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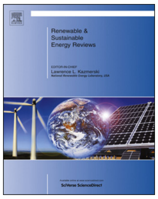

Challenges in the electrochemical modelling of solid oxide fuel and electrolyser cells

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ABSTRACT

Computational fluid dynamics (CFD) tools for the modelling of solid oxide fuel cells (SOFC), solid oxide electrolyser cells (SOEC) or solid oxide regenerative fuel cells (SORFC) nearly always require a fitting process prior to its application for cell design or optimisation purposes. In this fitting, a set of experimental data is used to guess the value of those parameters of the model that cannot be either modelled or measured experimentally. This is crucially the case of the charge transfer coefficients $(\alpha_{b,a}, \alpha_{f,a}, \alpha_{b,c}, \alpha_{f,c})$ and the exchange current densities $(i_{o,a}, i_{o,c})$ in the Butler–Volmer equation (*i.e.* electrochemical model).

The fitting of the electrochemical parameters in the SOFC, SOEC and SORFC modelling literature is reviewed in this work. It is found that this process is only vaguely discussed, if mentioned at all. In the authors' opinion, this practice contributes with uncertainty rather than guidance, since this fitting process is of utmost significance for making reliable quantitative predictions.

In this work, we further introduce a comprehensive model for the simulation of solid oxide regenerative fuel cells, *i.e.* a model that simulates, without any ad hoc adjustments or tuning, both the SOFC and SOEC modes. We also describe in detail how the electrochemical parameters are fitted, and discuss the applicability of the values commonly used in the literature for these fitted parameters and their proper validation. Finally, the validity of the proposed model and fitted parameters is shown by comparison of the numerical results with experimental data.

Contents

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1. Introduction

Hydrogen has been identified as a promising energy carrier: it can be cleanly produced in a water electrolyser driven by renewable energy; it may be then stored or transported, and eventually converted back into water and electricity in a fuel cell. A Solid Oxide Regenerative Fuel Cell (SORFC) is an electrochemical device that allows both operating modes, *i.e.* it can operate reversibly either as a fuel cell or as an electrolyser.

An SORFC operating as a solid oxide fuel cell (SOFC) generates electricity, heat and water from hydrogen and oxygen. An SORFC operating as a solid oxide electrolyser cell (SOEC) produces hydrogen and oxygen when water, heat and electricity are supplied.

The reversibility of the solid oxide cells was first proved in the 1990s for both tubular and planar geometries [3–5]; however, research in this field subsided due to the low prices of fossil fuels. In recent years environmental, economic and geopolitical concerns over fossil fuels have rekindled the interest in this technology. This is evinced by the ongoing research work for both planar [6–8] and microtubular solid oxide regenerative fuel cells [9,10].

Numerical modelling is a primary tool to understand, and optimise, the operation of solid oxide cells, either in fuel-cell or electrolyser mode. The modelling of *either* SOFCs *or* SOECs has been the subject of many papers [11–19]. Often such models use computational fluid dynamics (CFD) to simulate all the relevant mass, heat and charge transfer processes. Wang et al. [1] present an overview of the several modelling alternatives, including: physical models (by which they mean those that represent, mathematically, the underlying physics, be it in zero, one, multiple spatial dimensions); equivalent circuit models (based on electrochemical impedance spectroscopy, or EIS, measurements); and “gray-” and “black-box” models (such as Artificial Neural Networks and neuro-fuzzy systems). The review paper by Hajimolana et al. [2] is a systematic inventory of the main submodels proposed for the mathematical representation of all the relevant physical processes in the several spatial domains (gas channels, electrodes, electrolyte, interconnects).

References reporting the modelling of *both* SOFC *and* SOEC operating modes (*i.e.* SORFC) with a *single* CFD model that works satisfactorily in both situations are very scarce. To the authors' knowledge only Jin and Xue [20] have presented a validated numerical tool for the simulation of SORFCs. (Ni et al. [21,22] address the modelling and validation of a reversible solid oxide fuel cell, but in fact they only report the SOEC behaviour.) If properly formulated, a CFD model for either SOFCs or SOECs should produce suitable results in the other regime without any modification to the laws (submodels) for the underlying fundamental physics. However, this is not the case for most models, as shown below. This paper reviews the challenges posed by the development of such a unified model, and how to overcome them.

Any comprehensive SOFC, SOEC or SORFC model relies to a certain extent on data fitting to find values for some of the physical parameters, as it is the case of the charge transfer coefficients ($\alpha_{b,a}, \alpha_{f,a}, \alpha_{b,c}, \alpha_{f,c}$) and the exchange current densities ($i_{o,a}, i_{o,c}$) in the electrochemical model. This fitting, when properly resorted to, is the consequence of the incomplete knowledge of the underlying physical phenomena, or of the excessive complexity of such phenomena for them to be accommodated within a fluid-flow model. The disparity of spatial scales between these phenomena and the device to be simulated is often one of the sources of this complexity.

However, often this fitting process is only vaguely discussed in the literature. Table 1 summarises the common practices in the SOFC, SOEC and SORFC modelling literature to evaluate the

Table 1
Review of the evaluation of the electrochemical parameters in SOFC, SOEC and SORFC modelling literature.$f(\odot)$ means “calculated as a function of $\odot$”.

Model	Fitting	$\alpha_{b,a}/\alpha_{f,a}$	$\alpha_{b,c}/\alpha_{f,c}$	$i_{o,a}/i_{o,c}$	Value source
SOFC					
[25]	No	0.5/0.5	0.5/0.5	f(T)	From [56]/ guessed
[57]	No	0.5/0.5	0.5/0.5	5300/2000 A m^{-2}	From [58]
[50]	No	0.5/0.5	0.5/0.5	5300/2300 A m^{-2}	Not justified
[12]	No	0.5/0.5	0.5/0.5	7460/10090 A m^{-2}	Not justified
[59]	No	0.5/0.5	0.5/0.5	5300/2000 A m^{-2}	From [57]
[60,15]	Yes	0.5/0.5	0.5/0.5	Both f(T, species)	Fitting
[16]	Yes	0.5/0.5	0.5/0.5	Both f(T, species)	Fitting
[45]	Yes	1.5/0.5	0.75/0.25	Both f(T, species)	Fitting
[28]	Yes	2/1 [23]	1.5/0.5 [24]	Both f(T, species)	Fitting
SOEC					
[61,62]	No	0.5/0.5	0.5/0.5	Both from [25]	SOFC
[29]	Yes	0.5/0.5	0.5/0.5	Kinetics/fitted	Poor fitting
[63]	No	–	–	–	Not mentioned
[21,17,26]	No	0.5/0.5	0.5/0.5	2000/5300 A m^{-2}	From [57]
[22]	Yes	0.5/0.5	0.5/0.5	200 A m^{-2}/	Not mentioned
[19]	Yes	0.5/0.5	0.5/0.5	Fitted	Poor agreement
[51]	No	0.5/0.5	0.5/0.5	Both f(T, species)	Literature
SORFC					
[20]	Yes	0.5/0.5	0.5/0.5	1/0.1 A m^{-2}	Fitting