



Telescopic projective Adams multiscale modeling of electrochemical reactions in tubular solid oxide fuel cells

Chen Yang^{a,b,*}, Hangxing He^{a,b}, Nana Zhou^{a,b}, Wei Peng^{a,b}, Ke Yang^{a,b}

^a Key Laboratory of Low-Grade Energy Utilization Technologies and Systems, Chongqing University, Ministry of Education, Chongqing 400030, PR China

^b College of Power Engineering, Chongqing University, Chongqing 400030, PR China

ARTICLE INFO

Article history:

Received 3 November 2015

Received in revised form 22 June 2016

Accepted 12 July 2016

Available online 14 July 2016

Keywords:

Solid oxide fuel cell

Electrochemical performance

Multiscale modeling

Coarse projective integration

ABSTRACT

In order to predict the electrochemical performance of Solid Oxide Fuel Cells (SOFCs), a telescopic projective Adams (TPA) multiscale simulation method is proposed in this work. This method is constructed on the basis of the equation-free method (EFM). A lattice Boltzmann model is used as the fine-scale simulator of the proposed method. The electrochemical reaction-diffusion process was simulated by the TPA and the lattice Boltzmann method (LBM). The results of the two methods were found to be in good agreement, and the TPA method can give accurate results with lower computational costs. The electrochemical reactions were also simulated based on the TPA method. The results were consistent with the experimental data, indicating that the proposed TPA method is an effective tool to simulate the electrochemical reactions of SOFCs. Also, the proposed method is suggested to be helpful in multiscale modeling of other energy systems.

© 2016 Elsevier Ltd. All rights reserved.

1. Introduction

The demand for power-generation systems of high efficiency and low emission is growing. Fuel cells, unlike conventional energy-conversion systems, are more efficiently and environmental-friendly, by converting the chemical energy from fuels into electricity directly through electrochemical reactions. Meanwhile, fuel cells are complex devices that involve various physicochemical phenomena and processes. Due to the temporal-spatial multiscale characteristics of the electrochemical reactions inside the fuel cells, it is difficult to reveal the electrochemical mechanisms through experimental observations and to determine the internal states of fuel cells experimentally. Therefore, numerical simulations of the electrochemical reactions have received extensive attention (Singhal and Kendall, 2003). Numerical simulations are efficient ways to study these complex problems and direct the experiments. However, the effect of multiscale poses many difficulties for conventional numerical solutions.

Multiscale systems are those systems in which there is a direct linkage between the physics at very small lengthscales/fast timescales and the behavior at large lengthscales/slow timescales (Shay et al., 2007). Traditional macroscopic modeling encounters

many obstacles when dealing with multiscale systems. For example, many macroscopic equations cannot be obtained in closed forms although they exist conceptually. Besides, most of them are nonlinear evolution equations which are probably impossible to be solved. Likewise, for many practical problems, full representations of the fine-scale (mesoscale, microscale, etc.) system are somehow impossible for the foreseeable future, because each evolutionary step must be explicitly calculated by the fine-scale simulator, which results in the overwhelming computational costs (Weinan and Engquist, 2003).

In recent years, a framework for computer-aided multiscale analysis, called “equation-free” method (EFM) has been proposed and developed (Kevrekidis et al., 2003). This framework is built around the central idea of a coarse time-stepper (CTS), which allows the researchers to perform macroscopic tasks by acting on the microscopic models directly, circumventing the derivation of macroscopic-level descriptions. It constitutes a bridge between traditional, continuum numerical analysis and fine-scale simulation, and provides a new idea for multiscale simulations of complex processes. Therefore, this framework has been gaining widespread attention by researchers related to complex system simulation and has been applied to a variety of problems over the last few years (Erban et al., 2006; Rico-Martinez et al., 2004; Lee and Gear, 2007; Shay et al., 2007; Kavousanakis et al., 2007; Maluckov et al., 2008; Kevrekidis et al., 2003; Gear, 2001; Gear and Kevrekidis, 2003; Kevrekidis and Samaey, 2009; Yang and He, 2015).

* Corresponding author at: College of Power Engineering, Chongqing University, 174 Shazhengjie, Shapingba, Chongqing 400044, PR China.
E-mail address: yxtyc@cqu.edu.cn (C. Yang).

