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Dynamic simulation and analysis of a Solid Oxide Fuel Cell (SOFC)

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Abstract:

Dynamic simulation of an anode-supported tubular SOFC is performed to study the transients of current and the transport fields in the cell. The time constants of the system are studied and the possible explanations for their variation within the cell and at various overpotentials are presented. It was observed that the gain of the system varies depending upon the operating conditions of the system and the directionality of the step.

Keywords: SOFC, Dynamic simulation, Transient, Time constant, Gain

1. Introduction :

Different types of fuel cells are being widely explored for efficient utilization of fuels in various applications. SOFC is a high temperature (600-1000 °C) fuel cell, which is an ideal choice for large scale stationary applications. Because of its high operating temperature and fast transients, a properly implemented controller is essential for efficient use of the fuel and higher life-expectancy. A detailed analytical study is presented in this paper which is useful for the synthesis of such a controller.

2. Literature survey:

Several models have been studied in literature [1-3] for dynamic simulation of SOFC. The models vary from each other in terms of their complexities, physical phenomena considered and the operating range in which the model is validated. In [2], the transients in hydrogen, oxygen and water have been presented. But a detailed study on the variations of time constants depending upon the spatial locations and the operating conditions has not been done yet. Also to the best of the authors' knowledge, there has been no study yet on the behavior of various process gains in a SOFC.

3. Modeling Approach

The dynamic model with the numerical approach for solution is presented. The transients in the transport fields are compared and discussed. The reasons for the variations in the time constants are provided. The process gains of the system are studied.

3.1. Modeling of SOFC

The assumptions for the model are as below:

- The flow is Newtonian with constant viscosity in the gas channels.
- Radial variations of transport fields inside the flow channels are ignored.
- The model is isothermal.

The system of equations is solved by a Control Volume (CV) approach [1, 3]. The following phenomena are considered:

Anode gas flow channel

Hydrogen Conservation:

As hydrogen flows through the channel, it diffuses into the porous anode to take part in the reaction. Hydrogen conservation equation can be written as:

$$\frac{\partial C_{H_2,ac}}{\partial t} = -\frac{\partial (C_{H_2,ac} u_{z,ac})}{\partial z} - \frac{2J_{H_2,ac}}{r_{in,ac}} \tag{1}$$

Where C represents concentration (mol/m^3), r is the radius (m), u is the velocity (m/s) and J is the flux. Suffixes H_2 represents hydrogen, z and r denote axial and radial directions respectively, 'ac' represents anode channel and 'in' represents inner. Water conservation equation is written in the same manner considering the fact that the water diffuses into the anode channel from the porous anode.

Momentum Conservation:

Because of the previous assumptions, Navier-Stokes equation becomes:

$$\frac{\partial(\rho_{ac}u_{z,ac})}{\partial t} = -\frac{\partial(\rho_{ac}u_{z,ac}u_{z,ac})}{\partial z} - \frac{\partial p_{ac}}{\partial z} - \frac{\partial \tau_{zz,ac}}{\partial z} \tag{2}$$

Where ρ is density (kg/m3), p is the pressure (Pa), and τ_{zz} is the normal stress term.

Anode:

Hydrogen conservation:

$$\frac{\partial C_{H_2,an}}{\partial t} = -\frac{1}{r}\frac{\partial(rN_{H_2,an})}{\partial r} \tag{3}$$

Where the molar flux of hydrogen is given by [4]:

$$N_{H_2,an} = -D_{H_2,eff}\frac{\partial C_{H_2,an}}{\partial r} + \frac{C_{H_2,an}}{C_{H_2,an} + C_{H_2O,an}}(N_{H_2,an} + N_{H_2O,an}) \tag{4}$$

Where $D_{H_2,eff}$ is the effective diffusivity of hydrogen.

Similar equations are written for molar flux of water in the anode. The oxygen and nitrogen conservation equations along with the momentum balance are considered in the cathode flow channel in a similar manner. Although at steady state there won't be any flux of nitrogen in cathode, it may still show transient characteristics. Therefore both the oxygen and nitrogen conservations are considered in cathode.

