and air utilization, which in turn affects inner and outer stack temperature, ensures satisfactory prediction capabilities both in steady-state and transient operations.

Response to Load Change

The SOFC response to load change was investigated for three different step variations (i.e., case 1, case 2, and case 3, as shown in Fig. 2.25). The other input variables were set to the following nominal values:

- $T_{\text{in}} = 750 \text{ }^{\circ}\text{C}$
- $\lambda = 6$
- $U_f = 0.8$

Figure 2.26 shows V_{SOFC} and T_{out} responses. For all the simulated cases, load increase causes polarization losses to sudden increase, resulting in an

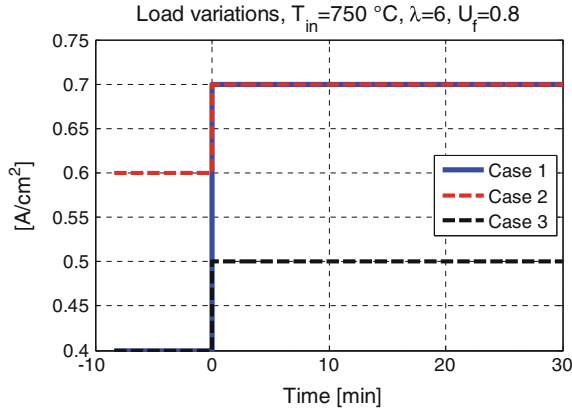


Fig. 2.25 Schematic illustration of load step changes considered in the response to load change analysis

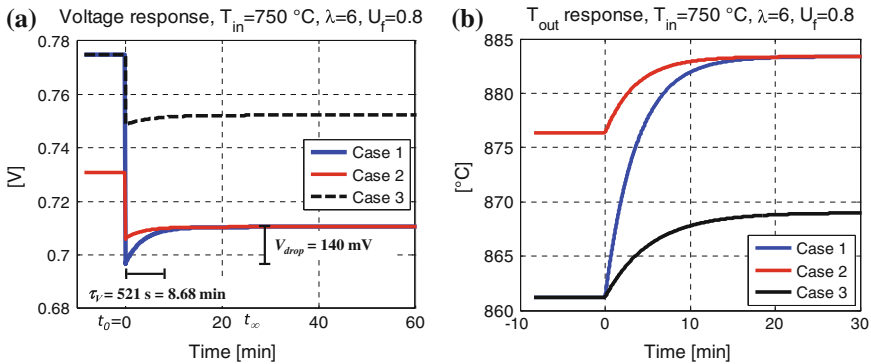


Fig. 2.26 Voltage (a) and outlet temperature (b) response to the load step-changes shown in Fig. 2.25. In (a) the values of t_0 and t_∞ resulting from cases 1 and 2 are indicated nearby the x -axis

undershoot-type voltage response, as shown in Fig. 2.26a. Such a behavior can be qualitatively explained considering the scheme shown in Fig. 2.27. At time $t = 0^-$, i.e., right before the load step change occurs, the voltage associated to current operating condition lies on the polarization curve associated to the given inlet temperature (i.e., $T_{in} = 750^\circ\text{C}$). Then, at time $t = 0^+$, i.e., immediately after the step change in load, the operating condition not only suddenly moves toward the new current density, but also deviates from the previous I-V curve; this latter phenomenon is due to the fact that the line corresponding to $T_{in} = 750^\circ\text{C}$ was obtained by modeling SOFC performance in steady-state conditions for current density varying between 0 and 1 A cm^{-2} . But when the load undergoes a step change, the subsequent thermal transient causes the temperature to slowly adapt to the next steady-state operating condition (see Fig. 2.27). Therefore, it can be assumed that at

time $t = 0^+$ the new operating condition corresponds to a lower T_{in} level, which actually well emulates the low average stack temperature obtained right after the step change. From this point forward, thanks to the slow temperature increase shown in Fig. 2.26b, polarization losses decrease, thus allowing for a slow voltage recovery, which in turn causes the operating condition to slowly move back to the initial $T_{in} = 750\text{ }^{\circ}\text{C}$ I–V curve, following the vertical line linking the points labeled $t = 0^+$ and $t = t_{\infty}$, respectively (see Fig. 2.27).

Table 2.5 summarizes the results obtained by simulating cases 1, 2, and 3 (see Fig. 2.25). The values of τ_V indicate that thermal dynamics is significantly slow, of the order of hundreds of seconds, thus achieving satisfactory accordance with the simulations performed in previous works (Achenbach 1995; Lukas et al. 1999; Larrain 2005). Moreover, τ_V tends to reduce as $\bar{J}(t_{\infty})$ increases. This behavior depends on the value of final current density reached after load step. In fact, the higher $\bar{J}(t_{\infty})$, the more heat is released by the electrochemical reaction, resulting in a more significant temperature increase, as it emerges from Fig. 2.26b. Such an effect allows for faster compensation of polarization losses due to load increase,

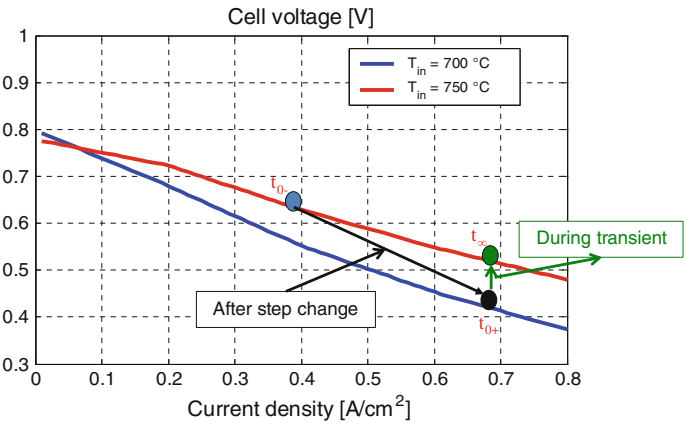


Fig. 2.27 Qualitative description of voltage evolution during a transient subsequent to a load step change

Table 2.5 Inputs and outputs of the response to load change analysis

Case	Step variables		Dynamic performance metrics	
	$\bar{J}(t_{\infty}) \left[\frac{\text{A}}{\text{cm}^2} \right]$	$\Delta \bar{J} = \bar{J}(t_{\infty}) - \bar{J}(t_0) \left[\frac{\text{A}}{\text{cm}^2} \right]$	$\tau_V \text{ (s)}$	$V_{\text{drop}} \text{ (mV)}$
1	0.7	0.3	525.4	140
2	0.7	0.1	525.1	44
3	0.5	0.1	775.7	36

which in turn results in shorter τ_V for case 1 and case 2 as compared to case 3 (see Fig. 2.27 and Table 2.5).

The values of voltage drop, listed in Table 2.5, indicate a significant dependence of such a variable on both magnitude of load step (i.e., $\Delta\bar{J} = \bar{J}(t_\infty) - \bar{J}(t_0)$) and final current density (i.e. $\bar{J}(t_\infty)$). This can be explained considering that if $\bar{J}(t_\infty)$ is a few percent higher than $\bar{J}(t_0)$ (i.e. small $\Delta\bar{J}$ in cases 2 and 3, see Table 2.5 and Fig. 2.26a), steady V_{SOFC} and T_{out} variations are not so significant, thus resulting in small V_{drop} , as shown in Table 2.5. Moreover, the higher $\bar{J}(t_\infty)$, the larger difference between voltage values at different temperatures, as shown in Fig. 2.17. Thus, since immediately after the load step T_{out} remains still closer to $T_{\text{out}}(t_0)$ than $T_{\text{out}}(t_\infty)$, the higher $\bar{J}(t_\infty)$, the larger voltage drop.

