Issues Related to the Modeling of Solid Oxide Fuel Cell Stacks

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This work involves a method for modeling the flow distribution in the stack of a solid oxide fuel cell. Towards this end, a three dimensional modeling of the flow through a Solid Oxide Fuel Cell (SOFC) stack was carried out using the CFD analysis. This paper examines the efficacy of using cold flow analysis to describe the flow through a SOFC stack. It brings out the relative importance of temperature effect and the mass transfer effect on the SOFC manifold design. Another feature of this study is to utilize statistical tools to ascertain the extent of uniform flow through a stack. The results showed that the cold flow analysis of flow through SOFC might not lead to correct manifold designs. The results of the numerical calculations also indicated that the mass transfer across membrane was essential to correctly describe the cathode flow, while only temperature effects were sufficient to describe the anode flow in a SOFC.

Key Words : SOFC Manifold Design, Temperature and Mass Transfer Effects

1. Introduction

In future, with the fast depleting oil reserves, countries will be forced to look at alternative energy sources. The future energy needs of countries of the world will have to depend on vast coal reserves, Hydrogen reserves and also on renewable energy options. With these options, one has to also explore ways of using the energy reserves in a more efficient and effective manner. Fuel cell with its high energy conversion efficiency is a promising option.

Fuel cells have a structure similar to that of a battery, with two porous electrodes separated by an electrolyte. Electricity is produced by a chemical reaction between a fuel (usually Hydrogen or a hydrocarbon) and an oxidant (usually Oxygen) inside the fuel cell. Figure 1 shows the schematic diagram of the electrochemical processes that take place inside a fuel cell. Hydrogen (H_2) flows over the anode (the negative electrode) and splits into positively charged hydrogen ions and electrons, which carry a negative charge. The electrons flow

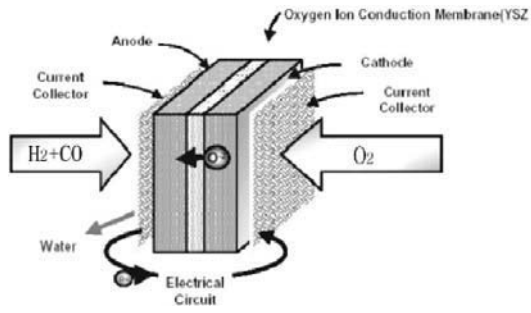

Fig. 1 The schematic diagram depicting the electrochemical processes occurring in a fuel cell

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through the anode to the external circuit, performing useful work (this is the electric current generated) while the hydrogen ions pass through the anode and into the electrolyte, moving towards the cathode (the positive electrode). The electrons eventually return to the cathode which is supplied with oxygen (O_2). At this point the electrons, hydrogen ions and oxygen react to form water (H_2O) and heat. In stationary fuel cell power plants the heat can also be captured and used as process heat in industries or space heating (co-generation). As long as the fuel cell is supplied with hydrogen and oxygen, the electrical energy production can continue indefinitely.

Fuel cell has also several advantages; It has no moving parts, its reliable, its efficiency is not limited by Carnot cycle and has usually very high efficiencies, if the heat generated can be captured for other uses. It operates cleanly and quietly.

A solid oxide fuel cell operates at around 1273 K. The output voltage of individual fuel cells are quite low, hence large stacks of individual fuel cells are needed to get the desired output voltage. A uniform distribution of fuel & oxidizer flow into the individual fuel cells in a stack is desired, as it enhances the effectiveness of the fuel cell system. Besides, the spatial non-uniformity in temperature could lead to thermal stresses being developed within the SOFC stack that could reduce its lifespan. Hence, a careful design of manifold is imperative. The geometries utilized in industries are complex, as high compactness is a desirable feature. This makes the task of designing the manifold a very challenging one. Figure 2 shows a simple geometry of the manifold design.

