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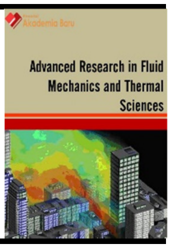

Overview of Computational Fluid Dynamics Modelling in Solid Oxide Fuel Cell

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ABSTRACT

Owing to the complexity and high cost of solid oxide fuel cell (SOFC) experiments, computational fluid dynamics (CFD) simulation is frequently performed for SOFC analysis. This paper provides an overview of the application of CFD modelling for the development of SOFC performance analysis. First, CFD modelling, materials and flow properties and boundary conditions required for modelling are discussed on the basis of our understanding of transport processes in SOFC. Available CFD software and models for SOFC analysis are then listed, and their applications are discussed. Finally, advancement in CFD modelling application is addressed to understand the CFD modelling ability.

Keywords:
solid oxide fuel cell, computational fluid dynamics, modelling, performance analysis

1. Introduction

Alternative energy sources, especially solid oxide fuel cells (SOFCs), are gaining popularity because of increase in power demands and depletion of fossil fuels. SOFCs are among the fuel cell technologies that use solid-state components and operate at high temperature (800–1000 °C). SOFCs possess several advantages, including high electrical efficiency (~50%), eco-friendliness, silent operation, fuel versatility, and potential for cogeneration [1–3]. However, the commercialization of SOFCs is currently difficult because of cost and durability limitations at high operating temperatures [4,5].

High operating temperature is one of the significant features of SOFCs. The dense ceramic electrolyte in SOFCs requires high temperature to achieve optimum ionic conductivity for electrochemical reactions. At high temperature, the catalytic properties of the electrodes are high and thus increase the electrochemical reaction rate [6]. However, high operating temperature

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requires the use of expensive materials especially for the interconnects. Besides, thermal stress generation is severe at high temperature and unfavourable to cell life [7, 8]. Therefore, the current aim of SOFC research is to reduce the operating temperature to an intermediate range (500–750 °C) [9].

Decreasing SOFC operating temperature to an intermediate range can offer several advantages, such as decreased operation and material cost, reduced thermal stress generation, and increased start-up speed [10]. Nevertheless, the challenge lies in maintaining SOFC performance at the reduced temperature. Yttria-stabilized zirconia (YSZ) has been long used as the SOFCs electrolyte because of its excellent ionic conduction. However, its performance drop at reduced operating temperature an [9,10]. Therefore, new materials are required for the intermediate temperature application. Several studies showed that samarium-doped ceria has great potential for intermediate temperature application because of its higher conductivity and lower ohmic losses compared with traditional YSZ electrolyte [7,11].

Apart from the excellent material properties, the overall performance of SOFCs is also dependent on the operating conditions (temperature and inflow rate) and design (components and assembly) of the cell. However, the interactions among these parameters occur at the micro level and are hardly observed through experiments. Experimental setups for the overall performance analysis of SOFCs are often complex and thus are often expensive. Moreover, these setups produce undesirable results in some cases. Therefore, computational fluid dynamics (CFD) is used as a tool to predict the overall performance of SOFCs (single cell or stack) at low cost and decrease the reliance on trial-and-error methodology [14]. The aim of this paper is to provide an overview of CFD modelling for SOFCs and its development in SOFC performance analysis.

2. CFD Modelling In SOFC

In CFD modelling, finite volume method and applied boundary conditions are used to solve the governing equations related to SOFC transport processes [15]. During simulations, various distributions (such as temperature and current density) can be obtained and used to calculate power densities or thermal stresses.

2.1 Transport Mechanism in SOFC

An SOFC assembly consists of a porous cathode and anode, which sandwich a dense electrolyte with interconnects that support and channel the reactants to the electrodes at both sides. Transport phenomena in SOFCs are complex because of the interrelation among several multiphysical processes and chemical and electrochemical processes during system operation [16]. In addition, the overall transport phenomenon are nearly impossible to study through experimental methods because electrochemical reactions occur simultaneously with transport processes [17]. The transport mechanism inside SOFCs must be determined before CFD modeling to obtain a suitable fluid model and the desired output and identify material and flow properties.

