Study of the tortuosity factors at multi-scale for a novel-structured SOFC anode

This content has been downloaded from IOPscience. Please scroll down to see the full text.
2017 J. Phys.: Conf. Ser. 849 012020
(http://iopscience.iop.org/1742-6596/849/1/012020)

View the table of contents for this issue, or go to the journal homepage for more

Download details:

IP Address: 128.41.35.98
This content was downloaded on 04/08/2017 at 12:11

Please note that terms and conditions apply.

You may also be interested in:

**Dynamic Capillary Pressure in Porous Media**
P. G. de Gennes

**A two-dimensional model for densification behaviour of C/SiC composites**
Xi Wei, Lai-Fei Cheng, Li-Tong Zhang et al.

**Experimental study of multi-scale heat transfer characteristics at pool boiling**
V Serdyukov and A Surtaev

**Preparation of Ni–YSZ Cermet through Reduction of NiO–YSZ Ceramic for SOFC Anode**
P.S.N. Baity, B. Budiana and S. Suasmoro

**Multi-scale model of the dynamic fracture of molten and solid metals**
A E Mayer, P N Mayer, V S Krasnikov et al.

**Multi-scale problem in the model of RNA virus evolution**
Andrei Korobeinikov, Aleksei Archibasov and Vladimir Sobolev

**Multi-Scale Visualization Analysis of Bus Flow Average Travel Speed in Qingdao**
HAN Yong, GAO Man, ZHANG Xiao-Lei et al.

**LBM for multi-component, non-continuum mass diffusion**
Abhijit S Joshi, Aldo A Peracchio, Kyle N Grew et al.

**Correlation between surface properties and wettability of multi-scale structured biocompatible surfaces**
S N Gorodzha, M A Surmeneva, O Prymak et al.
Study of the tortuosity factors at multi-scale for a novel-structured SOFC anode

X Lu¹, T Li², O O Taiwo¹, J Bailey¹, T Heenan¹, K Li², D J L Brett¹ and P R Shearing¹

¹Department of Chemical Engineering, University College London, London, WC1E 7JE, UK
²Department of Chemical Engineering, Imperial College London, London, SW7 2AZ, UK
Email: xuekun.lu@ucl.ac.uk

Abstract. Gas transport properties are closely related to the tortuosity of the pore network within porous materials. For the first time, this study explores a multi-scale imaging and modelling method to measure the tortuosity of an Solid Oxide Fuel Cell (SOFC) electrode material with pore sizes spanning over hundreds of orders of magnitude. This analysis is normally challenging using image-based techniques, as pores of different sizes may not be easily resolved at the same time using X-ray computed tomography (CT). In this study, a tubular SOFC anode, fabricated by a phase inversion technique, is used to illustrate this approach. A heat flux analogy is used to simulate mass transport and the results show that the embedded large-scale finger-like pores can significantly improve mass transport by providing less tortuous pathways.

1. Introduction
Gas transport through porous anodes is critical to the electrochemical performance of solid oxide fuel cells (SOFC) as the partial pressures of the reactants and products are closely related to the anode polarization, which significantly contributes to the loss of operating voltage. The porosity ($\epsilon$) and tortuosity of the gas transport path each play a significant role in determining the diffusivity of the fuel gas in the porous anode [1]. The tortuosity factor ($\tau$) is a material parameter used to characterise gas diffusion resistance due to the tortuous pore volume [2, 3]. This effective transport parameter can be obtained by the modelling of mass/heat flux through a 3D porous phase using computational fluid dynamics (CFD) methods [4].

A newly developed tubular SOFC fabricated by phase inversion technique has attracted considerable attention [5]. Apart from the controllable pore size in the spongy layer, the exchange of solvent and non-solvent in the hollow fiber generates micro-channels which grow in the radial direction, with a diameter of approximately 20 $\mu$m. This design can significantly improve gas transport in the anode with little sacrifice of mechanical robustness. In this study, non-destructive X-ray CT is used to image the SOFC anode at micrometer and nanometer resolution for the whole anode and the porous phase in the spongy layer, respectively. The tortuosity factor extracted from the high resolution scan was subsequently used for the simulation of the entire anode.

