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Short Review on the Suitability of CFD Modeling for Proton Conducting Fuel Cell Performance

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ABSTRACT

Electrochemical performance optimization of a conventional solid oxide fuel cell (SOFC) has been massively performed with computational fluid dynamic (CFD) modelling but it's usage in a proton conducting fuel cell (PCFC) is still minimal. PCFC is a category of SOFC but with proton conductor as electrolyte instead of oxygen-ion conductor in a conventional SOFC. The fabrication of high electrochemical performance of PCFC is desirable because of its ability to operate at lower temperature. The objective of this short review study is to explore the possibilities of CFD modelling application to improve electrochemical performance of a PCFC system. Some CFD study that have been done to SOFC and PCFC were reviewed. One main finding from this short review is that the application of CFD modelling in PCFC design optimization is still minimal. There is a lack of studies that focus on the impact of PCFC anode microstructure on transport phenomena of the PCFC; for example on gas diffusion. It was also found that CFD modelling software Ansys Fluent with add-on Fluent SOFC module that is widely applied to conventional oxygen-ion SOFC need to be modify using User Defined Function (UDF) in order to be used in PCFC system.

Keywords: CFD model; SOFC; PCFC; single cell

INTRODUCTION

Development of fuel cell integrates knowledge of the material science for powder synthesis and characterization, and engineering knowledge for the fabrication of the devices. For theoretical studies, it is also an integration of micro-models or small-scale system on the material part and macro-models or large-scale system on the device part (Klotz, 2014, Djilali & Sui, 2008, Becker et al. 2011, Mozdzierz et al. 2019, and Shimpalee et al. 2019). The experimental process of fuel cell materials and devices development may take a long time but the optimization process can be speed up with Computational fluid dynamic (CFD) modelling (Al-Baghdadi & Al-Janabi 2007; Andersson et al. 2014; Sui et al. 2019; Tikiz et al. 2019).

Computational Fluid Dynamic (CFD) modelling are a powerful numerical tool to study the transport phenomena parameter that is difficult to do experimentally. It is used across all fields of science and engineering that involve fluid like water and gas and how it behaves in a system. The heart of CFD modelling is mathematical and physical laws of fluid; for example; conservation equation of mass and energy, and thermodynamics law. CFD modelling software will calculate the fluid flow, mass and heat transfer and other phenomena including chemical reactions by solving the mathematical equation using a numerical calculation process. The results can be used to optimize the system's engineering design and operation parameter without the need of expensive, tedious and complicated experiment except for validation purposes.

Computational fluid dynamic (CFD) modelling has been massively used to optimize the transport phenomena in a conventional oxygen-ion conductor solid oxide fuel cell (SOFC) but it's usage in the proton conducting fuel cell (PCFC) is still minimal (Milewski et al. 2019 and Ghorbani & Vijayaraghavan 2019). PCFC is the same as SOFC but the difference is only that it uses proton conductor as it electrolyte instead of oxygen ion conductor and enable the lowering of operating temperature to 500-800^{o}C from ~1000^{o}C for SOFC. Lower operating temperature is desirable because it will save operating cost and enable the usage of cheaper interconnect materials which can also contribute to lower fabrication cost of PCFC. In SOFC and PCFC, CFD modelling can be used to investigate computationally what is happening inside the cell for example transport processes such as chemical species transport, electronic and ionic transport, and also mass, heat and momentum transfer. It can also be used to couple study at different scale. For

example, instead of modelling mass diffusion in SOFC and PCFC anode at microscale and thermal stress of entire SOFC and PCFC stacks at macroscale separately, these two can be coupled and modelled as entire system. This model can really benefit the optimization of the SOFC and PCFC design and accelerates the commercialization of this renewable energy device.

For conventional oxygen-ion conductor solid oxide fuel cell (SOFC), the CFD modelling research activities are matured enough to the point that there are a lot of commercial software that is designed according to SOFC transport equations. Because the charge transfers equations between SOFC and PCFC are different, the modification of commercially available coding or in-house developed code need to be done before the CFD can be used for PCFC. The PCFC charge transfer, mass transfer and other transport equations need to be translated into coding language before the performance data can be simulated for optimization purposes.

The objective of this short review is to explore the possibility of using Computational Fluid Dynamic (CFD) modelling software for performance enhancement of PCFC system.

LITERATURE REVIEW

CFD modeling have been massively used to optimize various transport phenomena in conventional SOFC with oxygen-ion conducting electrolyte. Table 1 shows some CFD study that have been done to oxygen ion SOFC using commercial (Ansys Fluent and Comsol Multiphysics) and open-source (OpenFoam) CFD softwares. This list is not including all CFD studies that have been done to SOFC and interested reader can refer to recently published review on CFD modelling softwares that have been used in performance modelling of hydrogen-fueled SOFCs (Ghorbani & Vijayaraghavan 2019).

As have been mentioned before, CFD modelling in PCFC design optimization is still minimal. There is a lack of studies that focus on the impact of PCFC anode microstructure on transport phenomena of the PCFC for example on gas diffusion. Table 2 shows mathematical and numerical modelling of anode-supported proton conducting fuel cell (PCFC) that have been done till date and according to Zhu & Kee (2017), only one PCFC CFD modelling study by Menon et al. (2015) that use Dusty Gas Model (DGM) to explain microscale porous media transport in their anode and couple it with other macroscale studies for their PCFC system.