Transport processes in a porous medium start when fuel and air are introduced to the surfaces of anode and cathode, respectively, resulting in gas diffusion, which leads to mass, momentum, and chemical species transport in SOFCs. In the cathode, oxygen reduction occurs and results in ionic transport across the electrolyte. In the anode, fuel is oxidized and electrochemical reactions occur between hydrogen and oxygen ions transported at the TPB, producing water, heat, and electrons [18]. In a SOFC, the amount of redox reaction products at the anode and cathode depends on the fuel used. Table I show the equations for reactions using different types of fuel. The heat generated is then transported to the flow through convection and to the solid part through conduction, whereas electrons are transported back to the cathode through an external circuit, thereby producing electricity [19]. The summary of the SOFC transport processes using hydrogen as fuel is shown in Figure 1. For the solution of the transport processes, CFD solves several governing equations including the following [20].

- Mass continuity equations
- Momentum conservation equations (combination of Navier–Stokes equation and Darcy law for porous medium effect)
- Ion and electron transport
- Electrochemical reactions

From the transport processes, material and fluid properties required for the modeling can be generated. The list of properties with respect to the transport processes are listed in Table 2.

Table 1
Equations for reactions using different type of fuels[21]

Type of fuel	Reaction at anode		Reaction at cathode		Overall reaction	
Hydrogen	$H_2 + O^{2-} \rightarrow H_2O + 2e^-$	(1)	$0.5O_2 + 2e^- \rightarrow O^{2-}$	(2)	$0.25O_2 + H_2 \rightarrow H_2O$	(3)
Carbon monoxide	$2CO + 2O^{2-} \rightarrow 2CO_2 + 4e^-$	(4)	$O_2 + 4e^- \rightarrow 2O^{2-}$	(5)	$2CO + O_2 \rightarrow 2CO_2$	(6)
Hydrocarbon (C_nH_m)	$C_nH_m + (2n + 0.5m)O^{2-} \rightarrow nCO_2 + (0.5m)H_2O + (4n + m)e^-$	(7)	$(n + 0.25m)O_2 + (4 + m)e^- \rightarrow (2n + 0.5m)H_2O$	(8)	$C_nH_m + (n + 0.25m)O_2 \rightarrow nCO_2 + (0.5m)H_2O$	(9)

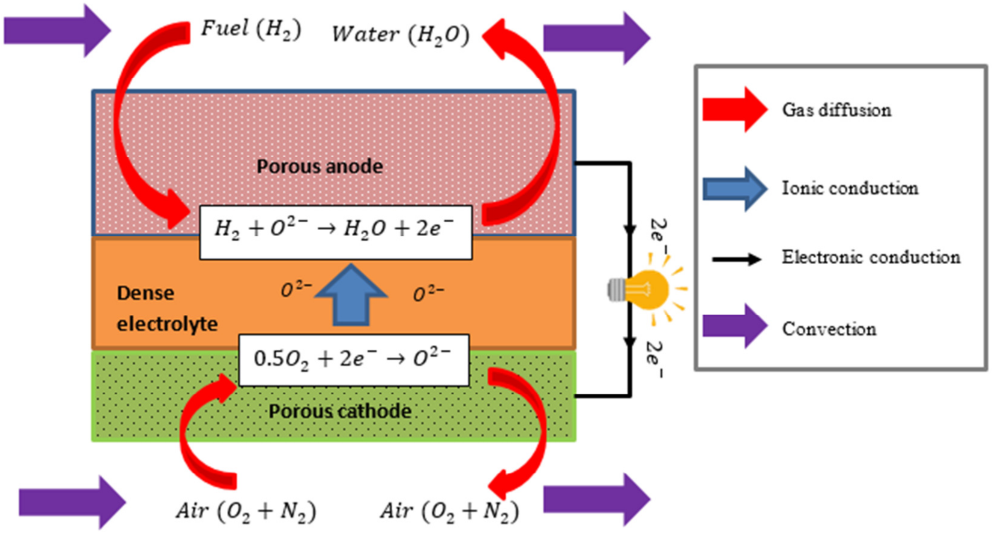

Fig. 1. Transport processes inside the single anode-supported SOFC using hydrogen

