SOFCs use a solid ceramic electrolyte which is sandwiched between two porous electrodes. In a typical SOFC, fuel is provided at the anode which undergoes an oxidation reaction releasing electrons to the external circuit and oxidant is provided at the cathode which accepts electrons from the external circuit and undergoes a reduction reaction. Thus electrons flow from the anode to the cathode in the external circuit and electricity is produced.

In anode supported SOFC, hydrogen is provided at the anode flow channel which diffuses through the anode support layer towards the electrolyte. The support layer provides mechanical support to the cell and facilitates uniform distribution of the reactant. At the support layer-electrode interface, the hydrogen reacts with the oxygen ions coming from the cathode to form water according to Eqn. (1).

$$H_2 + O^2^- \rightarrow H_2O + 2e^- \tag{1}$$

Since SOFC works at high temperature (>700°C), the water formed will be in gaseous state. The water formed will diffuse out to the channel and gets removed from the outlet. However, the maximum power output is limited by the concentration over-potential due to the mass transport limitation of the reactant to the reaction surface. At high output rates, the consumption of reactants is faster than the rate at which the reactant gas diffuses through the gas diffusion layer. This induces an electric potential drop limiting the maximum output current density obtainable. The formation of product also dilutes the fraction of reactants available. Moreover, the slow rate of diffusion of the reactant in the gas diffusion layer can cause a non-uniform distribution of reaction rate along the flow direction. This results in non-uniform heat generation and temperature distribution in the electrodes. These temperature gradients can lead to hot-spot formation and induce high thermal stresses affecting the life of the cell components. Hence, the mass and heat transport in the electrodes play the major role in the improvement of performance and life of a fuel cell. In the present work, the focus is given to the mass transport of hydrogen and water in the anode of a planar anode supported SOFC using multi-relaxation time lattice Boltzmann method. In the present work, a pulsating inlet provides a steady output from the cell.

The performance curves obtained show that for same flow rate, performance decreases as pulsatile inlet is given to the flow channel. With either increase in Womersley number or decrease in amplitude of pulsation, a decrease in performance has been observed. It can be concluded that the flow pulsations affect the performance adversely as the steady flow ensures a constant supply of reactant to the reaction sites providing a steady output from the cell.

Keywords: Planar anode supported solid oxide fuel cell, Porous support layer, Lattice Boltzmann method, Pulsatile flow

ABSTRACT

Solid oxide fuel cells (SOFCs) have been subject of keen interest due to their high efficiency, eco-friendliness and fuel flexibility. In the present work, the focus has been given to the mass transport of hydrogen and water in the anode of a planar anode supported SOFC using multi-relaxation time lattice Boltzmann method. In the present work, a pulsating inlet condition is given for flow at anode. By the solution of transport in the clear channel and the porous support layer, the hydrogen diffusion rate and the water formation and removal rate is studied. From the study the effect of Womersley number and amplitude of pulsation on the cell performance has been obtained and performance has also been compared with that obtained in the case of steady flow. The performance curves obtained show that for same flow rate, performance decreases as pulsatile inlet is given to the flow channel. With either increase in Womersley number or decrease in amplitude of pulsation, a decrease in performance has been observed. It can be concluded that the flow pulsations affect the performance adversely as the steady flow ensures a constant supply of reactant to the reaction sites providing a steady output from the cell.

INTRODUCTION:

As a highly efficient and environment-friendly energy source, fuel cells are very promising energy conversion devices which convert chemical energy of fuel directly into electrical energy without involving any thermo-mechanical energy conversion step. Among variety of fuel cells available, Solid Oxide Fuel Cells (SOFCs)[1-4] are particularly interesting because of their high electric efficiency, long term stability, low pollutant emissions and relatively low cost. They offer the possibility of using different type of fuels. It is considered to be well suited for large-scale power generation.
transport of hydrogen and water and the temperature
distribution in the anode of a planar anode supported SOFC.