Nomenclature

A_j	Constant
A_s	SOFC surface area (m^2)
A^*	Pre-exponential factor
B_j	Constant
D'	Diffusion coefficient
E	Reversible electrochemical cell voltage (V)
E_a	Activation energy ($J mol^{-1}$)
e_i	Discrete velocity in lattice unit
F_c	Faraday constant ($96487C mol^{-1}$)
f_i	Particle distribution function
f_i^{eq}	Equilibrium particle distribution function
G^0	Gibbs free energy ($J mol^{-1}$)
H	Enthalpy ($J mol^{-1}$)
I	Current density ($A m^{-2}$)
I_0	Exchange current density ($A m^{-2}$)
I_L	Limiting current density ($A m^{-2}$)
K	Reaction constant
K_p	Equilibrium constant
m	Number of directions of particle velocity
N	Total number of tubular SOFCs
n_{CH_4}	Mole concentration of methane
n_e	Number of electrons transferred per reaction
P	Partial pressure (Pa)
R	Universal gas constant ($8.314 J mol^{-1} K^{-1}$)
R^*	Reaction term
R_j	Ohmic resistance (Ω)
T	Temperature (K)
t	Time (s)
t_0	Initial evolution time
U_f	Fuel utilization rate
V	Cell voltage (V)
W_{SOFC}	Output power (kW)
x	Coordinate of the grid point
y	Coordinate of the grid point
Z_h	Molar flow-rate of hydrogen ($mol s^{-1}$)
Z_r	Molar flow-rate of inlet fuel ($mol s^{-1}$)

Greek letters

β	Electron transfer coefficient
δ_j	Thickness (m)
η_{act}	Activation overpotential (V)
η_{con}	Concentration overpotential (V)
η_{ohm}	Ohmic overpotential (V)
τ	Relaxation time in lattice unit
ρ	Reactant concentration in lattice unit
Ω_i	Collision term
ζ_{DA}	Efficiency of the converter
ζ_{SOFC}	Efficiency of the SOFC

Chemical

CH_4	Methane
CO	Carbon monoxide
CO_2	Carbon dioxide
H_2	Hydrogen
H_2O	Water
O_2	Oxygen

A detailed understanding of the electrochemical processes is the first step in developing a comprehensive mathematical model of the SOFC. A considerable amount of research has been conducted on SOFCs to date, and various numerical methods have been used.

Table 1

Values of equilibrium constants of reforming and shifting processes.

	Reforming	Shifting
A	-2.63121×10^{-11}	5.47301×10^{-12}
B	1.24065×10^{-7}	-2.57479×10^{-8}
C	-2.25232×10^{-4}	4.63742×10^{-5}
D	1.95028×10^{-1}	-3.91500×10^{-2}
E	-6.61395×10^1	1.32097×10^1

However, there exist a limited number of studies analyzing the performance of the SOFC at fine-scale. The LBM, which is a mesoscopic approach based on minimal lattice formulations of the kinetic Boltzmann equation, has shown promising simulation results of fluid flows and mass diffusion through complex geometries. And it has also been applied to simulate mass and charge transport in a SOFC anode structure successfully (Paradis et al., 2015). Therefore, based on the LBM, it is the attempt of this work to implement the TPA multiscale method to simulate the electrochemical reactions of the SOFC.

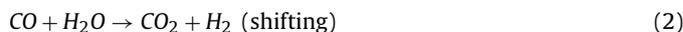
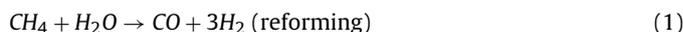
2. Model description

In this section, we will first give an introduction to the SOFC, the EFM and the LBM. Then a telescopic projective Adams multiscale method was proposed and developed based on the EFM. The model was executed directly on the mesoscopic lattice Boltzmann (LB) simulators. The second-order Adams–Bashforth method was used for the extrapolation of macroscopic solutions. The following is the introduction of the proposed method.

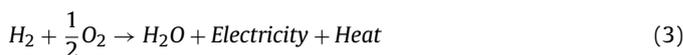
2.1. Solid oxide fuel cell

In general, a fuel cell is an electrochemical device that converts chemical energy to electrical energy directly and continuously as reactants (fuel and air) being supplied. The electrochemical reaction of the SOFC employs hydrogen fuel as the reducing agent and oxygen from the air as the oxidant. The electrochemical reactions, split into two half-cell reactions, are taking place at the SOFC electrodes. To complete the overall reaction, the oxygen anions (O^{2-}) migrate through the ion conductive electrolyte to the anode electrode, while the electrons are directed towards the cathode through an external circuit, as shown in Fig. 1.

The SOFC modeled in this work was fueled by natural gas to produce the hydrogen for electrochemical reaction. The internal reforming was needed. The reaction mechanisms for the internal reforming of the SOFC stack are:



The overall reaction is:



The equilibrium constants of reforming and shifting processes are temperature dependent, which can be obtained from the following equation:

$$\log K_p = AT^4 + BT^3 + CT^2 + DT + E \quad (4)$$

where constants A–E are listed in Table 1 (Chan et al., 2002).

The current density of the SOFC can be written as,

$$I = \frac{n_e Z_h F_c}{NA_s} \quad (5)$$

where n_e is the number of electrons transferred per reaction; F_c is Faraday constant; Z_h is molar flow-rate of H_2 participating in the

Download English Version:

<https://daneshyari.com/en/article/172000>

Download Persian Version:

<https://daneshyari.com/article/172000>

[Daneshyari.com](https://daneshyari.com)