Response to Excess of Air Change

An additional investigation was conducted on the voltage response to step changes in excess of air λ , which is commonly used as low-level control variable to keep the temperature increase from cell inlet to outlet in a safe range (i.e., $[100 \div 150]^\circ\text{C}$) (Zizelman et al. 2002). V_{SOFC} and T_{out} responses were simulated for the three cases listed in Table 2.6, each one referring to one of the three “effect-zones” (i.e., positive, no, and negative effect) highlighted in Fig. 2.21. Therefore, such an analysis allowed discussing the results with respect to the observations presented in the section devoted to steady-state parametric analyses. The other input variables were set to the following nominal values:

- $T_{\text{in}} = 750^\circ\text{C}$
- $U_f = 0.8$

Figures 2.29 and 2.30 show V_{SOFC} and T_{out} responses, respectively. Particularly, Fig. 2.28 indicate that, in all simulated cases, as λ increases T_{out} decreases, while V_{SOFC} always responds with an overshoot, which occurs because of the initial positive impact of higher amount of reactants (i.e., oxygen) in the cathode channel. Then, due to temperature reduction along the co-flow gas channels (see Fig. 2.29), V_{SOFC} slowly decreases down to the following stationary point (i.e., $V(t_\infty)$). As expected, current load $\bar{J}$, which is kept constant during the transient simulations

Table 2.6 Inputs and outputs of the response to change in excess air analysis

Case	Step variables			Dynamic performance metrics	
	$\bar{J} \left[\frac{\text{A}}{\text{cm}^2} \right]$	$\lambda(t_\infty)$	$\lambda(t_0)$	τ_V (s)	ΔV (mV)
4	0.1500	5	7	2466.2	4.7
5	0.3155			1100.9	0
6	0.7000			590.4	-13.4

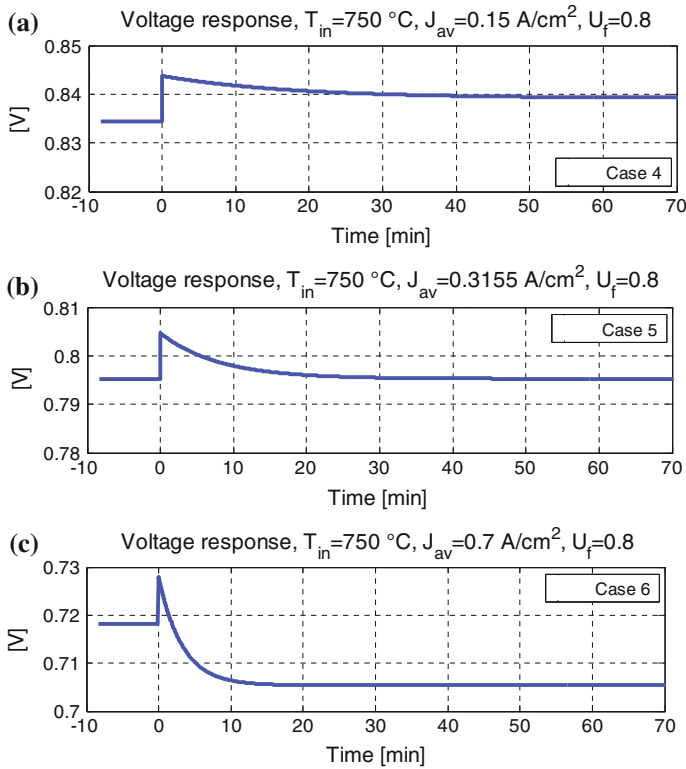


Fig. 2.28 Voltage trajectories simulated in the response to excess of air change analysis described in Table 2.6

here examined, strongly influences the response times, which decrease at high loads due to the higher amount of produced heat, as shown in Table 2.6.

Finally, as suggested by the steady-state parametric analysis carried-out in Sect. 2.2.1.7 (see Fig. 2.21), Table 2.6 and Fig. 2.28 show that ΔV varies from positive (i.e. case 4) to negative (i.e., case 6) values, as a function of the load. Therefore, this analysis not only allowed to investigate the dynamic effect of λ on cell performance, but also to further assess the accuracy of the black-box voltage correlation (i.e., Eq. 2.62) implemented in the lumped SOFC dynamic model.

2.3.1.3 Experimental Validation of the Lumped Model of Planar SOFC

The model presented and analyzed in the previous section was tested for experimental validation within the European project GENIUS (2013). Particularly, Eq. (2.58) was fed with all the inputs acquired by one of the industrial partners

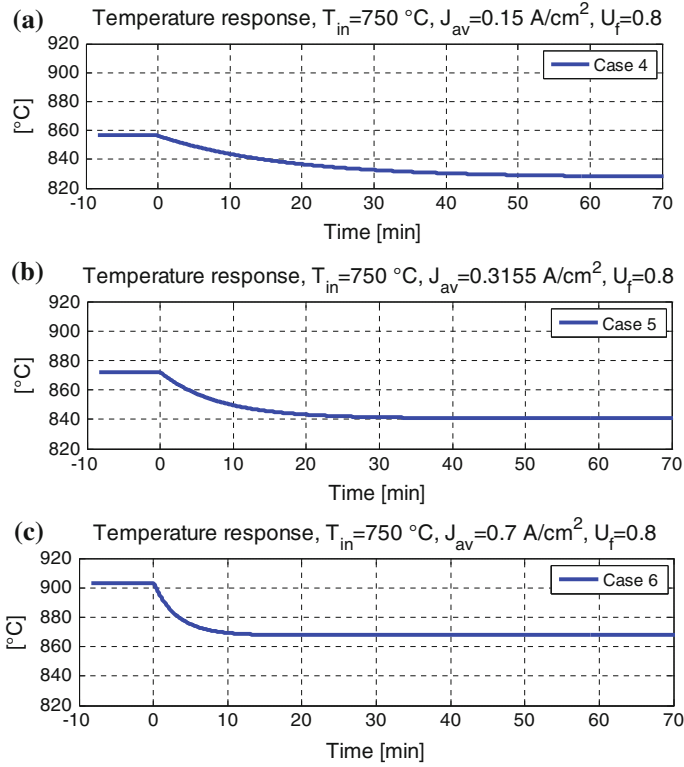


Fig. 2.29 Outlet temperature trajectories simulated in the response to excess of air change analysis described in Table 2.6

involved in the project, which include: inlet molar flows and temperature, voltage, and current density. Therefore, Eq. (2.58) allowed to estimate SOFC stack temperature and to compare it to the corresponding experimental measurement.

Figure 2.30 highlights the very good agreement achieved by extending the control-oriented modeling approach to a real system, thus confirming its suitability for on-field monitoring, control, and diagnostics of SOFC-based energy systems.