2. Methodology

2.1 Tortuosity Factor Measurement
The analogue between heat and mass transfer is well established \[ \text{[6]} \] and is regularly used to measure the tortuosity factor. The heat flow driven by a temperature gradient in a porous material is described using modified Fourier’s law as

\[
Q_p = -A\varepsilon k \frac{\Delta T}{\tau} L
\]

Where \( A \) is the cross sectional area of the flow volume, \( k \) is the thermal conductivity, \( \Delta T \) is the temperature difference and \( L \) is the length of flow volume, \( \varepsilon \) is the porosity and \( \tau \) is the tortuosity factor. As \( \varepsilon \) can be measured by image analysis, by dividing \( Q_p \) by the heat flow in a fully porous volume \( Q \) (i.e. \( \varepsilon = 1, \tau = 1 \)), \( \tau \) can be obtained. For simplicity, the thermal conductivity of the micro-channels are set to unity (i.e. \( k = 1 \)), so that the thermal conductivity is equivalent to the effective transport parameter \( \varepsilon / \tau \) for the spongy layer.

2.2 X-ray Computed Tomography

The entire tubular anode and the spongy layer were imaged using a Versa 520 and Ultra 810 X-ray microscope (Zeiss Xradia, Carl Zeiss, CA, USA) respectively \[ \text{[7]} \]. Detailed scanning parameters are shown in Table 1. FDK and filtered-back projection algorithms were used for the reconstruction of the full anode and the spongy layer scans respectively \[ \text{[5, 8]} \]. The reconstructed sample volumes were segmented using the Avizo V9.0 software (VSG, Bordeaux) package.

| Table 1. Scanning parameters for the spongy layer and entire anode |
|----------------------------------------------------------|
| Tube target | Voltage (kV) | Voxel size (μm) | Field of view (μm²) | Projections | Exposure time (s) | Camera binning |
|---------------|--------------|----------------|---------------------|-------------|------------------|----------------|
| Spongy | Cr | 35 | 0.032 (binned) | 16×16 | 1201 | 60 | 2 |
| Anode | W | 140 | 1.07 | 2000×2000 | 2001 | 18 | 1 |

2.3 Computed Dynamics Fluid (CFD) Simulation

The segmented porous phase of the spongy layer was imported into the CFD software Star-CCM+ (CD-adapco Inc.) for meshing followed by heat flux simulation. \( \varepsilon / \tau \) was then used to define the effective thermal conductivity of spongy layer in the simulation of the entire anode on a control volume with full radial thickness, an axial depth of 700 μm and 90° arc angle (see Figure 1). The detailed simulation parameters are shown in Table 2.

![Image](image-url)

**Figure 1.** The effective thermal conductivities of the micro-channels (red) and spongy layer (green) are assigned as unity “1” and \( \varepsilon / \tau \), respectively. Conformal meshes are generated between the two regions.
Table 2. CFD simulation parameters for spongy layer and entire anode

|                          | Spongy layer | Full anode |
|--------------------------|--------------|------------|
| Number of cells          | 1.2 million  | 1.6 million|
| Inlet temperature (°C)   | 1000         | 1000       |
| Outlet temperature (°C)  | 300          | 300        |
| Thermal conductivity ($\epsilon_s/\tau_s$) | 1            | 1          |
| Sample dimension ($\mu$m$^3$) | 9×6×4        | 800×800×800|

3. Results and discussion

A virtual slice of the anode is shown in Figure 2a. The radially aligned micro-channels are clearly resolved. The porous phase in the spongy layer, which appears as solid phase in Figure 2a, is segmented from the CT data and imported to Star-CCM+ to simulate the heat transfer driven by the temperature difference from 1000 K (LHS) to 300 K (RHS) (Figure 2b). The porosity and the mean diameter of the porous phase in the spongy layer are measured to be 0.19 and 200 nm respectively by image analysis. The heat flux in the 3D microstructure is shown in Figure 2c. It is observed that the tortuosity and constrictivity of the pore network generate a heterogeneous distribution of the flux, and the local flux maxima appear at the position where the transition of the pore thickness is sharp in the pathway. By integrating the heat flux on the cross-sectional plane, and dividing it by the heat flow on the cross-sectional plane of the empty volume, the material parameter $\epsilon_s/\tau_s$ is equal to 0.015, which is subsequently used as the thermal conductivity of spongy layer in the anode simulation.

