

교류 흐름 방식을 적용한 암모니아 공급 고체산화물 연료전지의 성능 분석

쿠 엔^{1,2}, 잡반티엔¹, 이동근¹, 이선엽^{2,3}, 배용균¹, 안국영^{1,2}, 김영상^{1,2†}

¹한국기계연구원 무탄소연료발전연구실, ²과학기술연합대학원대학교 융합기계시스템전공, ³한국기계연구원 모빌리티동력연구실,

Performance Analysis of Ammonia-Fed Solid Oxide Fuel Cell Using Alternating Flow

THAI–QUYEN QUACH^{1,2}, VAN–TIEN GIAP¹, DONG KEUN LEE¹, SUNYOUNG LEE^{2,3}, YONGGYUN BAE¹,
KOOK YOUNG AHN^{1,2}, YOUNG SANG KIM^{1,2†}

¹Department of Zero-carbon Fuel and Power Generation, Korea Institute of Machinery & Materials (KIMM), 156 Gajeongbuk-ro, Yuseong-gu, Daejeon 34103, Korea

²Mechanical Engineering, University of Science and Technology (UST), 217 Gajeong-ro, Yuseong-gu, Daejeon 34113, Korea

³Department of Mobility Power Research, Korea Institute of Machinery & Materials (KIMM), 156 Gajeongbuk-ro, Yuseong-gu, Daejeon 34103, Korea

†Corresponding author :
yskim@kimm.re.kr

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Abstract >> The effect of flow configuration in ammonia-fed solid oxide fuel cell are investigated by using a three-dimensional numerical model. Typical flow configurations including co-flow and counter-flow are considered. The ammonia is directly fed into the stack without any external reforming process, resulting in an internal decomposition of NH_3 in the anode electrode of the stack. The result showed that temperature profile in the case of counter-flow is more uniform than the co-flow configuration. The counter-flow cell, the temperature is highest at the middle of the channel while in the case of co-flow, the temperature is continuously increased and reached maximum value at the outlet area. This leads to a higher averaged current density in counter-flow compared to that of co-flow, about 5%.

Key words : Alternate flow(교류흐름), Ammonia(암모니아), Fuel cell(연료전지), Solid oxide fuel cell(고체산화물연료전지), Separator(분리판)

1. Introduction

Solid oxide fuel cell (SOFC) is one of the most promising alternative power generation device for sustainable power system, which can efficiently converse chemical energy to electrical power¹⁻⁴. Typical

power generation systems, such as steam turbines, gas turbines, and internal combustion engines, normally converse chemical energy from fuel to high temperature and high pressure, then turn to mechanical energy of the turbine shaft or crankshaft, finally turn to the electricity by the generator. SOFCs con-

sume hydrogen fuel and generate only water as by-product, leading to a great potential for reduction of CO₂ when using green hydrogen as fuel. In addition, since SOFCs operate at relatively high temperature (600-900°C), it is perfectly fitted with other power conversion cycles, i.e., Rankine cycle, Brayton cycle, or Carnot cycle, to form high efficiency SOFC-based combined power conversion systems⁵⁻⁷.

SOFCs can be fed by hydrogen, methane, ammonia, ethanol, methanol, etc. Among them, ammonia shows great ability to be an alternative for typical hydrogen fuel owing to its advantages in storage, transportation, and efficiency. Ammonia can be stored at pressure of 11 bar at ambient temperature whereas hydrogen fuel requires pressure of 350-700 bar⁸. Ammonia has a high energy density of 11.5 MJ/L in liquid form (15°C and 11 bar) while that of hydrogen is only 4.5 MJ/L (15°C and 690 bar), resulting in a more compact system when ammonia is used instead of hydrogen fuel. Ammonia can be directly fed into anode side of the SOFC where decomposition reaction of NH₃ occurs (NH₃ [g]→1.5H₂ [g]+0.5N₂ [g]). The decomposition reaction absorbs heat from electrochemical reaction of the SOFC, consequently the cooling power for the air blower can be significantly saved in comparison with hydrogen-fed SOFC case. In addition to above advantages, ammonia is a well-known species in industrial field, especially in fertilizer making process, therefore, mass production technologies, transportation methods, safety criteria, and policies for ammonia are extensively developed.