2.3.2 PostBurner Modeling

Figure 2.22 shows how the gases exhausting from anode and cathode channels are directly sent to the postburner, where they mix and react to produce additional heat for incoming fuel and air flows preheating and, eventually, to deliver useful heat when exiting the SOFC system. Moreover, since a highly toxic specie such as CO is

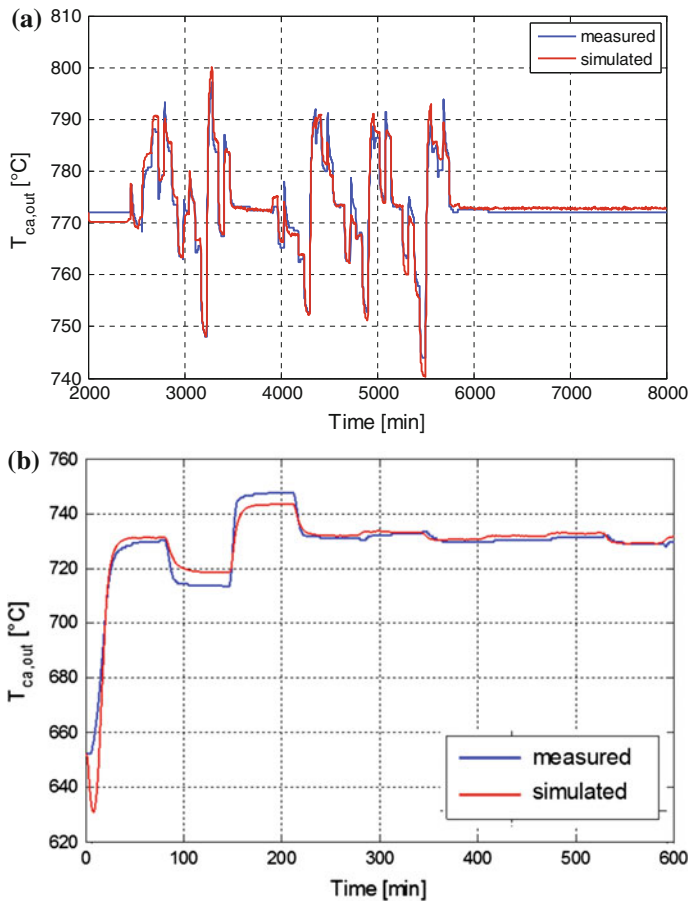


Fig. 2.30 Validation of the lumped model expressed by Eq. 2.58 against experimental transients consisting of a sequence of fast ramp changes in stack load

also present in the exhausts in a nonnegligible amount, its combustion contributes to lower the environmental impact of SOFCs.

Following the indications provided by Lu et al. (2006), the fact that cathodic channels are fed with extremely high excess of air (for SOFC internal cooling purposes) allows simplifying postburner modeling: it is therefore possible to assume that a complete combustion of H_2 and CO takes place inside this component, with a negligible impact of dissociation since outlet postburner temperatures are never so high (e.g., below 1400 °C). Moreover, the postburner is assumed adiabatic and its thermal dynamics considered negligible with respect to stack and heat-exchangers ones (Lu et al. 2006). Finally, the effect of combustion heat release rate can also be safely neglected. The above-introduced assumptions, as the ones that will be introduced later on for the heat exchangers (i.e., air preheater and steam

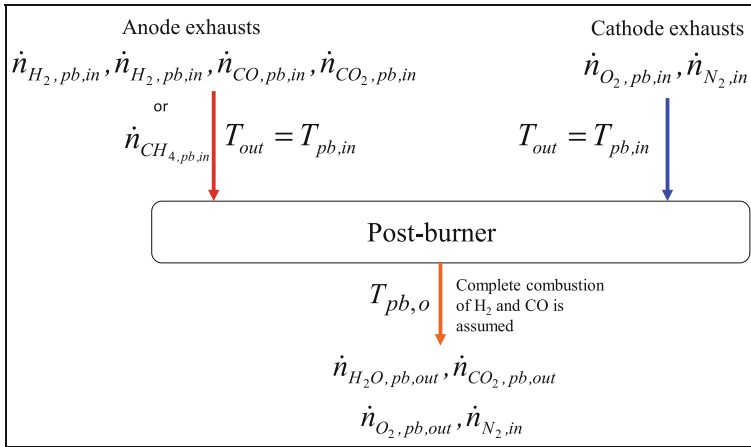
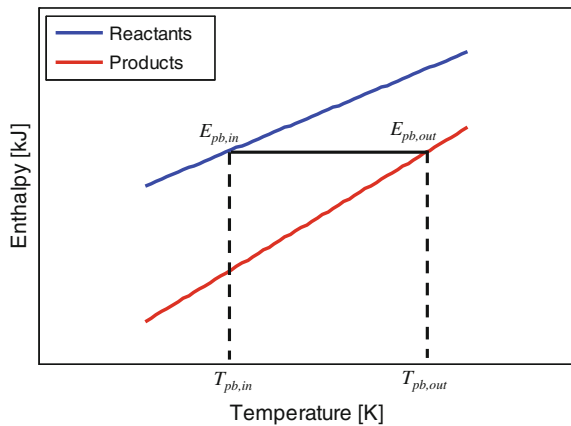


Fig. 2.31 Schematic representation of mass and energy flows entering and leaving the postburner used in a typical SOFC system (see Fig. 2.22). Note that nitrogen molar flows does never change going from SOFC system inlet to outlet, thus the corresponding notation did not change with respect to the control volume surrounding the SOFC stack, shown in Fig. 2.23

Fig. 2.32 Physical meaning of the energy balance over the postburner expressed by Eq. 2.63. The hypothesis of adiabatic flame temperature allows assuming that a constant enthalpy combustion process occurs inside the postburner (Heywood 1988)



pre-reformer), are in accordance with the aim of developing a comprehensive control-oriented model for an SOFC system, to be placed at the lowest level of the hierarchical modeling structure shown in Fig. 2.2.

As a consequence of the above hypotheses, the process occurring within the postburner can be treated, with a reasonable approximation, by applying the adiabatic flame temperature estimation method (Heywood 1988) to the inlet and outlet flows shown in Fig. 2.31. Particularly, the outlet temperature $T_{pb, out}$ can be estimated by iteratively solving the following equation, which derives from the consideration that combustion products enthalpy must equal reactants enthalpy, as shown in Fig. 2.32:

$$\begin{aligned}
\dot{E}_{\text{pb,in}}(T_{\text{pb,in}}) &= \sum_m \dot{n}_{m,\text{pb,in}} \cdot h_m(T_{\text{pb,in}}) = \dot{E}_{\text{pb,out}}(T_{\text{pb,out}}) \\
&= \sum_m \dot{n}_{m,\text{pb,out}} \cdot h_m(T_{\text{pb,out}}) m = [\text{H}_2, \text{H}_2\text{O}, \text{CH}_4, \text{CO}, \text{CO}_2, \text{O}_2, \text{N}_2]
\end{aligned} \tag{2.63}$$

where outlet molar flows are estimated as a function of inlet flows, through the following hydrogen (Eq. 2.64a), carbon (Eq. 2.64b) and oxygen balances (Eq. 2.64c). Equation 2.65 expresses the dependence of enthalpy on specific heat and enthalpy of formation of the generic species m :

$$\dot{n}_{\text{H}_2\text{O},\text{pb,out}} = \dot{n}_{\text{H}_2\text{O},\text{pb,in}} + \dot{n}_{\text{H}_2,\text{pb,in}} + 2 \cdot \dot{n}_{\text{CH}_4,\text{pb,in}} \tag{2.64a}$$

$$\dot{n}_{\text{CO}_2,\text{pb,out}} = \dot{n}_{\text{CO}_2,\text{pb,in}} + \dot{n}_{\text{CO},\text{pb,in}} + \dot{n}_{\text{CH}_4,\text{pb,in}} \tag{2.64b}$$