Hun et al.[5] investigated the effect of pulsating cathode flow
on the overall performance of a polymer electrolyte membrane
fuel cell (PEMFC) experimentally. They obtained that a
pulsating flow in the cathode improves the oxygen diffusion
rate across the cell. This resulted in a higher maximum current
density and power output. The increase in performance was
found more pronounced at low Womersley Number. To verify
the experimental results, they also implemented a theoretical
mass transport analysis in the pulsating cathode flow. The
present paper intends to address the impact of anode flow
pulsation on the SOFC performance. A pulsating input
condition is given for flow at anode. By the solution of
transport in the clear channel and the porous support layer, the
rate of hydrogen diffusion and the water formation is studied.
The fuel cell performance in this case is compared with that in
the steady non-pulsating flow.

\[ \mu_{\text{eff}} \text{ and } \rho_m \text{ are the effective dynamic viscosity and the density of the mixture respectively. } F \text{ is the sum of the Darcy term and the Forchheimer term accounting for the effect of porous media[7].} \]

\[ F = -\phi \nu K^{-1} \mathbf{u} - \phi F_\phi K^{-5} |\mathbf{u}| \mathbf{u} \]  

\[ F_\phi = 1.43 \phi^{1.5}, K = 0.067 \phi \left(1 - \phi^2\right) d_p^2 \]

The governing equations are solved using lattice Boltzmann
method (LBM) with multiple relaxation time collision. A
standard D2Q9 lattice structure is selected. The discretized
LBM equation can be written in the form:

\[ \mathbf{f}(\mathbf{x} + \mathbf{e}_i \Delta t + \Delta t) - \mathbf{f}(\mathbf{x}, t) = -M^{-1}S\left[\mathbf{m}(\mathbf{x}, t) - \mathbf{m}^{eq}(\mathbf{x}, t)\right] + \Delta t M^{-1} (1 - S/2) G \]

The transformation matrix \( M \) for D2Q9 model is

\[ M = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ -4 & -1 & -1 & -1 & -1 & 2 & 2 & 2 & 2 \\ 4 & -2 & -2 & -2 & -2 & 1 & 1 & 1 & 1 \\ 0 & 0 & 0 & 1 & 0 & -1 & 1 & -1 & -1 \\ 0 & 0 & 0 & 1 & 0 & 0 & -1 & 1 & -1 \\ 0 & 0 & -2 & 0 & 2 & 1 & 1 & -1 & -1 \\ -1 & 0 & 1 & 0 & -1 & 1 & 1 & -1 & -1 \\ 0 & 0 & 1 & -1 & 0 & 1 & 1 & -1 & -1 \\ 0 & 0 & 0 & 0 & 0 & 1 & 1 & -1 & -1 \end{bmatrix} \]

The products \( \mathbf{m} = M \mathbf{f} \) and \( \mathbf{m}^{eq} = M \mathbf{f}^{eq} \) are vectors in the
moment space and the components of equilibrium moments
for flow through porous media is given by

\[ \mathbf{m}^{eq} = (\rho_0, e^{eq}, \zeta^{eq}, \dot{j}_x, q_x^{eq}, \dot{j}_y, q_y^{eq}, p_x^{eq}, p_y^{eq})^T \]

\[ \rho_0 = \text{mean fluid density} = 1 \text{ in lattice unit}; \]

\[ e^{eq} = -4\rho_0 + 6\rho p + 3\rho^2 \phi^3 \rho_0 |\mathbf{u}|^2 \]

\[ \zeta^{eq} = 4\rho_0 - 9\rho p - 3\rho^2 \phi^3 \rho_0 |\mathbf{u}|^2 \]

\[ \dot{j}_x = \rho_0 u_x; \dot{j}_y = \rho_0 u_y; q_x^{eq} = -\rho_0 u_x \]

\[ q_y^{eq} = -\rho_0 u_y; p_x^{eq} = \rho_0 \phi^{-1} \left(u_x^2 - u_y^2\right) \]

\[ p_y^{eq} = \rho_0 \phi^{-1} u_x u_y \]

In MRT collision, \( S \), is a diagonal matrix with relaxation
times for each moment as the diagonal elements. The nine
diagonal elements are:

\[ 0, \frac{1}{\tau}, \frac{1}{\tau}, 0, 8\left(\frac{2-1/\tau}{8-1/\tau}\right), 0, 8\left(\frac{2-1/\tau}{8-1/\tau}\right), 1, \frac{1}{\tau}, \frac{1}{\tau} \]
Here, the force vector with components $F_x$ and $F_y$.