A detail mathematical model for PCFC single cell with configuration Ni-BZY | BZY | LSM – BZY was developed by Zhu & Kee (2017). First, they developed the gas-phase transport equation using Dusty Gas Model (DGM). This equation can be used to investigate hydrogen mass fluxes within the pore space. It was followed by defect transport equations, charge conservation and electric potentials, and reaction rate expressions. Gas-phase density, mass fraction, surface coverage, and electrostatic potential can be computationally solved from all these equations.

Various CFD modelling software are available either the commercial one where we need to buy the license (for example; Ansys Fluent and COMSOL Multiphysics; both come with add-on SOFC module) or freely available open source CFD software (for example OpenFoam and Cantera). Massive amount of CFD modelling studies have been done to conventional oxygen-ion conducting SOFC (Li et al. 2017, Lin et al. 2017, Pianko-Oprych et al. 2015a & 2015b, and Qu et al. 2011) but to the best of our knowledge, the possibilities of using CFD modelling software Ansys Fluent

TABLE 1. Computational fluid dynamic (CFD) study of SOFC

References	Title	Cell configuration	CFD Software
Li et al. 2017	A multiphysics fully coupled modeling tool for the design and operation analysis of planar solid oxide fuel cell stacks	Ni-YSZ |YSZ |LSM-YSZ	Ansys Fluent
Lin et al. 2017	Numerical simulation of cell-to-cell performance variation within a syngas-fuelled planar solid oxide fuel cell stack	Ni-YSZ |YSZ |LSM-ScSZ	Ansys Fluent
Pianko-Oprych et al. 2015b	Simulation of thermal stresses for new designs of microtubular Solid Oxide Fuel Cell stack	Ni-YSZ | YSZ | LSCF	Ansys Fluent
Pianko-Oprych et al. 2015a	Modeling of thermal stresses in a microtubular Solid Oxide Fuel Cell stack	Ni-YSZ |YSZ |LSCF	Ansys Fluent
Qu et al. 2011	Three-dimensional computational fluid dynamics modeling of anode-supported planar SOFC	Ni-YSZ |YSZ |LSM	Ansys Fluent
García-Camprubí et al. 2011	CFD analysis of cooling effects in H2-fed solid oxide fuel cells	-	OpenFoam
Nguyen et al. 2017	Three dimensional CFD modeling and experimental validation of a single chamber solid oxide fuel cell fed by methane	GDC-Ni| LDM | LSCF6482	COMSOL Multiphysics
Andersson et al. 2012	SOFC modeling considering electrochemical reactions at the active three phase boundary	Ni-YSZ | YSZ | LSM-YSZ	COMSOL Multiphysics

TABLE 2. Computational fluid dynamic (CFD) study of PCFC single cell

Reference	Title	Single Cell Configuration	Type of Model / CFD Software
Zhang et al. 2018	Mathematical modeling of a proton-conducting solid oxide fuel cell with current leakage	NiO-BZY | BZY |LSCF |	A one-dimensional (1D) framework of charge transports in an H-SOFC
Zhu & Kee 2017	Modeling Protonic-Ceramic Fuel Cells with Porous Composite Electrodes in a Button-Cell Configuration	NiO-BZY | BZY |LSM-BZY	Coupled nonlinear system of partial differential-algebraic equations (DAE)
Sailler et al. 2011	First 3D-Modeling of Proton-Conducting SOFC's Interconnect	NiO-BCY | BCY | Pr2NiO4	ESI Software CFD ACE+® commercial package.
Bavarian & Soroush 2012	Mathematical modeling and steady-state analysis of a proton-conducting solid oxide fuel cell	Pt | SCY | Pt	MATLAB
Menon et al 2015	Numerical analysis of mass and heat transport in proton-conducting SOFCs with direct internal reforming	NiO–BCSO | BSCF–BCSO | NiO–BCSO	Software package DETCHEM™
Menon et al 2015	Numerical analysis of mass and heat transport in proton-conducting SOFCs with direct internal reforming	NiO–BCSO | BSCF–BCSO | NiO–BCSO	Software package DETCHEM™

with add-on Fluent SOFC module for PCFC have yet to be explored. In the latest review paper that has discussed the numerical/CFD based software that have been used to study performance modelling of hydrogen-fueled SOFC, no PCFC CFD modelling studies were listed, although technically PCFC is also a hydrogen-fueled SOFC (Ghorbani & Vijayaraghavan 2019).

It was also found that in order to use CFD modelling software Ansys Fluent with add-on Fluent SOFC module for PCFC system, there was a need to write an in-house developed code using C Programming language that is unique for the PCFC system. This code can be written in User Defined Function (UDF) that came with Ansys Fluent software. Academic version of Ansys Fluent can be used freely in preliminary research stage by student, without purchasing of commercial license but with some processing limit. This CFD code must be validated with the experimental data. Validated CFD code can be used to simulated which one of various PCFC single cell parameter, for example the size, the cell's configuration, thermal stress, electrode thickness, porosity and tortuosity that will give the optimum electrochemical performance of PCFC system.

CONCLUSION

In this preliminary work, the possibility of using Computational Fluid Dynamic (CFD) modelling software for performance enhancement of PCFC system had been explored. It was found that CFD modelling software Ansys Fluent with add-on Fluent SOFC module that is widely applied to conventional oxygen-ion SOFC need to be modify using User Defined Function (UDF) in order to be used in PCFC system. The application of CFD modelling is believed to speed up the fabrication, testing, and commercialization of PCFC system.

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DECLARATION OF COMPETING INTEREST

None.

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