$$\dot{n}_{\text{O}_2,\text{pb,out}} = \dot{n}_{\text{O}_2,\text{pb,in}} - \frac{1}{2} \dot{n}_{\text{H}_2,\text{pb,in}} - \frac{1}{2} \dot{n}_{\text{CO},\text{pb,in}} - 2 \cdot \dot{n}_{\text{CH}_4,\text{pb,in}} \tag{2.64c}$$

$$h_m(T) = \bar{h}_{f,m}^0 + \int_{298}^T c_{p_m}(T) dT \tag{2.65}$$

It is finally worth here mentioning that the inlet flows shown in Fig. 2.31 are representative of both warmed-up and cold-start operations. Indeed, as it will be clarified in the next chapter, SOFC cold-start is here assumed being carried-out by directly feeding the postburner with methane; thus, in this specific working condition, the terms $\dot{n}_{\text{H}_2,\text{pb,in}}$, $\dot{n}_{\text{H}_2\text{O},\text{pb,in}}$, $\dot{n}_{\text{CO},\text{pb,in}}$ and $\dot{n}_{\text{CO}_2,\text{pb,in}}$ vanish in Fig. 2.31 and Eq. 2.64a–2.64c. On the other hand, during warmed-up phases, CH_4 normally gets completely reformed before leaving the SOFC anode channels (refer to the discussion made also in Sect. 2.3.1.1), thus leading to neglect the term $\dot{n}_{\text{CH}_4,\text{pb,in}}$ in such phases.

2.3.3 Heat Exchangers Modeling

Figure 2.22 indicates that there are two components, the air preheater and fuel pre-reformer, in which the hot gases exhausting from the postburner exchange heat with cold fluids, namely with the air and fuel flows entering the anodic and cathodic channels, respectively.

In order to cope with the purpose of developing a comprehensive dynamic model of SOFC systems, which is particularly required to fulfill the requirements, set at the control-oriented modeling level shown in Fig. 2.2, the zero capacity system approach proposed by Ataer et al. (1995) was here adopted. Such a modeling approach allows to describe, with a low computation effort, the response of

heat exchangers to variation in hot, and cold fluid temperature and flows. Therefore, a good compromise, similar to the one attained for the SOFC stack (see Sect. 2.3.1), between accuracy and computational burden can be achieved. Moreover, a proper modeling balance is ensured when coupling different submodels with each other (e.g., SOFC stack and air preheater).

According to Ataer et al. (1995), the following simplifying hypotheses can be assumed:

- temperature changes linearly within both hot and cold channels;
- the heat exchanged between hot and cold fluid is proportional to the difference between the hot (i.e., $T_{h,HE}$) and cold fluid (i.e., $T_{c,HE}$) mean temperatures;

Therefore, the dynamics of both hot and cold fluid can be modeled as follows:

$$\begin{aligned}
 \text{hot fluid: } (K_{HE} + C_h) \frac{dT_{h,HE}}{dt} &= \dot{E}_{h,HE,in}(T_{h,HE,in}) - \dot{E}_{h,HE,out}(T_{h,HE,out}) \\
 &\quad - U_{HE} \cdot A_{HE} \cdot (T_{h,HE} - T_{c,HE}) \\
 \text{cold fluid: } C_c \frac{dT_{c,HE}}{dt} &= \dot{E}_{c,HE,in}(T_{c,HE,in}) - \dot{E}_{c,HE,out}(T_{c,HE,out}) \\
 &\quad + U_{HE} \cdot A_{HE} \cdot (T_{h,HE} - T_{c,HE}) \\
 HE &= [\text{aph, pre}]
 \end{aligned} \tag{2.66}$$

where the energy flow terms (i.e., $\dot{E}$) are estimated by applying Eq. (2.63) to the control volumes surrounding either the air presheater or the pre-reformer (see Fig. 2.22). Furthermore, the terms C_h and C_c represent the hot and cold fluid heat capacity, respectively.

The molar flows entering and leaving the pre-reformer are to be estimated as detailed in Sect. 2.3.1.1. It is worth remarking that the specific pre-reformer here considered, i.e., the one used in the configuration of Fig. 2.22, only consists of the evaporator and reactor units. This is possible because the heat, required both to transfer water from liquid to vapor phase and to enable the endothermic steam-reforming reaction, is supplied by the hot fluid (i.e., postburner exhausts), flowing through the pre-reformer device (Sorrentino and Pianese 2009; Jahn et al. 2005).

The following subsection focuses on the methodology adopted to design heat exchangers destined to SOFC system integration.

2.3.3.1 Heat Exchanger Design

Heat exchangers design consists in finding the appropriate transfer area to ensure that the targeted heat transfer from hot to cold fluid takes place. Following a widespread practice, the method proposed by Kays and London (1964) for compact heat exchangers was here adopted. Particularly, the key parameter to be evaluated is the heat exchanger effectiveness ε , defined as the ratio between effective heat

transfer $\dot{Q}$ and the maximum heat transfer achievable by an ideal counterflow heat exchanger (Mastrullo et al. 1991):

$$\varepsilon = \frac{\dot{Q}}{\dot{Q}_{\max}} = \frac{\dot{C}_h \cdot \Delta T_h}{\dot{C}_{\min} \cdot \Delta T_{\max}} = \frac{\dot{C}_c \cdot \Delta T_c}{\dot{C}_{\min} \cdot \Delta T_{\max}} \quad (2.67a)$$

$$\Delta T_h = T_{h,HE,in} - T_{h,HE,out} \quad (2.67b)$$

$$\Delta T_c = T_{c,HE,out} - T_{c,HE,in} \quad (2.67c)$$

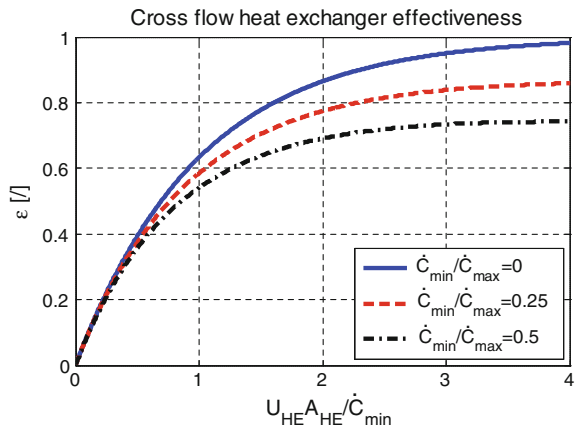
$$\Delta T_{\max} = T_{h,HE,in} - T_{c,HE,in} \quad (2.67d)$$

The terms $\dot{C}_c$ and $\dot{C}_h$ appearing at the right-hand side of Eq. (2.67a)–(2.67d) are estimated as the average heat capacity rate within the assigned temperature ranges. For the sake of brevity, Eq. 2.68 explains how such a calculation is performed for the sole hot fluid:

$$\begin{aligned} \dot{C}_h &= \frac{\dot{Q}}{(T_{h,HE,in} - T_{h,HE,out})} \\ &= \frac{\sum_m \dot{n}_{m,h,HE,in} \cdot h_m(T_{h,HE,in}) - \sum_m \dot{n}_{m,h,HE,out} \cdot h_m(T_{h,HE,out})}{(T_{h,HE,in} - T_{h,HE,out})} \end{aligned} \quad (2.68)$$