In the LBM equation, the variable being solved is the particle density distribution function, $f_i$. From this distribution function, the macroscopic velocity and pressure is obtained from the relations:

$$
u = \frac{\mathbf{v}}{l_0 + \sqrt{l_0^2 + l_1^2}}, \quad \mathbf{v} = \sum_{i=0}^{8} \mathbf{e}_i f_i$$

$$l_0 = \frac{2K + \phi \Delta T}{4K}, \quad l_1 = \frac{\phi \Delta T F_I}{2\sqrt{K}}$$

$$p = 0.06 \sum_{i=1}^{8} l_i - 6\rho_0 \|\mathbf{u}\|^2$$

**Scalar transport:**

$$\frac{\partial (\mathbf{c} \phi)}{\partial t} + (\mathbf{u} \cdot \nabla) \phi = D_{eff} \nabla^2 \phi$$

This equation is solved for both species transport and thermal energy transport [8]. Here, $D_{eff}$ represents the effective diffusion coefficient (mass or thermal according to the scalar function under consideration). The calculation of binary mass diffusivity (i.e. effective diffusivity for clear medium) is from the relation[6]:

$$D_k = \frac{0.0143 \gamma^{1.75}}{p(6.12^{1/3} + 13.1^{1/3})} \sqrt{\frac{1}{M_1 + \frac{1}{M_2}} \frac{1}{2000}}$$

In the above relation, $M$ is the molecular mass of the species and $T$ is the temperature. In porous media, the effective mass diffusivity is calculated as

$$D_{eff} = \frac{\epsilon}{\tau} \left( 1 - \alpha_{im} y_i \right) + \frac{1}{D_{k,m}}$$

$$D_{k,m} = \frac{2}{3} \left( \frac{8RT}{\pi M_m} \right)^{1/2}, \quad \alpha_{im} = 1 - \left( \frac{M_i}{M_m} \right)^{1/2}$$

Here, $\tau$ is the tortuosity of the porous medium and $y_i$ is the mole fraction of the species $i$.

For thermal transport, the effective thermal conductivity for the gas mixture is calculated from the relation:

$$k_m = \sum_{i=1}^{n} \frac{y_i k_i}{\sum_{j=1}^{n} y_j A_{ij}}$$

$$k_{eff} = \left[ 1 + \left( \frac{\mu M_j}{M_i} \right)^{1/2} \left( \frac{M_i}{M_j} \right)^{1/4} \right]^2$$

The effective thermal diffusivity for the porous medium can be found from the relation:

$$\alpha_{eff} = \left[ k_m \varepsilon + k_i (1-\varepsilon) \right] / \rho_n c_{pm}$$

The scalar transport equation is solved using the LBM equation given below in a D2Q5 lattice.

$$\mathbf{g}(x + \mathbf{e} \Delta t + \Delta t) - \mathbf{g}(x, t) = -N^{-1} \mathbf{Q} [\mathbf{n}(x, t) - \mathbf{n}^e(x, t)]$$

The transformation matrix for D2Q5 is

$$\mathbf{N} = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 0 & 1 & 0 & -1 & 0 \ 0 & 1 & 0 & -1 & 0 & 0 & 0 & 1 & 0 & -1 \ -4 & 1 & 1 & 1 & 1 & 0 & 1 & -1 & 1 & -1 \ 0 & 1 & -1 & 1 & 1 & 0 & 1 & -1 & 1 & -1 \ \end{bmatrix}$$

The diagonal terms of relaxation matrix and the equilibrium moment vector for this equation are given by

$$\mathbf{n}^e = (T, u_T, v_T, bT, 0)^T$$

$$\mathbf{Q} = \text{diag} \left[ 0, \frac{6}{3+\sqrt{3}}, \frac{6}{3+\sqrt{3}}, \frac{6}{3+2\sqrt{3}}, \frac{6}{3+2\sqrt{3}} \right]$$