Commercialization of ammonia-fed SOFC, however, are facing some problems. First, nitriding problem, which is a mandatory process of ammonia decomposition in Ni catalyst⁹, can degrade the triple phase boundary microstructure, resulting in a degradation of electrochemical performance of the fuel

cell. Second, agglomeration of nickel particles in YSZ based material, which is also called coarsening process^{9,10}. This phenomenon occurs due to high temperature operation of the fuel cell, causing a large-size nickel catalyst, consequently the active area of the catalyst layer is reduced, and then its performance is decreased. Finally, deformation of gas separator by nitriding reaction between iron (Fe) and nitrogen is a considerable problem. After a long period of operation, i.e., 1,000 hours, the iron particle can be pull out of separator surface, leading to possibility of local blockage which can immediately damage the stack^{10,11}. Interestingly, these three above problems are strongly dependent on local temperature inside the fuel cell stack. Therefore, understanding the temperature distribution in the cell is one of the most crucial requirements of stack development. In addition, since the temperature and current density are naturally coupled in the fuel cell, understanding current density distribution is also important. Unfortunately, studies of those for methane and hydrogen fuels are extensive while that of ammonia-fed SOFC is not considered. The decomposition reaction of ammonia is totally different compared to that of methane in terms of heat and activity, therefore, the result of methane case cannot be used to develop ammonia-fed fuel cell. Ammonia fuel cell must be investigated separately.

In this study, the temperature and current density of the ammonia-fed SOFC will be investigated. The 3D model of co- and counter-flow will be used to investigate ammonia decomposition reaction, which is coupled with electrochemical reaction in the fuel cell, by using ANSYS FLUENT commercial package^{12,13}. The model is then validated with experimental data to turn unknown electrochemical parameters, such as anode exchange current density, cathode exchange current density, and exponential factor of species. By

investigating temperature and current density of the two types of flow, an alternate co-flow configuration is proposed to improve the performance of the SOFC stack. Alternate co-flow might have a great potential to enhance the SOFC stack performance.

2. Design descriptions

2.1. Geometry

A full cell design size is normally 100×100 mm². To reduce calculation cost, however, a single channel is used for CFD analysis for two types of flow, which are co- and counter-flow. The calculation domain includes two bipolar plates at the top and bottom, fuel flow, air flow, and electrodes, as shown in Fig. 1. The bipolar plates directly connect to electrodes to collect electrical current from electrochemical reaction. Dimension and characteristic of geometry component are available in the Table 1. Electrolyte is omitted from the model and replaced by a virtual interface in the calculating program (see section 2.2).

2.2. Numerical model

The calculation was done using commercial SOFC

package in ANSYS FLUENT software (<https://www.afs.enea.it/>). In the SOFC model, the typical continuity equation, momentum equation, and energy equation are solved in the calculation domain. After that, the local species concentration at the interface of anode and cathode electrodes are used for solving electrochemical reaction using a virtual electrolyte. Finally, the species and heat fluxes from electrochemical reaction solver will be returned to the fluid domain, as shown in the Fig. 2.

The decomposition reaction of ammonia only occurs in the anode electrode. The Arrhenius expression Eq. 1 is used for calculation reaction rate.

$$k_{f,r} = A_r e^{-E_r/RT} \tag{1}$$

Table 1. Geometry parameters

Parameters	Unit	Value
Anode electrode thickness	m	0.7e-3
Cathode electrode thickness	m	0.04e-3
Anode electrode width (one channel)	m	2e-3
Cathode electrode width (one channel)	m	2e-3
Porosity of anode electrode	-	0.5
Porosity of cathode electrode	-	0.5

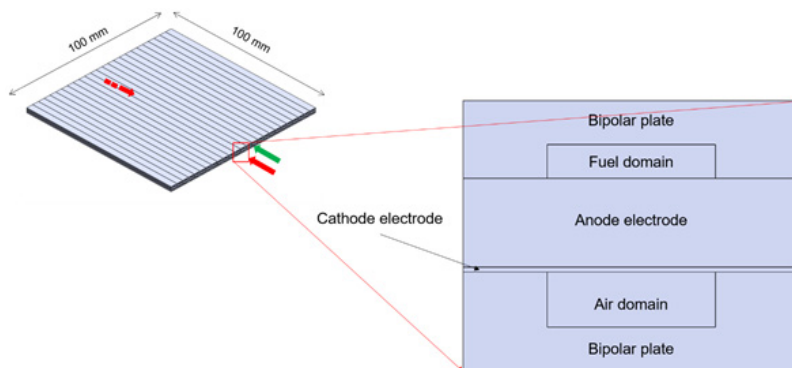


Fig. 1. Geometry of the single channel SOFC model

where

$k_{f,r}$: forward rate constant

A_r : pre-exponential factor¹⁴⁾ (1e12)