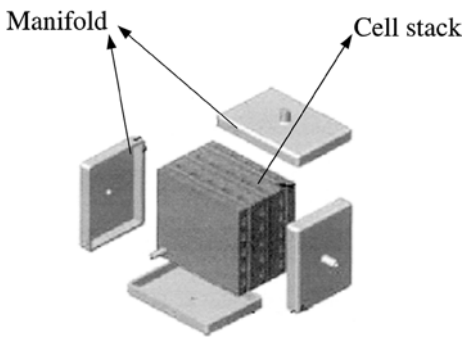

Fig. 2 Details of a manifold of the fuel cell stack

Some of the previous models (Achenbach and Reus, 1999; Boersma and Sammes, 1996; 1997; Haruhiko et al., 2001, Ma et al., 2002; Koh et al., 2003) of a fuel cell stack describe the flow through it by treating the stack as a network of hydrodynamic resistances. Recent experimental and modeling studies by Wattana et al.(2004) have considered cold non- reacting case to investigate the flow through the manifold of a SOFC fuel cell system. Kee et al.(2002) have modeled the flow through a SOFC stack by considering only the momentum and continuity equations, neglecting temperature and mass transfer effects. Their analysis cannot account for mass transfer across the electrolyte membrane. Burt et al.(2004) have carried out numerical investigation of cell-to-cell voltage variation considering the impact of flow distribution and heat transfer on a SOFC stack utilizing a one-dimensional co-flow cell model. Their model accounts for the transfer of mass across the membrane in a limited manner. Koh et al.(2002) have proposed a two-dimensional model for Molten Carbonate Fuel Cells (MCFC), but their model cannot account for variations in flow in the manifold.

From the above it is evident that certain aspects of modeling of SOFC stack have to be examined more carefully. Hence, the objectives of the current study are to model the phenomenon that occurs inside a SOFC, to examine if the cold flow studies suffice in suggesting a manifold design, to study the relative importance of temperature effects and the mass transfer effects on the SOFC manifold design and to suggest a methodology using statistical techniques for selecting a manifold design that accounts for varying mass flow conditions.

2. Mathematical Model

2.1 Geometry of the stack

CFD-ACE commercial package was utilized for the SOFC simulations. The geometry of stack used in the present calculations is as shown in Fig. 3. Only a single layer of the stack has been considered here. There are 6 individual fuel cells in a layer. The inset shows the arrangement of

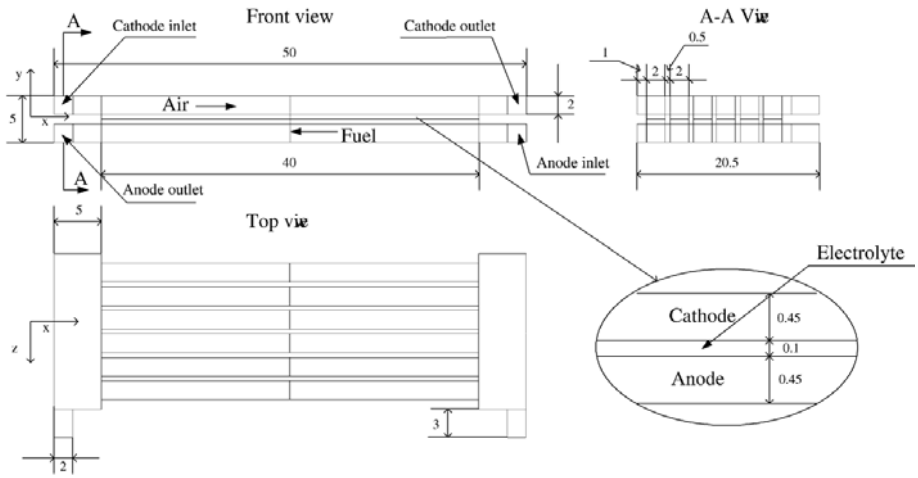

Fig. 3 Geometry of the stack utilized in the current calculations (All the dimensions are in mm)

anode, cathode and the electrolyte. The dimensions are as indicated in Fig. 3. The air enters the fuel cell through the cathode inlet from the left and goes out through the right. The fuel enters the fuel cell from the right and goes out through left side. The fuel channel is at the bottom and that of air is at the top.

