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An advanced numerical model for energy conversion and crack growth predictions in Solid Oxide Fuel Cell units

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ABSTRACT

A dynamic mathematical model capable of predicting the energy conversion and crack propagation in Solid Oxide Fuel Cell (SOFC) unit is developed. Finite Element Method (FEM) and eXtended Finite Element Method (XFEM) are used to solve the multiphysics phenomenon taking place in the SOFC during service. A pre-existing crack is assumed lying within one of the cell's porous electrodes and far from the cell's electrochemically active sites (electrodes/electrolyte interfaces), and thus it is assumed to not affect the electrochemical reactions. The pre-existing crack propagates instantaneously once the crack-tip equivalent stress intensity factor (SIF) overcomes the porous electrode material toughness. Due to their small opening, cracks are assumed to affect only the heat conduction within the solid phase of the porous electrodes. The coupled fluid flow, fluid's energy transfer in the porous electrodes, and mass transport are solved using advanced FEM based schemes, where transition between SOFC interfaces (mainly porous electrodes/flow channels) does not require any special treatment. The heat transfer in the solid phase of the porous electrodes and the thermo-mechanical problem are solved using the XFEM. The predicted energy conversion is validated using experiments from the literature as well as our previously published experiments [J. Power Sources 272 (2014) 233–238]. The developed FEM/XFEM numerical tool is used to investigate the effect of temperature gradients on the propagation path of a pre-existing crack within an anode-supported SOFC. The crack propagation path is found to depend on the position of the pre-existing crack relative the SOFC interfaces as well as its initial orientation.

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Introduction

The demand for clean energy generation has been increased dramatically over last decades. Fuel cell systems are one of the most promising technologies that can help achieve these objectives. Among the existing fuel cell systems, Solid Oxide Fuel Cell (SOFC) is a cleaner alternative to conventional power generation due to its fuel flexibility, its high electrocatalytic activity and its fuel reforming within the cell unit. A SOFC unit consists of a solid dense gas-tight electrolyte sandwiched by two electrodes, an anode and a cathode, which present enough porosity allowing the flow of gases going into and back from the cell active sites. The particularity of SOFC is its high operating temperature that has numerous advantages. For instance, the kinetic activity is high and nickel is a sufficiently good catalyst, eliminating the need to use costly precious metals. However, the thermal gradients developing during service as well as reduction and oxidation processes can lead to a build-up of residual mechanical stresses that might trigger electrode delamination and/or nucleation of cracks within the electrodes [1–6]. Other degradation modes that lead to loss of cell active area include anode nickel sintering, cathode chromium poisoning and anode sulphur poisoning [7–9]. To enhance SOFC mechanical properties, a new generation of SOFC called microstructured metal-supported SOFC is being investigated [10]. Microstructure optimization of SOFC's anode and cathode components was also considered by Ruiz-Morales et al. [11–13] and by Lashtabeg et al. [14] to enhance the SOFC energy conversion efficiencies. Along with experimental investigation, different modelling efforts are being developed to identify an optimal design of SOFC. In the last few years, significant multi-physics models are introduced to simulate SOFC in service [15–23]. Most of the models cited above are used to predict the flow, utilization and distribution of anode and cathode gases, as well as the temperature and the current distributions. Further, numerical models describing the effects of cell degradation on its energy conversion performance are developed by Gazzarri and Kesler et al. [24–26] and then used as a tool for identification of the cell degradation modes.

In the present paper, an advanced FEM/XFEM numerical tool is developed to solve the multiphysics phenomena taking place in a SOFC unit (anode/electrolyte/cathode) during service. The main objective of the present work is to investigate the effect of stresses, induced by temperature gradients, on the onset of crack propagation and the crack propagation path of a pre-existing crack within the cell. Note that temperature gradients within the cell can be developed during to the heating process and also during the steady state regime due to the heat generated by the electrochemical reactions. The pre-existing crack is assumed lying within one of the cell porous electrodes and far from the cell electrochemically active sites (porous-electrodes/electrolyte interfaces). The pre-existing crack is assumed to not affect the electrochemical reactions within the cell and its propagation is assumed instantaneous, and lead to a complete deterioration of the cell. Therefore in the present work, the effect of the crack on the electrochemical reactions is not addressed. Due to its small opening, the crack is assumed to affect only the heat conduction in the solid phase within the porous electrodes. Further, the interconnect was not taken into account, while simplified mechanical boundary condition are prescribed (see Fig. 1). Note that the model can support any boundary conditions for the fluid flow, heat transfer and thermo-mechanical equations. Also, the manufacturing residual stresses were not taken into account. The present work is novel for the following reasons:

(1) The numerical tool can predict the SOFC energy performance and possible crack propagation path of a pre-existing crack during service (heating period and steady state).
(2) The numerical schemes used to discretize the multi-physics equations can deal with the transition between the SOFC interfaces without any special treatment, avoiding numerical errors.

The paper is organized as follow: the multi-physics governing equations and their FEM/XFEM discretizations are recalled in Section 2. Validation of the numerical model is reported in Section 3. In Section 4, crack propagation is analyzed during the SOFC heating process and during the steady state. Finally, conclusions are drawn in Section 5.

Governing equations

The fluid flow, heat transfer, mass transport and thermo-mechanical equations as well as the electrochemical reactions within the SOFC unit are solved as following:

- Navier–Stokes and Darcy–Brinkman equations are solved respectively in the flow channel and in the porous electrodes (anode and cathode) using the nonconforming Couzeix–Raviart finite element method [27], with the nonlinear convective term being treated by an upstream approach with weight as in the previous work of Schieweck et al. [28].
- The heat transport is split into two equations: one describes the heat transfer in the solid phase (solved in the porous electrode and the electrolyte) which is solved using

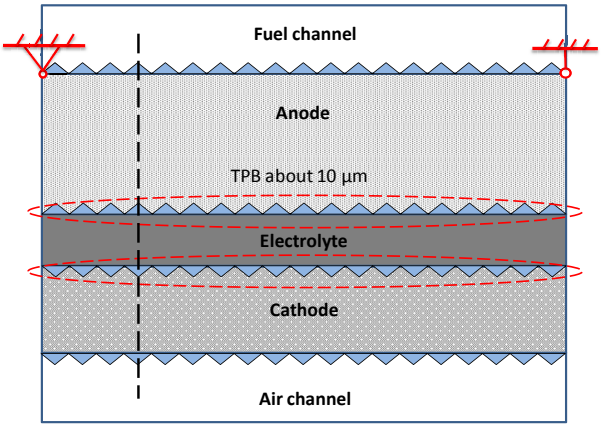

Fig. 1 – Mesh elements representing the three-phase boundaries.