The parameter $b$ is related to the diffusivity according to the relation,

$$b = \frac{60\alpha}{\sqrt{3}} - 4$$

In this equation, $\alpha$ represents mass diffusivity or thermal diffusivity depending on whether the equation solved is species transport or energy transport. The temperature or mass fraction of the species is obtained from the distribution function according to the relation

$$T = \sum_{i=0}^{6} \mathbf{g}_i$$

The LBM equations for fluid flow, hydrogen mass fraction and temperature are solved in the entire domain to obtain the macroscopic velocity, pressure, hydrogen concentration and temperature distribution. The consumption of hydrogen and generation of water and heat are simulated as boundary conditions in the anode functional layer, as discussed in the next section.
COMPUTATIONAL DOMAIN AND BOUNDARY CONDITIONS:
The computational domain shown in the figure 1 has the following dimensions. Length of the channel is 20mm, the thickness of porous support layer is 0.5mm and the width of the flow channel is 1mm. Hydrogen is provided as input into the anode at temperature, $T_{an}$ through the flow channel inlet at a specified velocity. The mole fraction of hydrogen at inlet is assumed to be 1.0. The velocity of the inlet feed for pulsating cases are given as

$$ U = u_0[1 + A \sin(\omega t)] $$  \hspace{1cm} (18)

Reynolds Number $(Re)$ and Womersley Number $(Wo)$ are defined as follows:

$$ Re = \frac{\rho u_a W}{\mu}; Wo = L \sqrt{\frac{\alpha \rho}{\mu}} $$  \hspace{1cm} (19)

Bounce back is employed for fluid flow on all solid surfaces and catalyst layer for no slip. For temperature and species transport no flux condition is given at all solid surfaces. Electrochemical reactions which result in the consumption of hydrogen and the generation of water and heat takes place at the catalyst layer ($Y=0$). As the catalyst layer is of negligible thickness when compared to the width of the support layer and channel, it is assumed as a surface and the reactions are implemented as boundary conditions.

$$ \frac{\partial C}{\partial x} = \frac{j}{nFD} $$  \hspace{1cm} (20)

For heat generation, temperature boundary condition is applied by same equations as in concentration boundary conditions.

The reaction is assumed to follow the modified Butler Volmer kinetics proposed by [9] and later applied by [10]. The reaction rate is then given by:

$$ j = j_{a0} \left\{ \exp \left(1 + \alpha_a \frac{F n_a}{RT}\right) - \exp \left(\beta_a \frac{F n_a}{RT}\right) \right\} $$  \hspace{1cm} (21)

In the equation, $j_{a0}$ is the exchange current density, $\eta_a$ is the activation overpotential, $F$ is the Faraday constant and $\alpha_a$ and $\beta_a$ are the transfer coefficients.

The local current density is calculated from the local mole fraction of hydrogen, the local temperature, pressure and the over-potential. The over-potential is calculated as [6]:

$$ \eta_a = \Delta V_{eq} + OCV - V_{cell} $$  \hspace{1cm} (22)

$$ \Delta V_{eq} = \frac{RT}{2F} \ln \left( \frac{1 - y_{H_2, in}}{y_{H_2}} \right) $$  \hspace{1cm} (23)

$$ OCV = E^0 - \frac{RT}{2F} \ln \left( \frac{1 - y_{H_2, in}}{y_{H_2}} \left( 1.013 \times 10^5 \right)^{1/2} \right) $$

$\Delta V_{eq}$ is the local thermodynamic equilibrium potential which is the energy barrier to be overcome for the reaction to take place. It implicitly accounts for the concentration over-potentials. $V_{cell}$ is the operating voltage of the SOFC and the difference between operating voltage and open circuit voltage, gives the activation overpotential. The local value of the overpotential is used to find the local current density in the functional layer.

Heat generation due to electrochemical reaction at the electrode is also considered. Joule heating is not considered in the present work. Heat generation takes place due to reversible entropic heating and irreversible heat of the electrochemical reaction. So the total heat generated due to the electrochemical reaction is given by [11,12]:

$$ Q_{gen} = j \left[ \eta_a + T \left( \frac{d(OCV)}{dT} \right) \right] $$  \hspace{1cm} (24)

The rise in temperature due to heat generation affects the reaction rate in the functional layer.

VALIDATION OF CODE:

For code validation, different cases were run and the results have been validated with that of published literature. Flow induced due to natural convection in a square cavity with heated walls is simulated for different Rayleigh and Prandtl numbers. The geometry and parameters used are similar to that used by Roy, Basak [13]. The bottom and left vertical walls of the cavity are heated. The right wall is kept at a lower temperature while the top wall is insulated. Plots of local Nusselt number distribution along the heated walls is plotted and compared with results of [13] as shown in Figures 2(a) and 1(b). The results obtained from LBM code are shown by lines and the symbols are data from [13].