Table 2
Materials and fluid properties and boundary conditions according to transport processes

Transport processes	Material properties	Fluid properties	Boundary conditions
Gas diffusion	Porosity Permeability Average pore size Effective diffusivity model	Density Viscosity Mass diffusivity	Reactants flow rate/velocity Operating temperature
Ionic conduction	Surface to volume ratio (ratio of active surface to volume)	-	Operating temperature Surface reaction (the half reaction at electrodes)
Electronic conduction	Electrical conductivity	Electrical conductivity	-
Convection	Thermal conductivity	Thermal conductivity Specific heat	Operating temperature
Chemical reactions	-	Species compositions	Operating voltage

3. CFD Software

The CFD modeling and simulations for SOFCs can be done using commercialized and open-source CFD software applications listed as follows.

- ANSYS FLUENT [20–22]
- STAR-CD [25]
- COMSOL Multiphysics [15,24,25]
- CFD-RC [28]
- CFD-ACE+
- OpenFOAM [29]

The requirements of SOFC CFD modeling are nearly the same for any CFD software. In the literature, among the most common software applications used in SOFC performance prediction are ANSYS FLUENT and COMSOL Multiphysics. ANSYS FLUENT is mainly used to predict the effect of geometry changes on cell performance, while COMSOL Multiphysics is often used to predict the effect of fuel composition on cell performance.

4. SOFC Models

SOFC models for CFD simulations can be categorized into zero-, one-, two-, or three-dimensional models based on the assumptions made and parameters to be studied. However, among the most used models for SOFC analysis are the two- and three-dimensional models.

Two-dimensional SOFC models are used to study the effect of parameters, such as fuel composition, electrode thickness, and reactant distributions. Kong *et al.,* [27] utilized a two-dimensional model to study the effect of interconnect rib on SOFC performance. Andersson *et al.,* [30] used the same model to study the effect of fuel composition on SOFC performance. Meanwhile, Barzi *et al.,* [31] studied the effect of reactant mass flow rate and anode thickness on the performance of a single planar button cell.

Three-dimensional models are extremely useful in studying the effect of flow distributions, flow configurations, and changes in geometry. Recknagle *et al.,* [25] and Zhang *et al.,* [22] used three-dimensional models to study the effect of three different flow configurations (co-, counter-, cross-flow) on the distribution of current and temperature inside SOFCs. Furthermore, three-dimensional models are also extensively used to test the effect of interconnect design on SOFC performance [13,22,25]. The effect of electrode microstructure on cell performance and reforming process was also studied by using a three-dimensional SOFC model [23]. Some of the studies that simultaneously used two- and three-dimensional SOFC CFD models are presented in Table 3.

