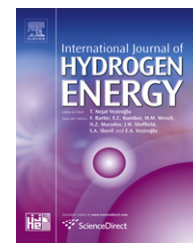


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# Prediction of the performance of a solid oxide fuel cell fuelled with biosyngas: Influence of different steam-reforming reaction kinetic parameters

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## ARTICLE INFO

### Article history:

Received 24 March 2012

Received in revised form

9 August 2012

Accepted 10 September 2012

Available online 6 October 2012

### Keywords:

SOFC

CFD

Simulation

3-D modeling

Biosyngas

Activation energy

## ABSTRACT

SOFCs are often designed to operate with specific fuels, quite often natural gas. CFD modeling is often used to arrive at efficient and safe SOFC designs. Therefore, when an SOFC is fed with different fuels, i.e., biosyngas, CFD can be used as a tool to predict whether the cell and stack will be safe and operate efficiently, and thus can give suggestions for the operation strategies for SOFCs. For that reason, a combined mass and heat transport model of an SOFC (single channel) has been developed for an anode-supported SOFC fed with biosyngas with special attention to the reaction kinetics of the direct internal reforming (DIR) reaction together with the water–gas shift reaction. An SOFC design jointly developed by ECN and Delft University of Technology is employed for the calculations. This work aims to predict the influence of different reforming reaction kinetic parameters on the cell performance by using an anode-supported intermediate temperature DIR planar solid oxide fuel single channel model, under co-flow operation. The DIR reaction of methane, the water–gas shift reaction and the electrochemical oxidation of hydrogen are being considered. As different reaction kinetic models are available in literature and employing them in CFD calculations will yield different results, a comparative analysis is carried out. Several cases were studied with a variety of DIR and water gas shift reaction kinetic parameters available from literature. For the different cases considered, the modeling results show differences in the current density distribution and temperature profile in the channel and in gas concentration profile along the channel. These differences are presented and discussed in detail. Predictions of the behaviors of internal reforming reaction in the reaction zone, and the possibilities of unwanted side reactions such as carbon deposition and Ni oxidation are given with constructive suggestions for future lab experiments.

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## 1. Introduction

Fuel cells are electrochemical devices which convert chemical energy to electrical energy through chemical reactions

directly and efficiently [1–4]. It is substantially different from the conventional thermal power plants, in which the fuel gas is oxidized in a combustion process and a thermal–mechanical–electrical energy conversion process is

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Nomenclature	
$C$	molar concentration
$C_p$	heat capacity at constant pressure
$C_v$	specific heat at constant volume
$D$	diffusion coefficient
$E_a$	activation energy
$E_{a,ele}$	electrochemical activation energy
$E_{rev}$	theoretical reversible voltage
$E^0$	standard electrode potential
$F$	Faraday constant
$f$	free
$g$	Gibbs energy
$H$	height
$h$	enthalpy
$i_{ele}$	current density
$I$	unit tensor
$k$	conductive heat transfer coefficient
$k_{0,ele}$	empirical parameter
$L$	cell length
$n_{mol}$	no. of moles
$n$	no. of species
$p$	pressure
$R$	universal gas constant
$r$	reaction rate
$S$	source
$t$	time
$T$	temperature
$U_L$	potential losses
$V$	voltage
$V_j$	Fuller diffusion volume
$W$	cell unit width
$Y$	species concentration
<i>Greek symbols</i>	
$\alpha$	permeability of electrodes
$\rho$	density
$\lambda$	thermal conductivity coefficient
$\varepsilon$	porosity
$\mu$	dynamic viscosity
$\tau$	thickness
$\nu$	velocity
<i>Subscripts</i>	
a	activation
atm	atmospheric
f	fuel
fl	fluid
i	species i
inlet	inlet of the gas channel
j	species j
M	momentum
ohm	ohmic resistance
rev	reversible
s	solid
tot	total
eq	equilibrium constant
wgs	water gas shift
<i>Superscripts</i>	
0	standard
reac	reacted

employed. Different from the conventional thermal power plants which are subjected to Carnot cycle efficiency, the high temperature solid oxide fuel cells are promised to be one of the most efficient device for direct conversion of fuel chemical energy into electricity [5,6]. The efficiency of the fuel cell based power plant can be further increased when coupled with a gas turbine cycle to about 70% [3]. Several studies have shown very high efficiencies with SOFC-GT system [6,7]. High energy-conversion efficiency and less noise production are the outstanding advantages of fuel cells. Easy maintenance and flexibility for a distributed energy system, and reduced environmentally harmful emissions, including greenhouse gases also make fuel cells attractive [8,9]. Fuel cell technology appears to be a promising generation of novel power sources.

The core component of an SOFC is a thin, gas-tight, ion conducting electrolyte layer sandwiched between a porous anode and cathode, shown in Fig. 1. The electrolyte in an SOFC is a solid oxide material which only lets the charge-carrying oxide ions go through [10]. Steam reforming and water gas shift reactions take place in the porous medium of the anode while electrochemical reactions are assumed to occur at the interface of the anode and the electrolyte [11]. During the electrochemical oxidation process, oxygen combines with electrons at the porous cathode and the ions thus formed are driven across the electrolyte by a chemical potential difference between the two sides of the electrolyte as a result of the fuel oxidation at the porous cathode [12]. Released electrons

are moving from the anode to the cathode through an external circuit because they are able to move through the electrolyte. The output potential of an SOFC is lower than the theoretical maximal value owing to a variable over potential or potential losses induced by activation polarization, ohmic losses, and concentration polarization by the resistance of mass transport. The ion conductivity in the electrolyte strongly depends on temperature and is reasonably high only as long as temperature is higher than 850 K, whereas high temperature induces an issue of safety along with the higher demands to the materials composing the SOFC [10]. Since the SOFC operates by transport of oxide ions, an SOFC can be fueled with reforming gas containing  $\text{CH}_4$ ,  $\text{CO}$ ,  $\text{H}_2$ ,  $\text{CO}_2$ ,  $\text{H}_2\text{O}$  and  $\text{N}_2$ , and the high operating temperature ensures the occurrence of rapid DIR and water gas shift reactions [13].

One of the essential aspects for the efficient operation of solid oxide fuel cells (SOFCs) is the suitable choice of fuel. The most commonly used fuel gas is hydrogen, which is mainly generated from steam reforming of  $\text{CH}_4$  on different catalysts, at temperatures ranging from 950 to 1100 K [14–16]. With internal steam reforming, solid oxide fuel cell (SOFC) systems have the potential to become a promising technology [17]. However, natural gas or biosyngas with  $\text{CH}_4$  can be introduced into SOFCs directly as fuel gases without any external reformers attached under certain conditions. This is because of the ability of the SOFC anodes to catalyze the steam reforming of  $\text{CH}_4$  as well as the water–gas shift reaction [15].

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