Electrochemical Reaction:

The cell terminal voltage can be expressed as:

$$E_{cell} = (E_{Nernst})_i - (R_A + R_\Omega + R_C)_i I_i \tag{5}$$

E_{Nernst} is the Nernst potential. R_Ω is the ohmic resistance. The activation overpotentials at the anode and cathode in terms of equivalent resistances are given by [5]:

$$R_A = [\frac{2F}{R_u T}k_A(\frac{p_{H_2}}{P})^{0.25}\exp(-\frac{E_{act,an}}{R_u T})]^{-1} \tag{6}$$

$$R_C = [\frac{4F}{R_u T}k_C(\frac{p_{O_2}}{P})^{0.25}\exp(-\frac{E_{act,cat}}{R_u T})]^{-1} \tag{7}$$

Where F is Faraday's constant and R_u is universal gas constant. T denotes temperature and p represents partial pressure. k_A and k_C are the pre-exponential factors and E_{act} is the activation energy.

3.2. Solution procedure:

The set of equations contains PDEs and algebraic equations. Method of lines is used for solution. The solution is done using a MAPLE-MATLAB combination. All the PDEs and algebraic equations are set up and normalized in MAPLE with the boundary conditions. The equations are disctretized generating a DAE system of 540 equations. The equations are exported to a MATLAB function to be used for dynamic simulation. The dynamic simulation is carried out in SIMULINK environment of MATLAB. The steady state solution generated by “fsolve” in MATLAB is passed on as the initial value for the dynamic simulation. Step inputs in voltage are given to study the system transients.

3.3. Results & discussions:

Steady state model is first validated by the experimental data. The experiments are carried out at a wide range of temperature (700-850 °C) and hydrogen flow (21-51 ml/min) to study the validity of the model. Figures 1 and 2 show that the simulation results match very well with the experimental data.

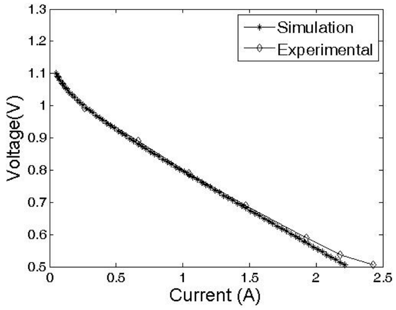


Figure 1. Comparison of I-V curves at 700 °C & 31 ml/min H_2 flowrate

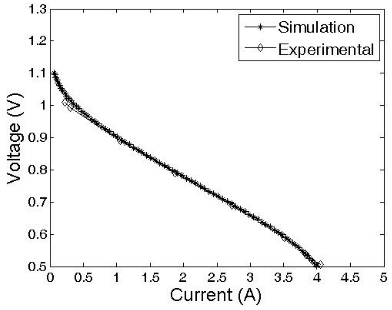
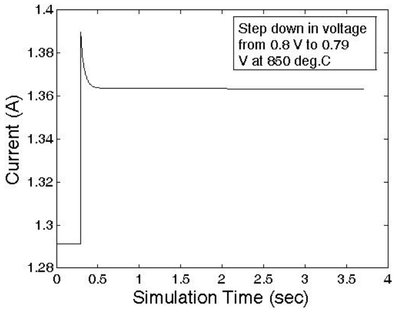


Figure 2. Comparison of I-V curves at 850 oC & 41 ml/min H_2 flowrate



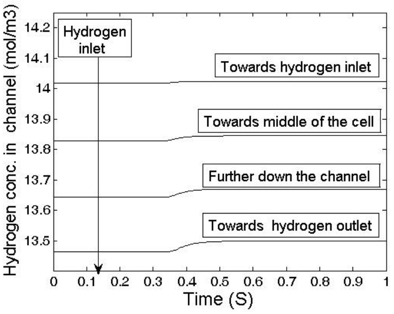


Figure 3. Transient response in current in response to stepdown in voltage

Figure 4. Transients in hydrogen concentration field in some CVs of anode channel

