



## Review

## Numerical thermomechanical modelling of solid oxide fuel cells



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## ABSTRACT

Over the last decade, many computational models have been presented to describe the complex thermomechanical behaviour of solid oxide fuel cells. The present study elucidates a detailed literature review of the proposed numerical models, ranging from a single channel or unit layer, up to coupled 3D high-end system models. Thermomechanical modelling foundations, including material properties and thermomechanical stress sources in SOFCs are emphasized. Employed material models for SOFC components are highlighted. Thermomechanical modelling issues such as geometrical idealisation, initial and boundary conditions for the highly coupled fluid and solid mechanics problem, as well as numerical solutions have been discussed. Thermomechanical stress–strain formulation of the common fuel cell components is highlighted. Finally, an overview of the numerically solved thermomechanical modelling studies in solid oxide fuel cells is given. Case studies are used throughout this review to exemplify and shed light on several modelling aspects.

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Nomenclature		Abbreviations	
$T$	temperature (K)	CFD	computational fluid dynamics
$x, y, z$	cartesian coordinates (m)	SOFC	solid oxide fuel cell
$k$	thermal conductivity (W/mK)	FEM	finite element method
$E$	modulus of elasticity (MPa)	MEA	membrane electrode assembly
$C_p$	specific heat capacity (J/kg)	CTE	coefficient of thermal expansion
		DSC	differential scanning calorimetry
		SEM	scanning electron microscopy
		FIB	focus ion beam
<i>Greek symbols</i>		<i>Subscript</i>	
$\mu$	viscosity (kg/ms)	<i>tot</i>	total
$\rho$	density (kg/m <sup>3</sup> )	<i>th</i>	thermal
$\lambda$	plastic multiplier	<i>m</i>	mechanical
$\epsilon$	strain (–)	<i>pl</i>	plastic
$\nu$	poisson's ratio (–)	<i>el</i>	elastic
$\sigma$	stress (MPa)		
$\alpha$	coefficient of thermal expansion (10 <sup>–6</sup> /K)		

## 1. Introduction

Fuel cells are one of the oldest energy conversion technologies, originating back to the 19th century [1–4]. Like batteries and wind power technologies they provide low CO<sub>2</sub> and SO<sub>2</sub> emissions. Their advantages, including high efficiencies, low pollutant emission, high volumetric and gravimetric power densities, no re-charge duration makes them attractive in terms of an electricity source, as well as an energy converter. This extendable list of traits makes the fuel cell technology a serious high-end competitor against technologies like batteries and internal combustion engines. One of the most important fuel cell types has been the high temperature operating solid oxide fuel cell (SOFC) technology. It has a wide range of application due to its compactness and ease of manufacturing [5]. It can be utilised as a combined heat and power generation system for stationary, military, portable or mobile applications [6–11]. The fundamental mechanism of a solid oxide fuel cell lies in the oxidation of a fuel at an anode electrode and the reduction of oxygen at a cathode electrode, as to generate a potential difference. More specifically, these phenomena occur among four major interacting components namely, the interconnector plates, electrolyte, cathode, and the anode. The electrolyte is a membrane that separates the oxygen electrode (called as cathode) and the fuel electrode (called as the anode). The exploded view of typical SOFC components is shown in Fig. 1.

Oxygen ions from air that are supplied to the cathode electrode via the channels present in the interconnector plates is reduced to O<sup>2–</sup> at the cathode side, transported across the dense electrolyte and reacts with H<sub>2</sub> fuel at the anode side releasing electrons [Fig. 2]. The electrons released at the anode are transported through an external circuit where electrical power can be drawn. The fuel cell can be typically operated at temperatures 600 °C–1000 °C. This is the range the electrolyte becomes conductive to oxygen ions, but nonconductive to electrons. The high operating temperatures of SOFCs have some advantages, including the minimisation of polarisation losses and fuel impurity tolerance [12,13].

In solid oxide fuel cells (SOFCs) several functional materials, including the electrolyte, cathode, anode interconnector plates, and sealants have to be joined together as to form an assembly. Therefore, effort has been given by many researchers to develop and investigate materials with similar thermomechanical properties. Each material has to fulfill different requirements, thus this has been a challenge for many years. Investigations about the compositions of those materials have been elucidated in several studies, in detail [14–20]. Today, it is commonly accepted that the dense electrolyte materials are usually made of yttrium stabilized zirconia (YSZ), or composite materials like nickel oxide and polycrystals of zirconia etc. [15,17]. The adjacent porous electrodes, namely the cathode and anode are variants of calcium doped manganite compositions and Ni-YSZ, respectively. The metal components i.e., the interconnector plates and frames are usually made of ceramics or of metallic alloys [20]. From a thermomechanical analyst point of view, the properties of the materials are of interest rather than which and why a particular material has been chosen. However, experienced scientists and engineers, particularly in research and development are strongly encouraged to read, understand and educate themselves in those areas, as to perform from scratch meaningful analyses. Hence, their contribution to the design and development of the technology will be extremely beneficial.

Despite the tremendous effort in many SOFC research areas, full commercialisation of the technology still encounters many technological problems. Apart from the large scale implementation problems, the reliability and robustness of an SOFC design are of concern. Thermomechanically induced stress within fuel cells have attracted the attention of the community after hermeticity problems or mechanical degradation issues became significantly present in practice. Thereby, two focal points are investigated. The mechanical stability of the membrane electrolyte assembly (MEA) is one area, as the failure of the MEA will lead to failure of the stack operation. Many researchers have been focused to this problem, as to gather detailed insight about the mechanical or thermo-mechanical behaviour of the MEA. The second important challenge

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