Empirical correlations are available (Lee et al. 2011) to express the functional relationship linking effectiveness to key heat exchanger parameters, such as the average heat transfer coefficient U_{HE} , the transfer area A_{HE} , and the terms $\dot{C}_c$ and $\dot{C}_h$. Such relationships are illustrated in Fig. 2.33, where $\dot{C}_{\min}$ and $\dot{C}_{\max}$ are defined as the minimum and maximum value between $\dot{C}_c$ and $\dot{C}_h$, respectively. Particularly, Fig. 2.33 qualitatively describes the dependence $\varepsilon = f(A_{HE} \cdot U_{HE} / \dot{C}_{\min}, \dot{C}_{\min} / \dot{C}_{\max})$ for a cross-flow heat exchanger, which is the type that most suitably fits the

Fig. 2.33 Variation of heat exchanger effectiveness as a function of both design and operating parameters (adapted from Mastrullo et al. 1991; Lee et al. 2011)



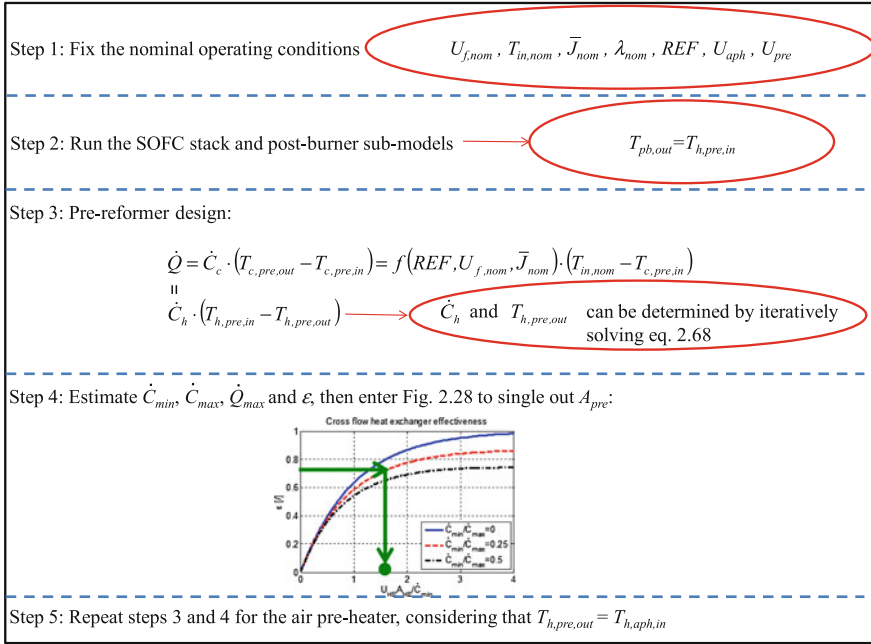


Fig. 2.34 Logic diagram synthesizing the model-based design of heat exchanger transfer area, for a given nominal operating condition established for the SOFC system

schematic layout of Fig. 2.22. Figure 2.33 also highlights that, once are assigned the heat transfer coefficient, the hot and cold fluid molar flows as well as the inlet and outlet temperatures, the values of effectiveness, and $\dot{C}_{min}/\dot{C}_{max}$ ratio can be computed through Eqs. (2.67a) and (2.68), thus allowing to enter Fig. 2.33 diagram and single out the current value of the abscissa $A_{HE} \cdot U_{HE}/\dot{C}_{min}$, which in turn can be used to estimate the transfer area.

Furthermore, upon the knowledge of the selected heat exchanger type (e.g., double pipe, shell and tube, plate, etc.), the surface to volume ratio can also be retrieved (NTNU 2013), thus allowing to determine heat exchanger volume. The latter variable, together with material properties knowledge, can be used to estimate (see Eq. 2.61) heat exchanger lumped capacity, whose evaluation is needed to correctly simulate temperature transients via Eq. (2.66).

The correct deployment of the method described above for an SOFC system is synthesized in Fig. 2.34.

2.3.3.2 Air Compressor

The air compression system has an important role in the design and control of SOFC systems. Particularly, it is required to supply air to the cathode in the right

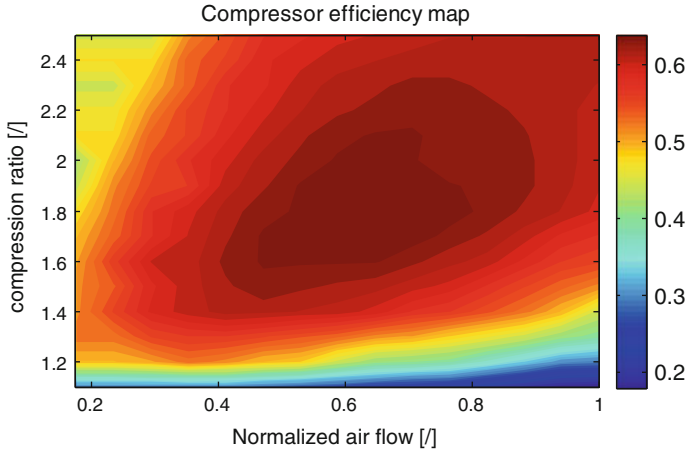


Fig. 2.35 Contour plot showing a normalized map linking compressor (i.e., Lyshom type, Miotti et al. 2006) efficiency to air flow and compression ratio

amount so as to guarantee, at the same time, the electrochemical reactions to take place appropriately and air-cooling of the SOFC stack to be safely performed.

Since the air compressor power represents the main loss within the entire SOFC system (see Fig. 2.22), its accurate estimation is needed to correctly estimate net performance. For the current study, a screw compressor (Miotti et al. 2006) was assumed. Compressor power is evaluated as a function of adiabatic efficiency and ideal compression work:

$$P_{cp} = \dot{m} \frac{c_p T_a}{\eta_{cp} \cdot \eta_{cm}} \left[\beta^{\frac{k-1}{k}} - 1 \right] \quad (2.69)$$

where β is the compression ratio, $\dot{m}$ is the inlet air flow processed by the compressor and η_{cp} and η_{cm} are the compressor and compressor motor efficiency, respectively. The last two efficiency terms are generally estimated via look-up tables, which are either supplied by manufacturers or developed by carrying-out suited experimental tests. Particularly, in this work η_{cp} is estimated as a function of mass flow and pressure ratio via an experimental efficiency map developed by (Miotti et al. 2006), as shown in Fig. 2.35.

Upon knowledge of compressor power adsorption via Eq. (2.69), net electric power yielded on output by the SOFC system (see Fig. 2.22) can be approximated as follows:

$$\begin{aligned} P_{net,AC} &= P_{net,DC} \cdot \eta_{DC/AC} = (P_{gross} - P_{aux}) \cdot \eta_{DC/AC} \cong (P_{gross} - P_{cp}) \cdot \eta_{DC/AC} \\ &= (n_{cells} \cdot V_{SOFC} \cdot I_{SOFC} - P_{cp}) \cdot \eta_{DC/AC} \end{aligned} \quad (2.70)$$

where the sole compressor parasitic contribution was considered, due to its much higher impact than other devices on net performance (Badami and Caldera 2002).