E_r : activation energy¹⁵⁾ (J/kgmol) (1.96e8)

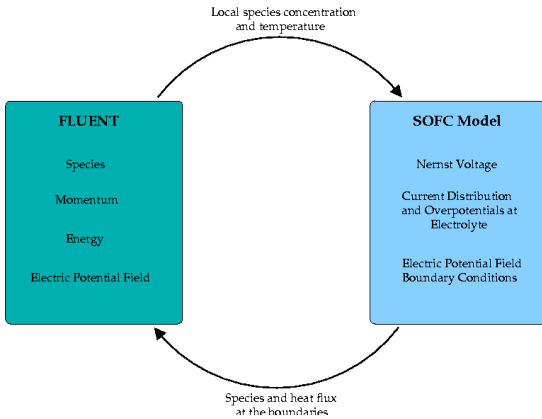
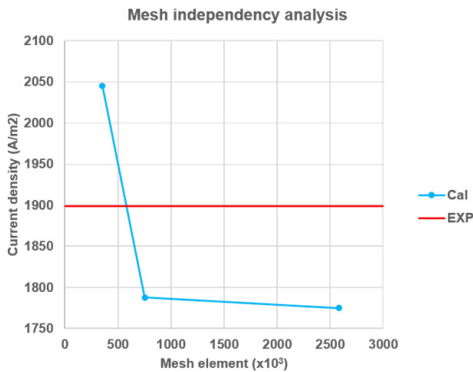
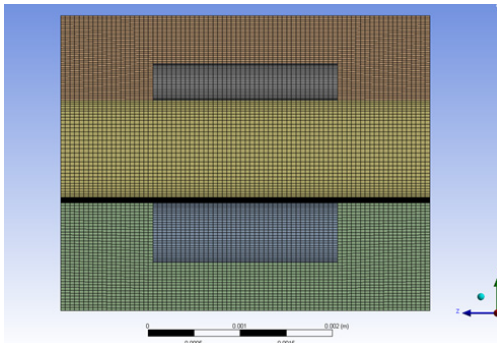


Fig. 2. Calculation process (<https://www.afs.enea.it/>)



(a)



(b)

Fig. 3. Mesh analysis results. (a) Mesh independent analysis. (b) Corresponding mesh quality.

Regard to meshing process, all hexahedral meshes were created using nonconforming mesh technique. Approximately seven hundred thousand mesh elements are generated for the entire calculation domain to reach acceptable accuracy. The accuracy was investigated by increasing number of mesh elements which is so called mesh independent analysis, as shown in Fig. 3.

3. Validation

The boundary condition for the calculation has been set as shown in Fig. 4. Since this is a single channel SOFC, the side walls will be defined as symmetry condition. To make result more close to reality, the top surface, bottom surface, and two ends are set as adiabatic condition¹⁶⁾.

The model was validated with experimental data from published paper¹¹⁾. The mass flow inlets of ammonia and air and working condition of the experiment are listed in the Table 2. Fig. 5 shows a comparison of calculation I-V curve and experimental data. The calculation curve well agrees with experimental points, showing a great ability of the SOFC single channel model in further investigation.

4. Results and discussion

The length of the single channel is 0.01 m while its width is only 2 mm. To make the picture easier to follow, the length of the channel was scaled by 10 times in Figs. 6-8.

Fig. 6 shows molar fraction of ammonia and hydrogen of co- and counter-flow. The fuel and air flow rate are 8.561e-8 kg/s and 1.647e-6 kg/s, respectively. Fuel direction is from left to right in all cases. In addition, the voltage of each cell is fixed at 0.83 V in all calculations as an input value. As you can see,

the ammonia is quickly fully decomposed at the entrance of the fuel side in both cases. In counter-flow case, however, ammonia is a little bit decomposed faster (Fig. 6[a] and [b]) owing to difference in local temperature, resulting in a higher hydrogen concentration at the entrance area (Fig. 6[c] and [d]) compared to that of co-flow case.

