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## Thermal shock resistance and failure probability analysis on solid oxide electrolyte direct flame fuel cells



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#### HIGHLIGHTS

• Thermal shock resistance was analyzed for direct flame fuel cells.

• Mass/charge/heat transport processes and thermal mechanical stress were coupled.

• Effects of cell structures (anode or electrolyte supported SOFC) were studied.

• Effects of flame temperature non-uniformity and heating process were studied.

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#### ABSTRACT

A detailed two-dimensional model of direct flame fuel cell (DFFC) was developed by considering the coupling effects of heterogeneous chemical and electrochemical reactions, electrode microstructure, transport processes of mass, charge and energy, as well as the thermal mechanical stress. The stress distribution was simulated at different heat-up rates which represent the typical DFFC and the common solid oxide fuel cell (SOFC) operation. Transient temperature field and associated thermal stress distributions are determined and analyzed for two different cell structures. The failure probability of the fuel cell is defined and estimated by employing the Weibull statistic. The model is demonstrated to be a useful tool for understanding the mechanical stress distribution within a DFFC cell and for the cell structure design and optimization. The results reveal that the failure probability of an SOFC cell plate working in flame conditions may be 6 orders higher than that in the common SOFC operation conditions. The anode-supported SOFC shows better thermal shock resistance compared with the electrolyte-supported SOFC. The uniformity of the flame temperature is vital in the DFFC system since the non-uniform distribution of the flame temperature greatly increases the failure probability.

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### 1. Introduction

Direct flame fuel cell (DFFC) is a kind of novel fuel cell, which combines the flame and the solid oxide fuel cell (SOFC) in a "nochamber" setup [1]. The flame consumes the oxygen at the anode side and provides the reacting heat for keeping the SOFC operating temperature. The cathode is exposed to the air to maintain the gas concentration gradient between the different electrodes [1–6]. Compared to the conventional dual-chamber and single-chamber SOFC, DFFC has the advantages in fuel-flexibility, sealing, simple setup and rapid start-up.

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Thermal stresses are the main factors for the failure of solid oxide fuel cells, especially for DFFC operation. During the operation of DFFC, the fuel cell plate is heated up much more rapidly by the flame compared to the temperature rising rate in common SOFC operating conditions and this may lead to significant thermal stress to the cell. In addition, the non-uniform temperature distribution of fuel cell generated of common flame can also lead to the variation of fuel cell temperature, which will lead to the thermal stress of SOFC as well. Thus, it is significantly important to analyze the thermal shock resistance and failure possibilities of SOFC for operating in typical flame conditions, which will be crucial for novel DFFC prototype design and performance optimization. Currently, although numerous studies have been carried out on thermal stresses for SOFC experimentally and theoretically, more specific models should be studied in order to quantify and predict the magnitude of the thermal stress in SOFC operating in flame conditions.

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In this study, a mechanistic model for DFFC by coupling the mass transport processes, the energy conservation, the electrochemistry and the mechanical stress is developed. The thermal shock resistance of the DFFC configuration is studied. Transient temperature field and associated thermal stresses are determined and compared for two DFFC structures which are based on the anode-supported SOFC (ASSOFC) and the electrolyte-supported SOFC (ESSOFC) separately. The influences of the flame non-uniformity on DFFC performance and the stress field are studied. The Weibull statistic is employed to estimate the failure probability of the DFFC during the start-up and operation period.

#### 2. Model development

#### 2.1. Model geometry

The geometry of the model exhibits a two dimensional (2D) planar type DFFC as seen in Fig. 1. In the DFFC setup, the fuel cell was located above the flame with the anode facing the flame front and the cathode exposed to ambient air. Two different cell structures (ASSOFC and ESSOFC) are studied and the dimensions are given in Table 1. The thicknesses of the cell layers ( $t_a$ ,  $t_e$ ,  $t_c$  in Fig. 1) are chosen as the configurations which are commonly used in published literature [7–9].