2.4 Black-Box Modeling

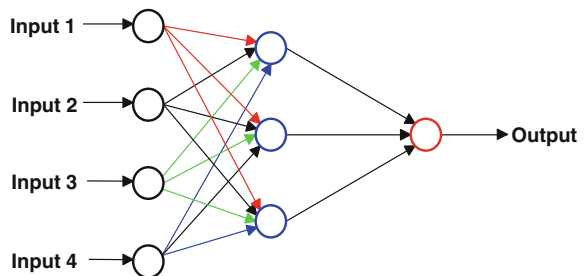
As already mentioned in Sect. 2.1.1 and schematized in Fig. 2.2, the availability of an extended experimental data set enables direct development of black-box models destined to either control or diagnostic algorithms development. Specifically in this section, the suitability of neural network (NN) models to fully exploit the knowledge content of highly informative data set is discussed.

Particularly, Sect. 2.4.2 focuses on the development of static neural networks for SOFC voltage modeling. Afterwards, Sect. 2.4.3 highlights how the availability of transient experiments enable the development of dynamic neural network models. The high accuracy granted by the latter models allows developing control algorithms that are as effective in transient maneuvers as in steady state, thus being more suitable than static black-box models for implementation in SOFC systems destined to load following applications (e.g., automotive, railway, marine propulsion, automotive, and airplane auxiliary power units).

2.4.1 Overview on Neural Network Models

Multi-layer-perceptron-feed-forward [MLPFF (Patterson 1995)] models are beyond doubt the most used artificial neural networks for fast and accurate steady-state prediction of highly nonlinear processes. Figure 2.36 provides a schematic representation of an MLPFF NN structure, highlighting the presence of nodes (i.e., processing units) and connections among nodes, to which the network parameters (i.e., the weights) are associated. For a deeper understanding of NN models features and basic theoretical principles, the reader is addressed to the abundant available literature (Patterson 1995; Haykin 1999; Ripley 2000). A brief overview on NN training and generalization is given below.

Fig. 2.36 Schematic representation of a generic multi-input single-output MLPFF NN structure. It is worth noting that the illustrated exemplary structure consists of four inputs, one hidden layer, and three hidden neurons



Network parameters are usually identified through a learning process, during which a set of training examples (generally experimental data) is fed to the NN to determine the weights of the connections linking network nodes. The most common approach adopted to identify NN parameters (i.e., connection weights) is the error backpropagation algorithm (Patterson 1995; Haykin 1999; Nelles 2000), due to its easy-to-handle implementation. At each iteration, the mean squared error (MSE, see Eq. 2.71) between experimental ($\hat{y}_l$) and NN output values (y_l) is propagated backward from the output to the input layer, passing through the hidden layers. The learning process is stopped when the MSE on a specified data set undergoes an assigned threshold.

$$\text{MSE} = \frac{1}{N} \sum_l (\hat{y}_l - y_l)^2 \quad (2.71)$$

The training process mainly aims at determining NN models with a satisfactory compromise between accuracy and generalization. The latter feature can be maximized by selecting a training data set enough extended, so as to cover most of the system/process operating domain (Marra et al. 2013). Moreover, selecting an appropriate termination criterion for the backpropagation algorithm allows preventing network overfitting (Nelles 2000), which in turn may result in a significant loss of generalization. The early stopping is one of the most effective method against overfitting (Patterson 1995; Haykin 1999; Nelles 2000; Nørgaard et al. 2000). Particularly, the early stopping criterion consists in interrupting the training process once the MSE computed on a data set, different from the training one, stops decreasing. Therefore, when the early stopping is used, network training and test require at least three data sets (Haykin 1999): training-set (set A), early stopping test-set (set B) and generalization test-set (set C).

As for dynamic NN, the literature proposes a high number of effective neural structures that enable dynamic nonlinear modeling of many systems/processes. Since the analysis of all dynamic NN models falls out of the scope of the present book, a brief description of the adopted modeling methodology is here presented. Particularly, recurrent neural networks (RNN) can be obtained by suitably modifying the MLPFF NN structure shown in Fig. 2.36 (Nørgaard et al. 2000). The main modifications consist of: (i) feeding current and past input values, (ii) introducing feedback connections among the neurons, and thus providing the NN with a memory capability enabling dynamic simulations (see Fig. 2.37, where a typical RNN structure is shown).

Depending upon the feedback typology, which can either involves each neuron or only the output and input layers neurons, RNNs are classified into local RNN and global or external RNN, respectively (Haykin 1999; Nørgaard et al. 2000). Specifically in this work, the external RNN type was selected for dynamic modeling of SOFC performance, as discussed in Sect. 2.4.3. Detailed descriptions of external RNN structure and related implementation issues were given by the authors in

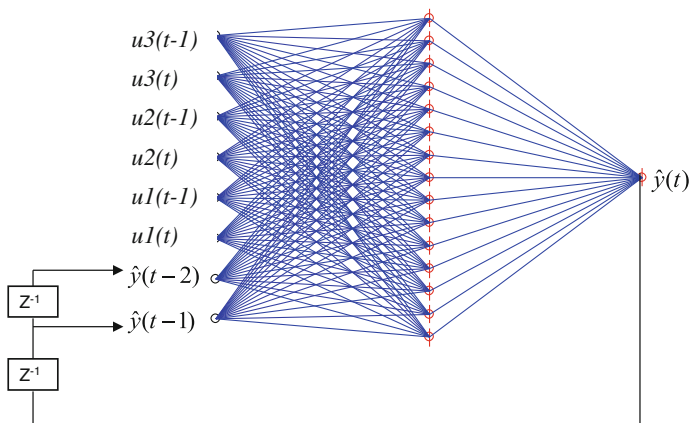


Fig. 2.37 Schematic representation of a generic RNN structure. It is worth noting that the illustrated exemplary structure consists of 3 inputs, 1 hidden layer and 15 hidden neurons. The memory effect, which provides dynamic simulation capabilities, is achieved by considering 1 past input and two output feedbacks $\hat{y}$

previous papers (Arsie et al. 2006, 2009, 2010), where the high potential of such models for control algorithm development in the automotive field was also demonstrated.

The neural network models developed and presented in the next two sections were trained applying the backpropagation algorithm in conjunction with the early stopping criterion, thus ensuring, as discussed above, both high accuracy and generalization. Moreover, trial and error analyses were carried-out to select NN structures with minimal number of parameters (weights), thus also allowing preventing network overparametrization, which can also result in generalization losses (Nelles 2000).

2.4.2 Development of Neural Networks for Steady-State Modeling of SOFC Performance

As shown in Fig. 2.2, the availability of a large number of experiments allows following the red path that directly links the real system, on which the experiments are gathered, to the control/diagnostics oriented modeling level. This case occurred in the framework of the GENIUS project (GENIUS 2013), which the authors participated in the timeframe 2010–2013. Particularly, several steady-state polarization curves were acquired on a fully experimented 5-cells short SOFC stack manufactured by Hexis, as described in a previous work (Marra et al. 2013).