Fig. 7 shows the temperature at the middle of the cell and current density at electrolyte of two types of flow. It is obvious that, the hottest temperature of the co-flow case is in the outlet of flows owing to exothermic electrochemical reaction of the fuel cell. In case of counter-flow, however, the hottest zone is in the middle of the channel. This is reasonable because in hydrogen-fueled fuel cell, the hottest area is at the

outlet of the air¹⁷⁾. In the case of ammonia, the decomposition reaction of NH₃ is endothermic which absorbs heat from fuel cell, consequently the hottest point moves to the center of the cell (Fig. 7[b]). The average temperature of co-flow case is 966 K while that of counter-flow is 988 K.

Regard to the current density, in both cases the current is highest at the entrance of fuel and then it is reducing along the channel because of reduction of hydrogen concentration. The averaged current density of co-flow is 3,036 A/m² whereas that of the counter-flow is 3,166 A/m², 4.3% higher than co-flow case.

It seems that co-flow is less efficient than counter-flow due to temperature distribution along the

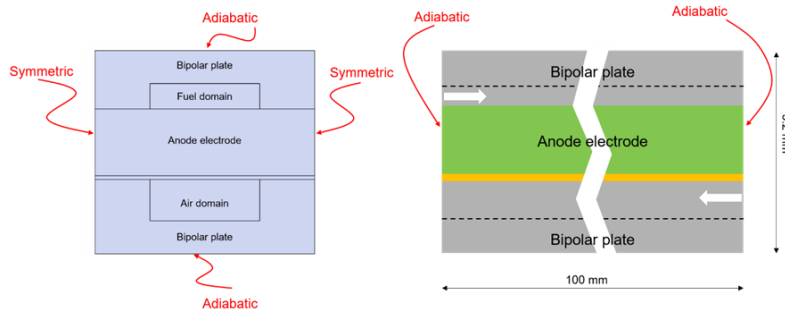


Fig. 4. Boundary conditions

Table 2. Working condition of SOFC cell for validation

Parameters	Unit	Value
Anode electrode tortuosity	-	3
Cathode electrode tortuosity	-	3
Fuel inlet temperature	°C	600
Air inlet temperature	°C	600
Mass flow of fuel (inlet)	kg/s	1.316e-7
Mass flow of air (inlet)	kg/s	1.367e-6