#### 2.2. Model assumptions

The main assumptions are listed as the following:

- (1) The electrochemical reactions spatially occurred along electrode thickness within the electrode. The reaction active sites are assumed to be uniformly distributed in each electrode layer. The two conducting phases (electronic and ionic) are considered to be continuous and homogeneous in each layer.
- (2) The charge transfer reaction is assumed to take place at the three phase boundary (TPB).
- (3) A mixture of H<sub>2</sub>, CO, H<sub>2</sub>O, CO<sub>2</sub> gases with a typical flame composition were chosen as the anode gases and the cathode gas was chosen as air. All of the gasses are considered as ideal gases.
- (4) The convection flux and pressure gradient in the porous electrodes are ignored.
- (5) Radiative heat transfer is neglected within the whole cell.
- (6) The temperature load is considered to be the only one in stress analysis.

#### 2.3. Governing equations

#### 2.3.1. Charge conservation

The governing equations for SOFC electrode transient charge balance were shown as follows [10,11]:

 Table 1

 Dimensions of the fuel cells

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	ASSOFC	ESSOFC
1	50 mm	50 mm
t <sub>a</sub>	1000 µm	50 µm
t <sub>e</sub>	20 µm	150 µm
t <sub>c</sub>	60 µm	50 µm

Ionic charge balance at the anode:

$$\frac{C_{dl,an}S_{act,an}\partial(V_{ion,an} - V_{el,an})}{\partial t} + \nabla \cdot \left(-\sigma_{ion,an}^{eff}\nabla V_{ion,an}\right) = Q_{ion,an} \\
= -\left(i_{0,an,H_2}\frac{c_{H_2}^{TPB}}{c_{H_2}^{H_2}} + i_{0,an,CO}\frac{c_{CO}^{TPB}}{c_{CO}^{bulk}}\right) \\
S_{act,an}\left(exp\left(\frac{\alpha n_e F\left(V_{el,an} - V_{ion,an} - V_{ref,an}\right)}{RT}\right) \\
-exp\left(-\frac{(1-\alpha)n_e F\left(V_{el,an} - V_{ion,an} - V_{ref,an}\right)}{RT}\right)\right) (1)$$

Electronic charge balance at the anode:

$$\frac{C_{\text{dl},\text{an}}S_{\text{act},\text{an}}\partial(V_{\text{el},\text{an}} - V_{\text{ion},\text{an}})}{\partial t} + \nabla \cdot (-\sigma_{\text{el},\text{an}}\nabla V_{\text{el},\text{an}}) = Q_{\text{el},\text{an}}$$
$$= -Q_{\text{ion},\text{an}}$$
(2)

Ionic charge balance at the cathode:

$$\frac{C_{\text{dl,ca}}S_{\text{act,ca}}\partial(V_{\text{ion,ca}} - V_{\text{el,ca}})}{\partial t} + \nabla \cdot \left( -\sigma_{\text{ion,ca}}^{\text{eff}} \nabla V_{\text{ion,ca}} \right) = Q_{\text{ion,ca}} \\
= i_{0,ca}S_{\text{act,ca}} \frac{c_{O_2}^{\text{TPB}}}{c_{O_2}^{\text{bulk}}} \left( \exp\left(\frac{\alpha n_e F\left(V_{\text{el,ca}} - V_{\text{ion,ca}} - V_{\text{ref,ca}}\right)}{RT}\right) \right) \\
- \exp\left( -\frac{(1 - \alpha)n_e F\left(V_{\text{el,ca}} - V_{\text{ion,ca}} - V_{\text{ref,ca}}\right)}{RT}\right) \right)$$
(3)

Electronic charge balance at the cathode:

$$\frac{C_{\text{dl,ca}}S_{\text{act,ca}}\partial(V_{\text{el,ca}} - V_{\text{ion,ca}})}{\partial t} + \nabla \cdot \left( -\sigma_{\text{el,ca}}^{\text{eff}} \nabla V_{\text{el,ca}} \right) = Q_{\text{el,ca}}$$
$$= -Q_{\text{ion,ca}}$$



Fig. 1. DFFC setup (left) and simplified 2D model geometry of planar SOFC (right).

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