Figure 2. (a) Virtual ortho slice of the anode; (b) simulation of heat transfer in the spongy layer; (c) heat flux in the spongy layer; (d) Heat transfer simulation on the anode with different thermal conductivity defined in the micro-channel and spongy layer.
The result of the heat transfer simulation for the whole anode is shown in Figure 2d. The temperature contour displays a non-uniform distribution with a ragged edge where there are isolated micro-channels. These are caused by the discrepancies of the effective thermal conductivity between the micro-channels and the spongy layer. As the heat flows from one micro-channel to the other, temperature gradient occurs at the spongy layer between them due to the low thermal conductivity.

The microstructure parameters extracted from the anode heat transfer simulation are compared with those in the spongy layer in Table 3. With the micro-channels embedded in the anode, the macroscopic material parameter for the whole anode $\varepsilon_a/\tau_a$ is approximately 4 times as large as $\varepsilon_s/\tau_s$, indicating a 300 % increase in terms of heat flow.

|        | $\varepsilon$ | $\tau$ | $\varepsilon/\tau$ |
|--------|---------------|--------|---------------------|
| Spongy | 0.19          | 12.1   | 0.015               |
| Anode  | 0.33          | 5.2    | 0.063               |

4. Conclusion
Multi-scale imaging and hierarchical simulation is an effective method to extract the material parameters (i.e. porosity and tortuosity) in the samples with distinctly different pore sizes spanning over several orders of magnitude, under which circumstances the porous phases cannot be resolved at the same time. These geometrical parameters are critical for effective diffusivity estimation in macroscopic electrochemical simulations. Results show that mass transfer in novel-structured tubular SOFC anodes embedded with radially aligned micro-channels is significantly improved four-fold due to the decrease of global tortuosity compared to the traditional homogeneous tubular SOFC anode with the pure spongy layer.

Acknowledgement
The authors acknowledge the sample provided by Dr. Tao Li from Kang Li’s research group in Imperial College London, and also appreciate support from the EPSRC under grants EP/N032888/1 and EP/M014045/1. PR Shearing acknowledges funding from the Royal Academy of Engineering.

References
[1] Virkar A V, Chen J, Tanner C W and Kim J-W, 2000 Solid State Ionics 131 189-198
[2] Iwai H, Shikazono N, Matsui T, Teshima H, Kishimoto M, Kishida R, Hayashi D, Matsuzaki K, Kanno D and Saito M, 2010 Journal of Power Sources 195 955-961
[3] Wilson J R, Kobisiphat W, Mendoza R, Chen H-Y, Hiller J M, Miller D J, Thornton K, Voorhees P W, Adler S B and Barnett S A, 2006 Nature materials 5 541-544
[4] Shearing P, Howard L, Jørgensen P S, Brandon N and Harris S, 2010 Electrochemistry communications 12 374-377
[5] Droushiotis N, Doraswami U, Ivey D, Othman M H D, Li K and Kelsall G, 2010 Electrochemistry Communications 12 792-795
[6] Tjaden B, Lane J, Withers P J, Bradley R S, Brett D J and Shearing P R, 2016 Solid State Ionics 288 315-321
[7] Schurch R, Rowland S M, Bradley R S and Withers P J, 2015 IEEE Transactions on Dielectrics and Electrical Insulation 22 709-719
[8] Scherl H, Koerner M, Hofmann H, Eckert W, Kowarschik M and Hornegger J, 2007 Medical Imaging 651058-651058-10