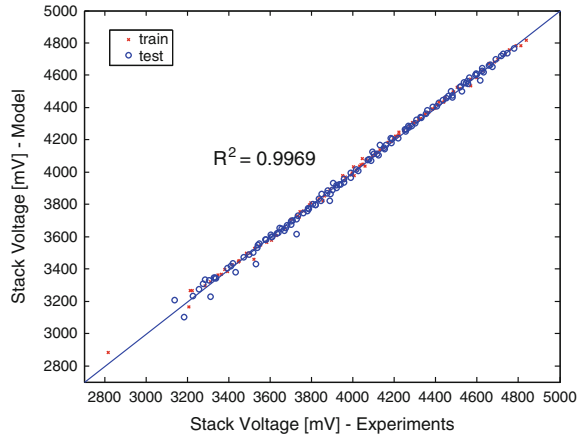


Fig. 2.38 Comparison between NN (i.e., model on the ordinates) outputs and measured voltage (i.e., experiments on the abscissa)

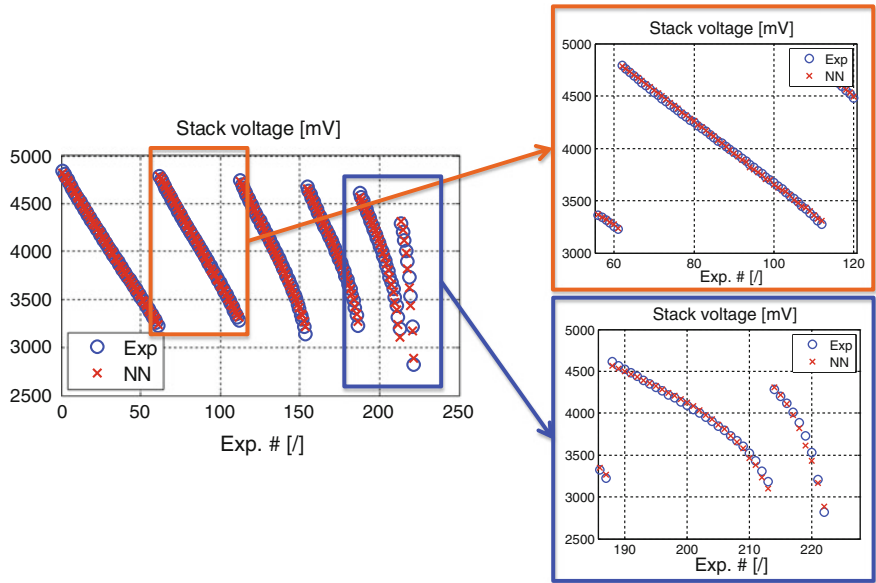


Fig. 2.39 Comparison of NN and experimental voltage over a voltage versus number of experiments domain

The stack was tested in such a way as to provide full I-V polarization curves at different operating conditions. For this specific application, an MLPFF NN (see Fig. 2.36) was selected to develop a black-box model linking voltage variation to

main operating conditions, namely current density, inlet temperature, and anode and cathode inlet flows.

Figures 2.38 and 2.39 highlight the high accuracy guaranteed by such an NN model over the entire available data set. Particularly, the two close windows, shown at the right-hand side of Fig. 2.39, clearly highlight the very good precision ensured by neural network models in predicting steady-state SOFC performance as a function of load. For further details on NN structure definition, inputs selection and conceptual arguments associated to neural network training and testing, the reader is addressed to a previous authors' contribution (Marra et al. 2013).

2.4.3 Development of Neural Networks for Dynamic Modeling of SOFC Performance

As discussed above, the large number of experimental data, gathered within the GENIUS project (GENIUS 2013), enhanced the development of black-box models such as neural networks. Beyond the steady-state data acquired in the form of I–V profile (see Fig. 2.39), several transient voltage profiles were also acquired within the GENIUS project (GENIUS 2013), particularly on a stack manufactured by Topsoe Fuel Cell. Therefore, it was possible to develop RNN suitable to simulate SOFC performance both in steady-state and dynamic conditions, as discussed in Sect. 2.4.1.

Figure 2.40 shows the specific RNN structure developed to simulate SOFC voltage variation as a function of several input variables. Such an RNN configuration was deployed to simulate voltage profiles acquired on different SOFC systems, as detailed in a previous authors' contribution (Sorrentino et al. 2014), to which the reader is addressed for further details on network development and experimental activity.

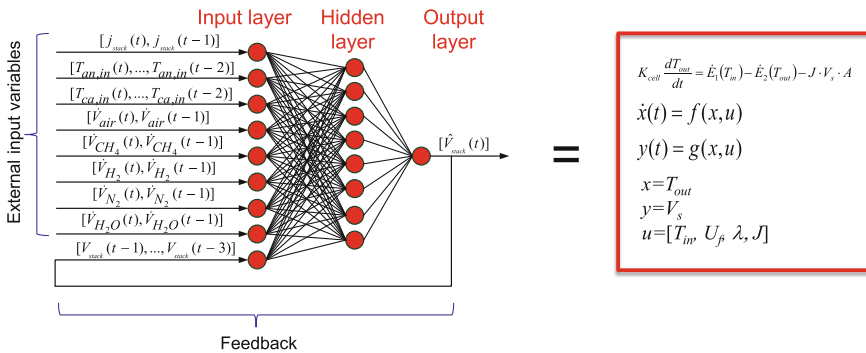


Fig. 2.40 RNN structure and qualitative equivalence between RNN and lumped models of SOFC dynamics

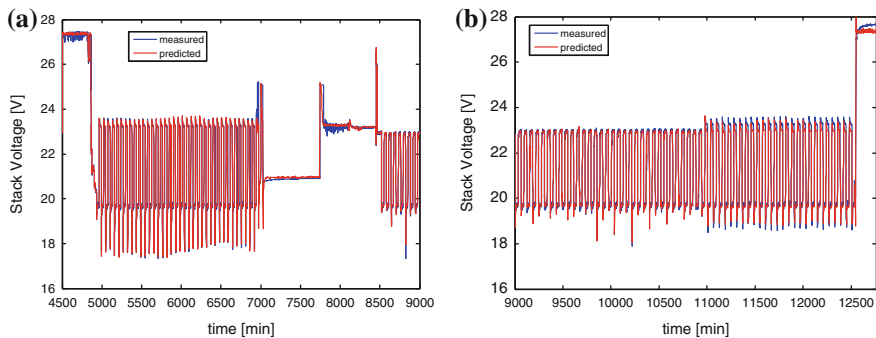


Fig. 2.41 Accuracy of the RNN SOFC performance simulator on the training (a) and test (b) data sets

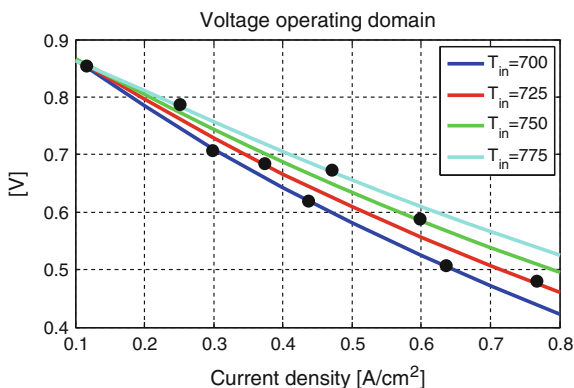
The high accuracy and generalization granted by RNN for SOFC dynamic simulation is confirmed by the comparative analyses illustrated in Fig. 2.41. Particularly, the voltage dynamics induced by both step and ramp load variations can be well captured thanks to the modeling equivalence shown in Fig. 2.40. Indeed, the latter figure evidences how the capability of the RNN, of learning the thermal dynamics associated to main operating variables variation (refer to the discussions made in Sects. 2.3.1.2.1 and 2.3.1.2.2), allows to directly estimate dynamic effects, without the need of solving an ordinary differential equation, as it happens when applying a lumped modeling approach as the one proposed in Sect. 2.3.1. Such an aspect may positively lead to fast development of control-oriented models, which also meet the conflicting needs of high accuracy and low computational effort.