2.2 Materials and property settings

The Anode (Ni/ZrO2 Ceramic Metal Composite (cermet)), Cathode (Doped Lanthanum Manganite (LaMnO3)) and Electrolyte (Yttria Stabilized ZrO2 (8 mol% Y2O3)) are modeled as porous media. The details of the porous media settings are as given in Table 1. The transport properties and conductance used in the current calculations are as given in Table 2.

2.3 Chemical reactions

The reactions in the anode and the cathode are modeled as surface reactions and are assumed to take place inside the pores according to the

Table 1 Porous media settings

Volume name	ε	κ	k	RXN	S/V	Pore	Diffusivity	σ
Anode	0.40	1e-12	6.23	anode	100	1e-6	Bruggman (2)	100000
Cathode	0.50	1e-12	9.6	cathode	100	1e-6	Bruggman (2)	7700
Electrolyte	0.01	1e-18	2.7	—	—	1e-6	Bruggman (2)	1e-20

ε-Porosity (fluid volume/total volume), κ-Permeability m^2 (total volume/surface area)^2, k-Thermal Conductivity W/m-K, S/V-Surface to Volume Ratio 1/m, σ-Electrical Conductivity $ohm^{-1}m^{-1}$.

Table 2 Transport property and conductance settings

Volume Name	ρ	μ	σ(1/ohm-m)	Cp	k	Γ
Anode	IGL	MixKin	10	JANNAF	MixKin	SCH (0.7)
Cathode	IGL	MixKin	10	JANNAF	MixKin	SCH (0.7)
Electrolyte	IGL	MixKin	10	JANNAF	MixKin	SCH (0.7)
Anode_channel	IGL	MixKin	1e-20	JANNAF	MixKin	SCH (0.7)
Cathode_channel	IGL	MixKin	1e-20	JANNAF	MixKin	SCH (0.7)

ρ-Density kg/m^3, IGL-ideal gas law, μ-Viscosity kg/m-s, MixKin-kinetic theory, σ-Electrical Conductivity 1/ohm-m, Cp-Specific Heat J/kg-K by JANNAF curve fits, k-Thermal Conductivity W/m-K and Γ-Mass Diffusivity kg/m-s by Schmidt number

following reaction. Oxygen ions are modeled as "Bulk Species"

Anode : $H_2+CO+2O\_BULK \rightarrow H_2O+CO_2$
Cathode : $O_2 \rightarrow 2O\_BULK$

The nominal values for the reference current J_0 and the Tafel constants for the two reactions are as follows ;

$J_0=1E+14$, $\alpha_a=0.7$, $\alpha_c=0.7$ for Anode reaction
$J_0=1E+10$, $\alpha_a=0.7$, $\alpha_c=0.7$ for Cathode reaction

2.4 Boundary conditions

The inlet and outlet boundary conditions are as given below. At the Cathode inlet the mass flow rate was 2.12×10^{-5} kg/s, the temperature was 1273 K and pressure was taken as 1 atm. At the Anode inlet mass flow rate : 4.415×10^{-6} kg/s, the temperature was 1273 K and pressure was taken as 1 atm. At both the Cathode and Anode outlet the fixed pressure boundary condition was utilized and the pressure was 1 atm. The exit temperature was given as 1273 K.

2.5 Grid structure and grid details

The number of grid points utilized in the present study is around 55000. The geometry is as shown in Fig. 4. The typical number of cells in the x, y and z-direction are 60, 30 and 30 respectively. The Calculations are carried out till the residuals associated with all variables decrease by at least 6 orders of magnitude. The results were verified to be grid size independent. The time taken for convergence is around 4hours on an Intel 4 pc with 1 GB Ram.