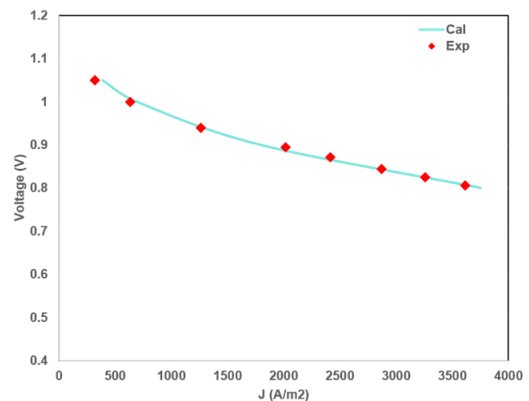


Fig. 5. Validation of SOFC model with experimental data

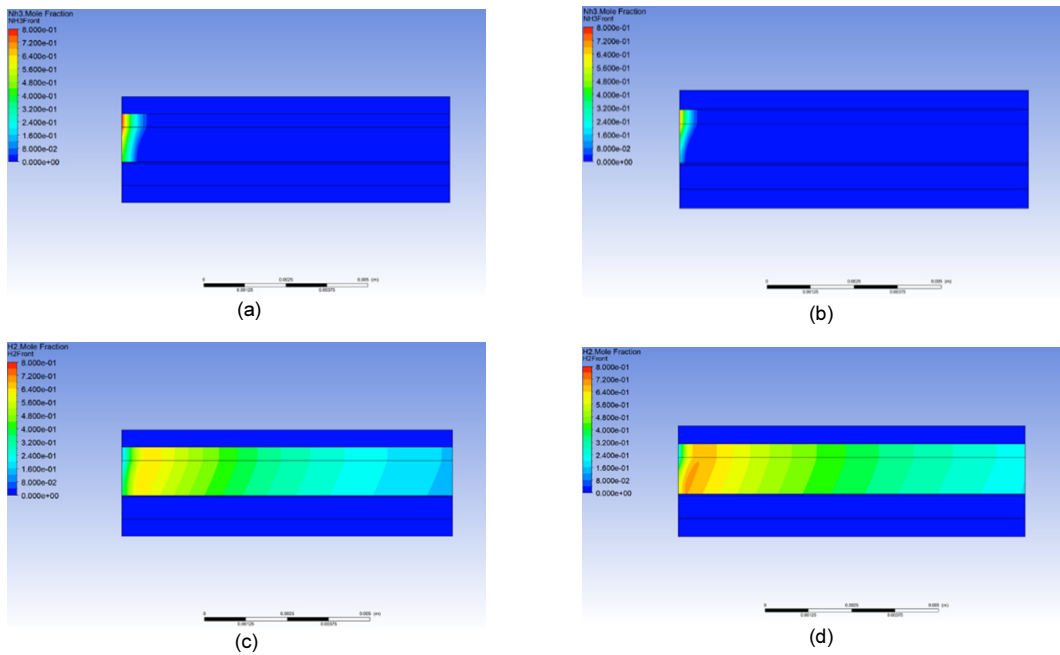


Fig. 6. Concentration of ammonia and hydrogen at the middle section of the cell. (a) Co-flow, NH₃ concentration. (b) Counter-flow, NH₃ concentration. (c) Co-flow, H₂ concentration. (d) Counter-flow, H₂ concentration.

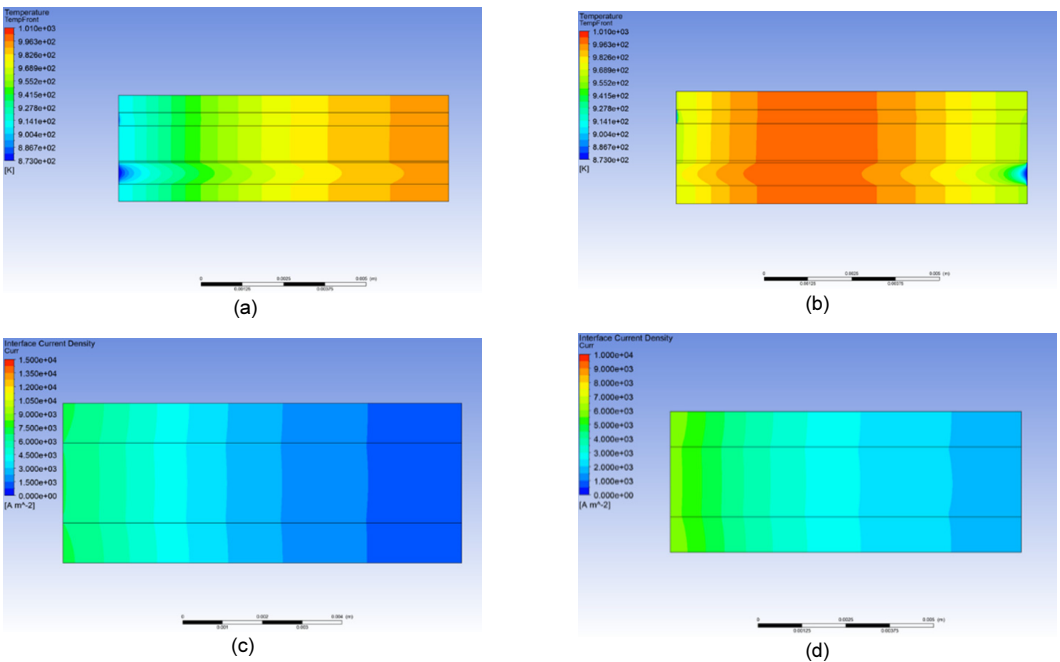


Fig. 7. Distribution of temperature at the middle section of the cell and current density at electrolyte. (a) Co-flow, temperature. (b) Counter-flow, temperature. (c) Co-flow, current density. (d) Counter-flow, current density.