A drawback can be associated to the number of parameters to be stored on electronic control unit when identifying a complex neural model, whose parameters can amount up to 100–200 overall (Arsie et al. 2006). However, such an issue can be mitigated by applying network size reduction methods, such as the well-known optimal brain surgeon method (Nørgaard et al. 2000), which was proved, by the authors themselves (Arsie et al. 2013), very effective in reducing network size and, thus, over-parametrization problems.

2.5 Required Experimental Activity

Following the outcomes and observations generated by the numerical analyses presented above, the objective of this section is to provide useful recommendations on the required experimental activity, depending on both selected modeling approach and real-world application of developed models.

Fig. 2.42 Experimental coverage (i.e. related to black-points location) of theoretically allowable voltage operating domain



Particularly, Sect. 2.5.1 highlights the importance of fully covering the SOFC working domain, whenever the aim is to develop highly general steady-state models. On the other hand, Sect. 2.5.2 indicates how to select the most suitable transient maneuvers, when aiming at developing dynamical models of SOFC behavior.

2.5.1 Definition of Steady-State Identification Domain

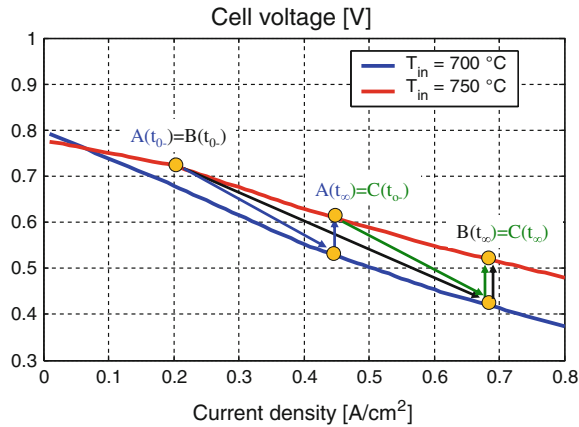
Figure 2.42 shows a generic I–V domain, which qualitatively holds valid in representing the whole theoretically allowable working region of an SOFC. As it is well known, the relatively high fragility of SOFCs makes really hard to fully explore such a domain by experimental activities only. Nevertheless, accurate cell design, as well as materials selection, often entail evaluating cell performance and other variables (e.g., internal temperature, current, and composition distributions) in a considerable number of operating conditions.

One suitable solution to the above issues is to refer to the hierarchical modeling approach shown in Fig. 2.2. Indeed, the black-colored points shown in Fig. 2.42 could be used to map the external perimeter and most significant internal points of the SOFC working domain. Afterwards, a physical model (e.g., the one presented and discussed in Sect. 2.2.1) could be developed, thus allowing to perform design-oriented simulations in a larger domain.

Moreover, the developed physical model can be exploited to create virtually extended data sets. This corresponds nothing but to adopting the hierarchical approach associated to the blue line of Fig. 2.2, thanks to which the rest of the working domain of Fig. 2.42 can be covered by performing a large number of virtual experiments.

One possible application of the above-described virtual data set extension is the development of black-box steady-state models, such as the ones presented in Sect. 2.3.1 (see Fig. 2.24) and Sect. 2.4.2. Furthermore, the virtually extended data

Fig. 2.43 Schematic representation of the transient maneuvers described in Table 2.7. Such a representation is in accordance with physical response subsequent to a load step change, as previously discussed in Sect. 2.3.1.2.1



set can be used to identify inverse models of SOFC behavior, e.g., able to estimate inlet fuel and air flows as a function of voltage and/or external temperature. Such inverse models are potentially very useful to assess the effect of cell to cell tolerance, as a function of measured performance, or, eventually, to verify maldistribution effects in multi-stack systems.

2.5.2 Transient Experiments

As deeply discussed in Sect. 2.3.1.2, transient response of SOFC voltage to load change strongly depends on the conditions before and after the transient maneuver. Figure 2.43 shows three possible load step-changes on a generic I–V domain. Particularly, maneuver A starts with low current density and ends with medium current, whereas maneuvers B and C end with high current density. The difference between maneuvers B and C lies in the fact that the former starts with a low current, while the latter with a medium current.

Table 2.7 Inputs and outputs of the response to load changes illustrated in Fig. 2.43

Case	Step variables		Dynamic performance metrics	
	$\bar{J}(t_\infty) \left[\frac{\text{A}}{\text{cm}^2} \right]$	$\Delta \bar{J} = \bar{J}(t_\infty) - \bar{J}(t_0) \left[\frac{\text{A}}{\text{cm}^2} \right]$	$\tau_V \text{ (s)}$	$V_{\text{drop}} \text{ (mV)}$
A	0.45	0.25	866.6	8.7
B	0.7	0.5	521.4	24.7
C	0.7	0.25	521.1	11.5

The simulations were carried-out assuming the same cell geometry and operating conditions of Sect. 2.3.1

The effect of different maneuvers on voltage response, which is based on the considerations already deepened in Sect. 2.3.1.2, is resumed by Table 2.7. The latter table must be considered of particular relevance when designing an experimental campaign aimed at identifying dynamic models of SOFC performance. Indeed, the fact that equal final current density values (i.e., cases B and C) are associated to equal voltage relaxation times and significantly different voltage drops (i.e., B more than doubles C, as shown in Table 2.7), clearly addresses the need for running quite various experimental transients. Particularly, not only most of the current density range must be explored, but also transient maneuvers have to be imposed in such a way as to ensure different load change as well as various initial and final load values be experimentally investigated. Of course the higher the number of combinations of the above mentioned variables values, the more informative the transient data set, which in turn will increase the generalization capabilities of black-box dynamic models, such as the RNN presented in Sect. 2.4.3.

2.6 Chapter Closure

This chapter presented in detail a hierarchical modeling structure, which is suitable to tackle main practical design problems associated to SOFC development and commercial success, namely system sizing as well as control and diagnostic strategies definition.

The compromise between physical content and computational burden of phenomenological and gray- and black-models was addressed and discussed with respect to their real-world potential deployment. Particularly, it was explained how the use of dimensional models is propaedeutic to performing parametric and scenario analyses of practical relevance, as well as to provide control-oriented model developers with key physical information, to be accounted for when selecting and developing less physical models. The latter modeling approaches were in turn proven effective as mathematical tools to be referred to when aiming at performing optimal balance of plant analyses, as well as single component sizing as a function of desired performance and fuel cell system nominal power.

All SOFC stack models were tested for validation against both reference numerical benchmarks and experiments. Numerical benchmarks were particularly useful in demonstrating the general validity and significant reliability granted by the developed 1D model. Particularly, main SOFC performance (e.g., voltage and fuel consumption), as well as spatial variations of most relevant operating variables, such as current density, temperatures, and species compositions, were accurately estimated. On the other hand, experiments gathered on different stacks confirmed the high potential offered by both black-box (including neural networks) and gray-box (e.g., lumped capacity models) to simulate voltage and outlet temperature in both steady-state and transient conditions.

The following two chapters focus on main methodologies and practical suggestions, to be accounted for when applying the proposed models hierarchy for model-based development of effective and reliable control and diagnostic tools.

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2016, XXII, 154 p. 86 illus. in color., Hardcover

ISBN: 978-1-4471-5657-4