Table 3
Examples of CFD modeling in SOFC

Ref.	Studied variable	Operating temperature (°C)	Fuel	CFD Software (model type)
[25]	Flow configurations (co-, counter-, and cross- flow)	595-625	Hydrogen (H_2)	Star CD (3D model)
[28]	1. Design of interconnect (addition of guide vanes) 2. Reynold number of fuel and air	~835	Hydrogen (H_2)	CFD-RC (3D model)
[32]	Type of porosity distribution (parabolic/linear/inverse parabolic)	800	Hydrogen (H_2)	COMSOL MULTIPHYSICS version 3.5 (2D model)
[31]	1. Fuel and air mass flow rate 2. Anode thickness	800	Hydrogen (H_2)	(2D models-button cell)
[29]	Reactants mass flow rate	850	Hydrogen (H_2)	OpenFOAM-1.5 (2D model)
[24]	Geometry of the gas channel (corrugated bi-polar plate)	700	Hydrogen (H_2)	ANSYS FLUENT (3D model)
[27]	Interconnect rib dimensions	700	Hydrogen (H_2)	COMSOL MULTIPHYSICS Version 3.5 (2D model)
[17]	Type of fuel used	900	1. Methane free biogas (H_2+CO^2) 2. Hydrogen (H_2)	COMSOL Multiphysics 4.2a (3D model)
[23]	1. Anode porosity 2. Anode pore size 3. Anode diffusion layer	700-1000	Methane (CH_4)	ANSYS FLUENT v13 (3D model)
[30]	Fuel compositions	750	Hydrogen (H_2), carbon monoxide (CO), carbon dioxide (CO_2), water (H_2O), methane (CH_4)	COMSOL Multiphysics v 4.3 (2D model)
[15]	1. Contact pressure 2. Interconnect design	800	Hydrogen (H_2)	ANSYS-FLUENT 14 (3D model)
[20]	Flow configuration (cross-flow)	800	Hydrogen (H_2)	ANSYS-FLUENT 14 (3D model)
[22]	Flow configurations (co-, counter-, and cross- flow)	800	Hydrogen (H_2)	ANSYS-FLUENT 14 (3D model)
[33]	1. Flow configurations (co- and counter- flow) 2. Air ratio 3. Carbon deposition	750	Syn-gas (CH_4 =21%, CO_2 =18%, CO =20%, H_2=40%, N_2 = 1%)	COMSOL Multi-physics 4.3.1 (3D model)
[34]	Gas distributor geometry	727	Hydrogen (H_2)	COMSOL 5.1 (3D model)
[2]	Geometry of flow channel (rectangle, triangle, and trapezoidal)	800	Hydrogen (H_2)	COMSOL Multiphasic 5.2 (3D model)

Two- and three-dimensional models both have their own advantages and disadvantages in SOFC modeling. Compared with two-dimensional models, three-dimensional models generate more accurate simulation results for the transport processes because the transport processes are three-dimensional in nature. However, the computational cost for a three-dimensional model is higher than that of a two-dimensional model especially during meshing. Therefore, two-dimensional models are preferred in SOFC simulation. In addition, with appropriate assumptions, three-dimensional models can be reduced to two-dimensional models without considerably affecting the simulation results. Therefore, depending on the parameters to be studied, both models can be used to obtain the desired output.

5. Advancement in SOFC CFD Modeling

Most CFD models for SOFC analysis were mainly used for performance analysis on a single SOFC stack. However, given the necessity for proper heat management within the stack, CFD modeling is now actively used for stack analysis. Pianko-Oprych *et al.,* [35] used CFD modeling to predict heat transfer between the cooling air and heat generated by 16-anode-supported microtubular SOFC sub stacks. Meanwhile, Dong *et al.,* [36] conducted CFD simulation on a five-cell planar SOFC stack to study the uniformity of the supply of the reactants in the stack. The aim of stack performance analysis is to distinguish SOFC performance of a single SOFC stack from that of multiple SOFC stacks. It also aims to distinguish the effect of heat management on the thermal stress generation. CFD stack modeling in SOFCs plays an important role in the commercialization of SOFCs, particularly in the prediction of total energy and cost of the overall system [37].

Currently, CFD modeling is used to predict carbon formation during internal reforming and irreversible nickel re-oxidation inside SOFCs, especially internal-reforming SOFCs. For example, Choudhary and Sanjay [33] performed CFD modeling to study the effect of steam recirculation ratio to carbon formation at the anode, while Schluckner *et al.,* [38] studied several carbon gasification strategies. Using CFD modeling for carbon formation is important for SOFC fuelled by hydrocarbons as carbon formation can reduce cell performance and has adverse effects on electrodes.

6. Conclusion

CFD modeling is important to performance analysis of SOFC because it enables the investigation of parameters that cannot be tested through experimental methods. This paper covers some parts of CFD modeling for SOFC analysis and includes important modeling parameters, CFD software applications, and SOFC models for CFD simulation. In addition, the advancement in SOFC CFD modeling is discussed briefly. For future work, the effects of assumptions made on CFD models should be discussed in detail, as assumptions play a major role in any CFD model.

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