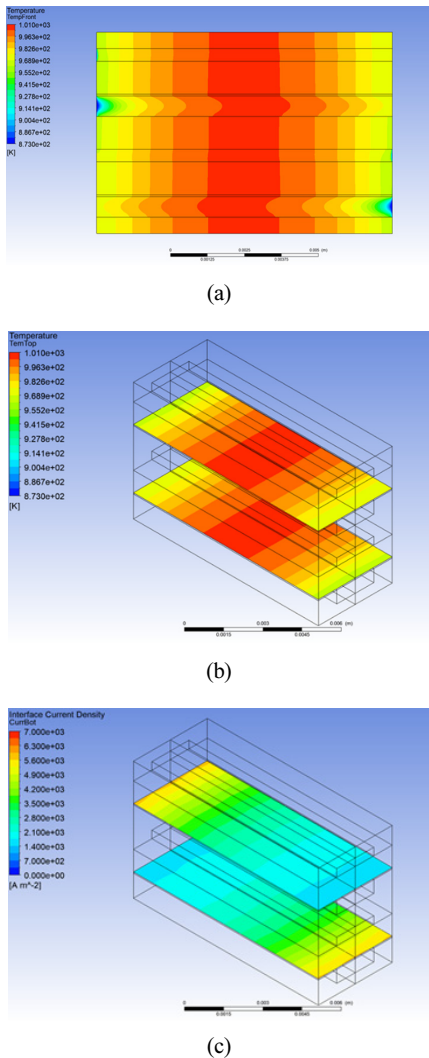


Fig. 8. Current density and temperature distribution in the alternate co-flow design. (a) Temperature at the middle section of the cells. (b) Temperature at electrolytes. (c) Current density at electrolytes.

channel. To overcome this, an alternate co-flow is proposed, as shown in Fig. 9. Two adjacent cells have difference flow directions, which can help their hottest and lowest temperature zones compensate each other, resulting to a more flatten temperature distribution. Temperature and current density distribution of the proposed design is on Fig. 8.

As a result of alternate flows, the temperature is symmetric to the center line of the channel as shown in Fig. 8(a) and (b). In addition, current density distribution is more uniform than the single flow cases, as shown in Fig. 8(c).

Fig. 10 compares temperature variation along with channel of three flow types. The alternate co-flow

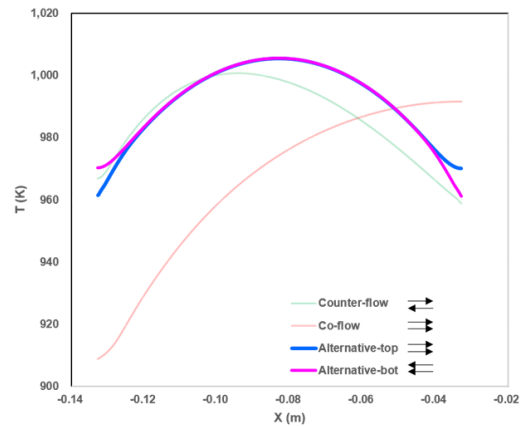


Fig. 10. Comparison of co-flow, counter-flow, and alternate co-flow in terms of temperature

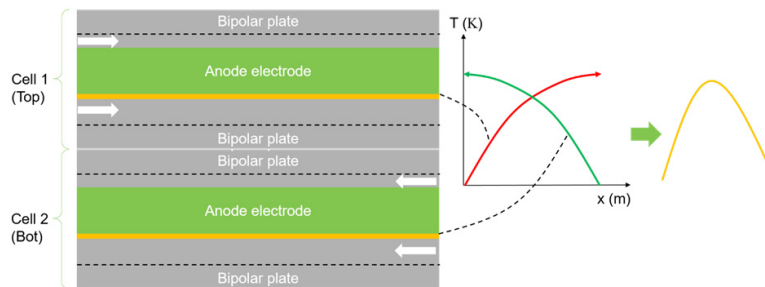


Fig. 9. Alternate co-low concept

case shows symmetric curve to the center of the channel. Although its peak is higher than the other cases, the higher averaged temperature of the alternate co-flow case results in a higher averaged current density, 5.3% higher than that of single co-flow.

5. Conclusions

Effects of co- and counter-flow in single channel cell to the temperature and current density distribution of ammonia-fed SOFC has been investigated. A three dimensional model, which includes decomposition reaction of ammonia and electrochemical reaction of fuel cell, has been used. An alternate co-flow has been proposed to enhance cell performance. Some useful information has been derived that can be summarized as follows.

If all things being equal, such as working voltage, fuel and air flow rates, input temperature of gases, and the cell geometry, counter-flow is better than co-flow in NH_3 -fed SOFC. Counter-flow shows 2.3% higher in averaged temperature and 4.3% higher in current density than those if co-flow.

The proposed alternate co-flow can significantly improve the temperature distribution and averaged current density of the SOFC compared to singled flows.

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