To validate flow through porous media, simulations of flow and heat transfer in a cavity filled with porous media is simulated. The left wall is heated and the right wall is at a lower temperature. The top and bottom walls are insulated. The buoyancy force due to density gradients induces natural convection. Simulations are conducted for different values of Darcy and Rayleigh numbers. Results are compared with that of[7]. Temperature distribution at mid-height of the cavity is plotted as shown in Figure 2(c). The lines show LBM results and symbols are result by[7].

For validation of surface reaction, results are validated with [14] as shown in Figure 2(d). The left wall has a constant concentration. The right and the bottom walls are insulated to mass diffusion. The species reaching the top wall undergoes reaction as follows.
\[-D \frac{\partial C}{\partial y}_{\text{top wall}} = k_r \left(C_{\text{top wall}} - C_{\text{eq}}\right) \quad (25)\]

The simulation was done for Damköhler number, \( Da = \frac{k_r d}{D} = 48 \). Here \( d \) is the height of the cavity. The dotted lines in the figure are results from [14] and the solid lines show LBM results.

![Figure 2](image-url)

**Figure 2.** (a) & (b) COMPARISON OF FLOW AND HEAT TRANSFER RESULTS WITH [13]: NUSSELT NUMBER DISTRIBUTION ALONG HEATED WALLS OF A SQUARE CAVITY WITH NATURAL CONVECTION INDUCED FLOW. (c) COMPARISON OF RESULTS OF FLOW THROUGH POROUS MEDIA WITH [7]: TEMPERATURE PROFILE AT MIDDLE HEIGHT OF A CAVITY FILLED WITH POROUS MEDIA WITH WALLS AT DIFFERENT TEMPERATURES. (d) COMPARISON OF PRESENT RESULTS (SOLID LINES) OF [14] SURFACE REACTION WITH (DOTTED LINES).

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>( E_{a}^{\text{act}} )</td>
<td>( 1.2 \times 10^{5} ) J/mol</td>
</tr>
<tr>
<td>( T_{\text{ref}} )</td>
<td>800 °C</td>
</tr>
<tr>
<td>( A_{\text{des}} )</td>
<td>( 5.59 \times 10^{15} ) s-m²/mol</td>
</tr>
<tr>
<td>( \Gamma )</td>
<td>( 2.6 \times 10^{-5} ) mol/m²</td>
</tr>
<tr>
<td>( \gamma_{0} )</td>
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<tr>
<td>( E_{\text{des}} )</td>
<td>( 8.812 \times 10^{4} ) J/mol</td>
</tr>
<tr>
<td>( \epsilon_{0} )</td>
<td>0.978 V</td>
</tr>
<tr>
<td>( P_{a,\text{in}} )</td>
<td>( 1.01325 \times 10^{5} ) Pa</td>
</tr>
<tr>
<td>( P_{c,\text{in}} )</td>
<td>( 1.01325 \times 10^{5} ) Pa</td>
</tr>
<tr>
<td>( \gamma_{H_{2},\text{in}} )</td>
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</tr>
<tr>
<td>( \gamma_{O_{2},\text{in}} )</td>
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<tr>
<td>( k_{H_{2}} )</td>
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</tr>
<tr>
<td>( k_{H_{2}O} )</td>
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<td>( k_{s} )</td>
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<td>( c_{p,H_{2}O} )</td>
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<tr>
<td>( L )</td>
<td>( 2000 \times 10^{-5} ) m</td>
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<tr>
<td>( W )</td>
<td>( 150 \times 10^{-5} ) m</td>
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</table>

### RESULTS AND DISCUSSIONS:

For simulations, the initial conditions used are, \( T=\text{Top,} \gamma_{1}=0.0 \) and \( u=0.0 \) throughout the domain. The values of parameters used in the simulation are given in Table 1. A pulsating flow with parabolic profile is given at inlet. In order to study the effect of this pulsating flow, various parameters like time-averaged fluid flow rate and frequency are varied. The performance of the fuel cell for the pulsatile flow is compared with that of steady non-pulsating fluid flow. The results obtained are discussed in the subsequent sections.