A step decrease in the cell terminal voltage is introduced. The transient response in current is shown in Figure 3. Because of the decrease in the cell terminal voltage, the overpotential increases, therefore generating more current. After an initial jump, the current reaches a new steady state value quickly. Figure 4 shows that the time constant in hydrogen concentration field keeps increasing down the channel. The increasing time constant can be attributed to the transport lag in the channel and the mass transfer resistances inside the porous anode. Effective diffusivity of hydrogen is much higher than oxygen. Therefore the time constant is very low for the CVs towards the hydrogen side inlet. Figure 5 shows that in the cathode channel, the time constants in the CVs towards the oxygen side inlet are higher than the inlet side CVs of hydrogen. This can be attributed to the slower diffusivity of oxygen. Figure 6 shows the transients of oxygen concentration inside the cathode. The settling time is much higher than the hydrogen concentration field inside the anode. Table 1 shows how the time constant varies with spatial location inside the cell. Time constants also vary significantly depending upon the operating conditions, magnitude of the step and the variable in which the step is given.

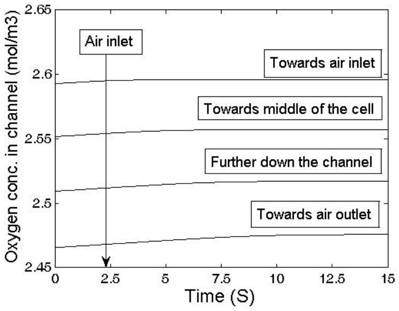


Figure 5. Transients in oxygen concentration field in some CVs of cathode channel

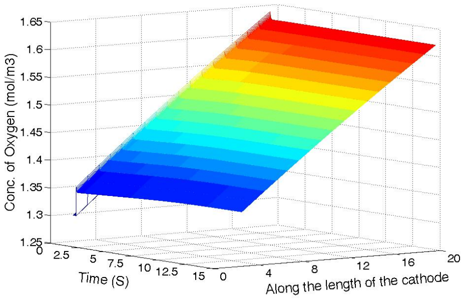


Figure 6. Oxygen concentration field inside cathode

The gain is calculated by the following equation:

$$Gain = \frac{\%\ change\ in\ output\ variable}{\%\ change\ in\ input\ variable}$$

Therefore the gain between the current and voltage is always negative. Steps of ± 0.01 V and ± 0.03 V are given at 700 ^{o}C and 850 ^{o}C for the hydrogen flow rate of 36 ml/min. The corresponding gains are presented in Table 2. It can be observed that for steps of ± 0.01 V at both 700 ^{o}C and 850 ^{o}C, the corresponding gains are not much different. But for steps of ± 0.03 V, the respective gains are different for both the temperatures. The corresponding gains at 850 ^{o}C are higher than that at 700 ^{o}C mainly because of the faster kinetics of the system.

Table 1: Variation in time constants with spatial locations inside the cell:

In anode channel:		
Towards H_2 inlet	Towards middle	Towards H_2 outlet
0.062	0.074	0.083
In cathode channel:		
Towards O_2 inlet	Towards middle	Towards O_2 outlet
5.336	3.412	1.408

Table 2: Gain between voltage and current

Temperature (^oC)	ΔV (V)	ΔV (%)	ΔI (A)	ΔI (%)	Gain
700	+0.01	+1.25	-0.0544	-5.504	-4.403
700	-0.01	-1.25	+0.0545	+5.510	-4.408
700	+0.03	+3.75	-0.1615	-16.341	-4.358
700	-0.03	-3.75	+0.1647	+16.665	-4.444
850	+0.01	+1.25	-0.0721	-5.577	-4.462
850	-0.01	-1.25	+0.0721	+5.577	-4.462
850	+0.03	+3.75	-0.2120	-16.421	-4.379
850	-0.03	-3.75	+0.2161	+16.739	-4.464

4. Conclusions and future work

It has been shown that the time constants of the SOFC system change widely depending upon the input, operating conditions, the spatial location and the transport field that is considered. We have also studied the varying gains of the system depending upon the operating conditions and the directionality of the step. The results from this study will be used in controller synthesis.

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