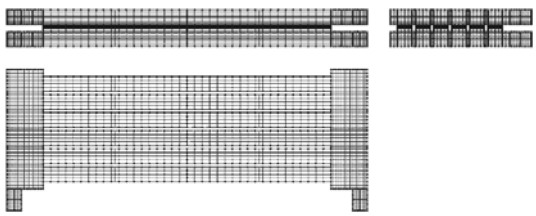

Fig. 4 Grid structure utilized in present study

3. Results and Discussions

The modeling of the flow through a single layer of SOFC stack consisting of 6 fuel cells was carried out at atmospheric pressure. The three basic designs on which numerical studies have been conducted are shown in Fig. 5. The composition of the fuel used was 0.096 H_2+0.428 H_2O+0.26 CO+0.216 CO_2 and air composition was taken as 0.79 N_2+0.21 O_2. Most calculations other than the results of obtained to verify the dependence of voltage on the current density, were carried out at 0.5 V.

In order to examine the correctness of the results, the variation of voltage with the current density (Ref. Fig. 6) was plotted. The results show a qualitative agreement with those reported in the experimental study by Jiang and Virkar (2003). The higher values of current density seen in Fig. 6 are to be expected as the cells are connected in parallel in the current study.

With the results thus verified, numerical experiments were carried out to examine if cold flow

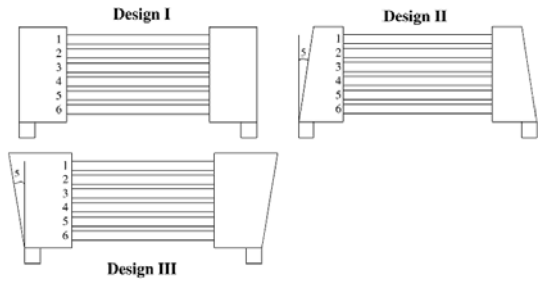

Fig. 5 The three basic designs considered in the present study

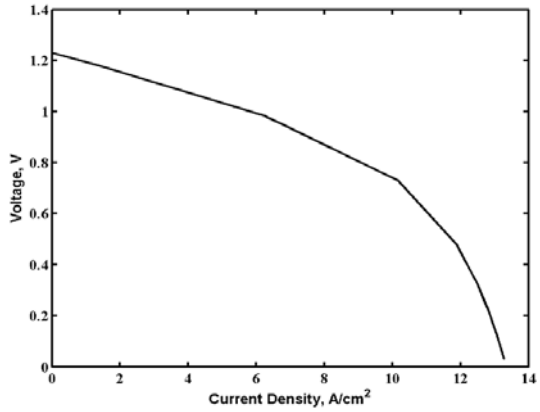

Fig. 6 The variation of voltage with current density for the fuel cell

studies suffice in suggesting a manifold design. Two different cases were studied to ascertain the above, one a cold non-reacting flow case with temperature being maintained at 300 K and a hot reacting flow with the temperature being around 1273 K. The difference between the hot reacting case and the cold non-reacting case is that in the former in addition to higher temperatures, reaction and diffusion of gas species into the anode, cathode and across the membrane is allowed. In the latter, the temperature is fixed at 300 K and the mass diffusion has not been considered. The above cases were verified for all the three design indicated in Fig. 5.

To understand the relative importance of the thermal effects and the mass transfer across the membrane on flow rates through the fuel cells, a hot (temperature 1273 K) non-reacting flow case was considered in addition to the cold non-reacting case and the hot reacting case described previously. The difference between the hot reacting case and the hot non-reacting case being that in the former, the mass diffusion of gas species into the anode, cathode and across the membrane is allowed. In the latter, the temperature is fixed at 1273 K and reactions have not been considered. Without the reactions, the oxygen ions are not produced in the cathode region and as the membrane is selectively permeable only to oxygen ions, there is no diffusion of species across the membrane in the hot non-reacting flow case. These calculations were carried out for all the three designs indicated in Fig. 5.