Before the discussion of cases of pulsatile inlet flow, the results for constant inlet are given in figure 3. The figure shows contours of X direction velocity, mole fractions of hydrogen and water and temperature are given. The figure shows that the electrochemical reactions taking place at \( Y=0 \), results in the lowering of hydrogen mole fraction and the increase in water mole fraction and temperature in that region. The aim of further simulations is to study the effects of pulsations on mass and heat transport and electrochemical performance.
The variations in hydrogen concentration and temperature with the phase angle due to pulsation of flow can be observed from figure 4 and 5. The flow pulsations are such that the maximum velocity of flow is for the phase 90° and the minimum is at 270°. The variations in hydrogen concentration and temperature also show the same trend. This shows that the temporal variations of all the three variables are in phase and the local values of the scalar variables depend strongly in the instantaneous local velocity value.

The effect of the pulsation on performance can be predicted from observing the instantaneous concentration profiles along the catalyst layer (Figure 6). The plots also show that the concentration profiles go to below the average value at phase angle between 180° and 360°. This implies that the rate of reaction will also decrease in this phase range as the reaction rate strongly depends on the reactant concentration at the reaction sites.
In addition to the output current density, the maximum temperature in the fuel cell components and its location are also very important factors determining their life. Maximum temperature in the computational domain is observed at the rightmost point of anode functional layer \((x=1000, y=1)\). Its variation with time is analysed and found to be pulsating with time as shown in Figure 8.

![Figure 8: VARIATION OF MAXIMUM TEMPERATURE WITH PHASE FOR Wo = 1.13, A = 0.25 AND V_{\text{cr}} = 0.6 V](image)

From the plots till now we have been observing the temporal variations of the major parameters of interest. It is seen that all these parameters showed pulsatile behaviour. The effect of these pulsations on the performance of the cell will now be analysed by plotting the performance curves from the time-averaged values.

The performance curves for \(Re=5\) (defined based on inlet height and average inlet velocity) and operating temperature, 1073K, are plotted in Figures 9 for different Womersley Numbers (\(Wo\)) keeping non-dimensional amplitude (\(A\)) constant. It is interesting to note that the time-averaged value of output current for a particular operating voltage is almost independent of the \(Wo\), for the range of values simulated in the present work. The results for three amplitudes plotted in Figures 9a, 9b and 9c also show the same trend. But a more intriguing trend observed is that as the amplitude of the flow pulsations is increased, the output current decreases meaning the performance is adversely affected.

![Figure 9. PERFORMANCE CURVE OF SOFC FOR (a) A=0.25 (b) A=0.50 (c) A=0.75 (d) Wo=0.80 (e) Wo=0.98 (f) TIME-AVERAGED CURRENT DENSITY VS NON-DIMENSIONAL AMPLITUDE A AT OPERATING VOLTAGE 0.6, OPERATING TEMPERATURE 1073K](image)

Tests are conducted for varying amplitudes for different \(Wo\). All cases showed that with increasing amplitude of pulsation of inlet flow the performance is adversely affected, as shown in Figure 9d and 9e. The output current density is lowered than that for steady inlet flow condition. The variation of the time-averaged output current density with amplitude for different \(Wo\) is plotted in Figure 9f. The figure shows that the decrease in the output current density with amplitude is considerable.

**CONCLUSIONS:**

The effect of the pulsatile anode flow on the overall performance of a SOFC cell has been investigated. Performance curves are plotted for different Womersley number and amplitude of pulsation of flow. The results show that pulsations in flow cause deterioration of performance, unlike the case of proton exchange membrane fuel cells (PEMFC). The major reason for this should be presence of liquid water in PEMFCs. The removal of liquid water is facilitated by flow pulsations in PEMFC. The present work was attempted to study whether such effect will be noticed in SOFC where the water produced is in gaseous state. In SOFC
it is seen that the flow pulsations adversely affect the reactant transport to the reaction sites affecting the output of the cell. From this, it is concluded that, for the values considered in the present work, the reaction transport to the reaction site is the major factor of concern and that the flow pulsation will affect this transport, and hence the performance, adversely.

REFERENCES:

[10] !!! INVALID CITATION !!!