Figure 7 shows the variation of mass flow rate through the individual fuel cells for cold non-reacting flow (temperature 300 K), hot non-reacting flow (temperature 1273 K) and a hot reacting flow (temperature 1273 K) for both the anode and the cathode when the geometry corresponds to Design I. The flow pattern changes from cold non-reacting case to hot reacting case in both the anode and cathode flow channels. The hot non-reacting flow case follows the hot reacting flow case in the flow through anode flow channel, while it follows the cold non-reacting flow case in the flow through cathode flow channel. The mean and standard deviation (STD) of

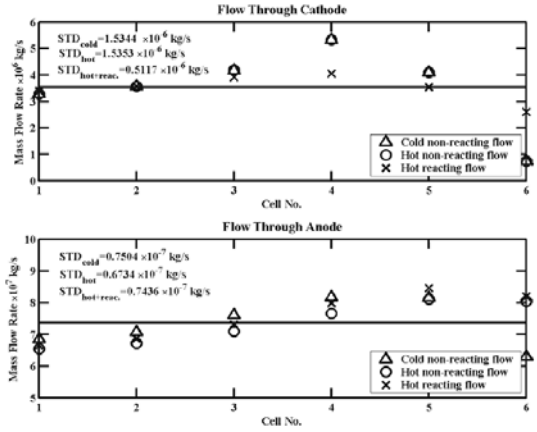

Fig. 7 The variation of mass flow rate in the individual fuel cells for design I

the distribution are introduced to obtain a quantitative measure of the cell to cell variation of mass flow rate. The mass flow rate of air through the cathode is closer to the mean and hence better in the hot reacting case compared to the cold non-reacting case. Consequently, smaller STD is associated with the hot reacting flow case. In the flow through the anode, although the STD is nearly the same due to the flow rate through Cell 6 being on either side of the mean. The cell to cell variation of mass flow rate is smaller for the hot reacting flow case.

The difference between the hot reacting case and the cold non-reacting case seems to arise basically from the large variation in flow rates through cell 6 in both the anode and the cathode flow channels. To obtain an insight into this, velocity vectors (Ref. Figs. 8 and 9) for the flow through the cathode and anode flow channels for both the hot reacting and cold non-reacting case were plotted. It is evident from Fig. 8 that for the cathode flow, the recirculation zone near the inlet to Cell 6 is quite large for the cold non-reacting flow case, when compared to hot reacting flow case. This causes a lower mass flow rate to enter Cell 6 in the cold non-reacting case. This phenomenon could be due to either thermal effects or the mass transfer effects that are not considered in the cold non-reacting flow case.

Interpreting Fig. 8 in conjunction with Fig. 7, it is evident that the reduction in the size of the

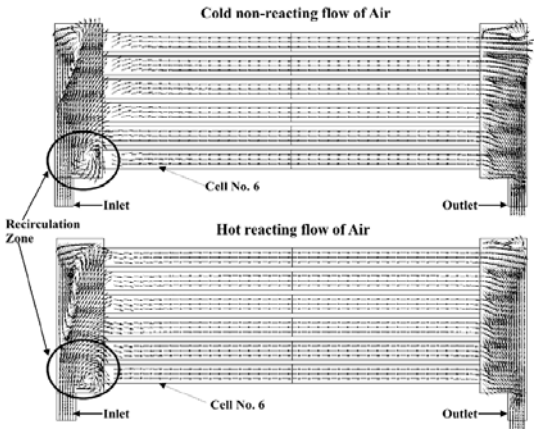

Fig. 8 The velocity vectors for the flow through the cathode flow channel center plane at $y=1$ mm

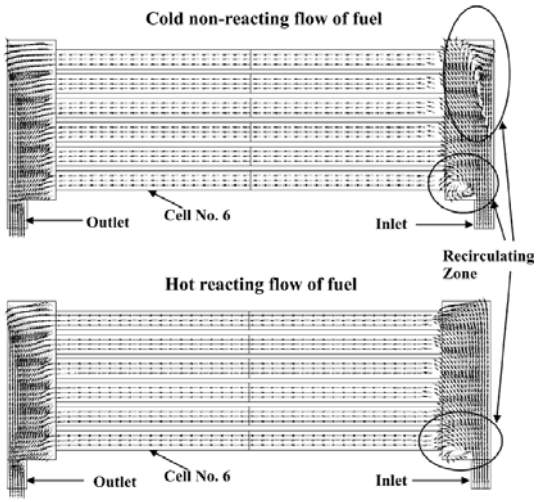

Fig. 9 The velocity vectors for the flow through the Anode flow channel center plane at $y=-1$ mm

recirculation zone at the entry to the Cell 6 (Ref. Fig. 8) in the flow through the cathode in the hot reacting flow case is not due to temperature effects (hot non-reacting flow case results are similar to those obtained with the cold non-reacting case, Ref. Fig. 7). It is because of a suction pressure developed in the cathode flow channel due to the transfer of oxygen ions from cathode to anode.

In the velocity vector plot of flow through the anode flow channel (Ref. Fig. 9), the cold non-reacting flow case has two recirculation zones compared to the single one in the hot reacting flow case. The recirculation zone near the entry to Cell 6 is also smaller for hot reacting flow case as compared to the cold non-reacting case. This can be ascribed to thermal effects as hot non-reacting flow case results are similar to those obtained with the hot reacting case (Ref. Fig. 7). From this it can be deduced that the mass transfer across membrane needs to be considered in order to correctly describe the cathode flow in SOFC, while only thermal effects are suffice to describe the anode flow in SOFC. This is to be expected as there is a significant transfer of mass (Oxygen) accompanying the current flow across the membrane in a Solid Oxide Fuel Cell. Thus, to describe the flow through a SOFC correctly, it is imperative to consider both thermal and mass transfer effects.

The variation in the mass flow rate through the individual fuel cells for the cold non-reacting case (temperature 300 K), hot non-reacting flow (temperature 1273 K), and the hot reacting case for Designs II and III are as shown in Figures 10 and 11. It is clear from these figures that the variation in the mass flow rate through the individual fuel cells for the hot reacting case is quite different from those obtained for the cold non-reacting case. Thus, cold non-reactive flows cannot describe completely the processes inside a fuel cell stack and it is imperative to consider hot reacting flow when deciding on a manifold design. The hot non-reacting flow case for design II and III also is similar to the hot reacting flow case in the flow through anode flow channel, while it is similar to the cold non-reacting flow case in the flow through cathode flow channel. Some of the differences between a full numerical simulation of a fuel cell stack and the results obtained based on the hydrodynamic network of resistances reported above have also been discussed in Beale et al.(2003).

Finally, a particular design of the manifold is considered good only if it performs better than the competing designs over a wide range of inlet mass flow conditions. The inlet mass flow rate here was varied $\pm 30\%$ over the values given in Section 2.4. The results of variations in the STD

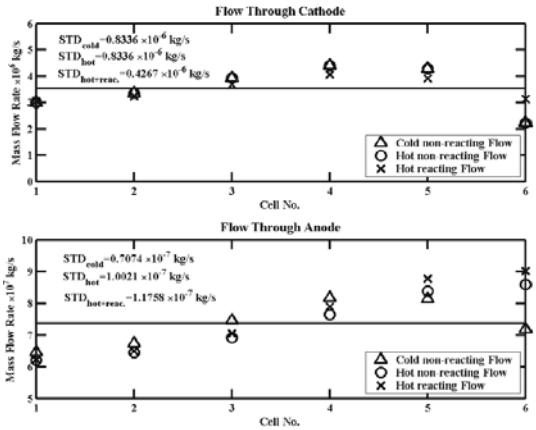

Fig. 10 The variation of mass flow rate in the individual fuel cells for design II

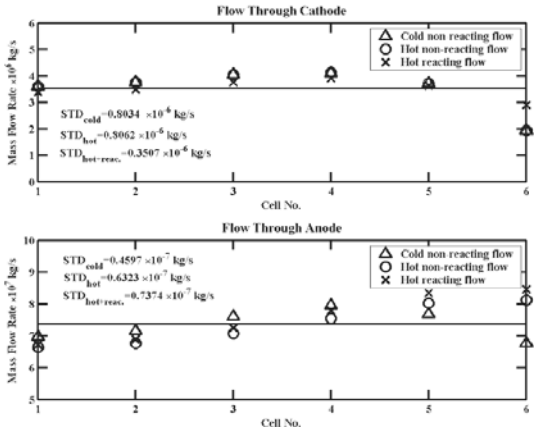

Fig. 11 The variation of mass flow rate in the individual fuel cells for design III

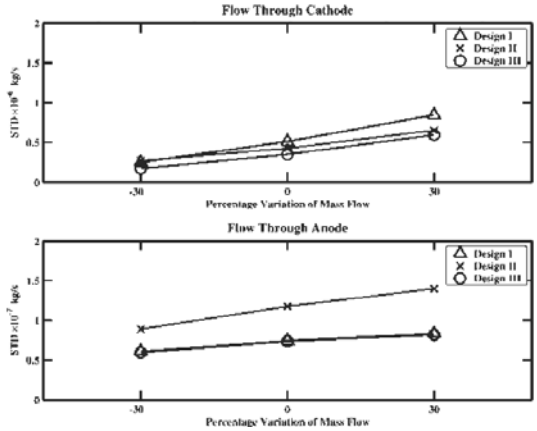

Fig. 12 The variation of STD for the different designs considering the hot reacting case

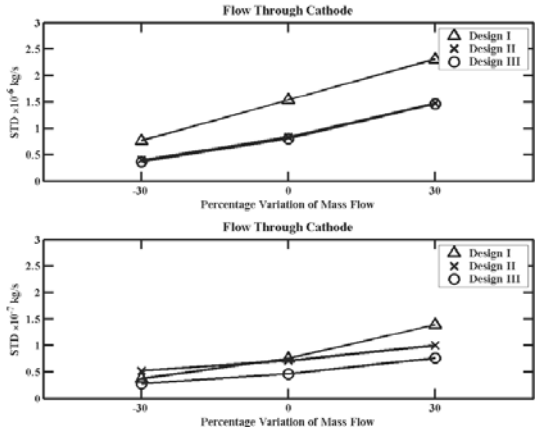

Fig. 13 The variation of STD for the different designs considering the cold non-reacting case

for each design under these conditions are depicted in Fig. 12 (hot reacting case as criteria). It is apparent from Fig. 12 that Design III is best among the three at all conditions and Design I is the second best. Thus, through the use of STD it is possible to quantify the variation of mass flow rates from cell to cell. Its appropriate use, as demonstrated above can help pin-point the best among the competing manifold designs.

The perils of utilizing the cold non-reacting case on deciding on the best design is brought out in Fig. 13, which shows the variations in STD for the different designs considering the cold non-reacting flow case. From Fig. 13 it can be inferred that Design III is the best. Also, Design II has a lower STD compared to Design I under most conditions, thus making Design II better than Design I. Now hypothetically speaking, if Design III is difficult to fabricate, then one has to choose Design II as the next best. But, intuitively one knows that Design II cannot be better than Design I as it has a convergent section in the manifold. This demonstrates that using cold non-reacting flow case to decide the best design might under some circumstances lead to wrong choices.

4. Conclusions

Three dimensional modeling of the flow through a SOFC stack was carried out using the

CFD-ACE package.

(1) It was demonstrated that cold flow analysis of SOFC might not lead to correct manifold designs.

(2) The mass transfer across the membrane is required to correctly describe the cathode flow in SOFC, while only temperature effects are sufficient to describe the anode flow in SOFC. Thus, it is essential to consider both thermal and mass transfer effects in order to correctly describe the flow through an SOFC stack.

(3) A methodology has been suggested though the use of STD to pin-point the best among the competing manifold designs.

Acknowledgments

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