INVERSE PROBLEM METHOD: THE CASE OF PLANAR SOLID OXIDE FUEL CELL

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Abstract

Fuel cells are energy conversion devices for combined heat and power generation. Different types of fuel cells have been studied and developed in the past decades. Among them are solid oxide fuel cells (SOFCs), which present the highest working temperature. Mathematical modeling is an essential tool for the analysis and design of fuel cells. This is particularly appropriate for SOFCs, where localized experimental measurements are difficult due to the high operating temperature. Inverse problems are important when direct measurements of the desired quantities are not possible. In this paper we present a mathematical model based on inverse method for finding heat flux and temperature over a SOFC.

Keywords:
Solid oxide fuel cell**,** inverse method**,** heat flux**,** temperature

1. Introduction

The performance of a fuel cell is strongly influenced by the temperature distribution. Therefore, it is essential to accurately calculate the temperature profile in any relevant part of the cell. For this purpose, four energy balances, to the air and fuel channels, PEN structure, and interconnect based on figyre1 are considered.

Dynamic SOFC model: energy balances are given: [Ioraa, 005]

Fuel channel

$$\frac{\partial \rho_f e_f}{\partial t} = -\frac{\partial (u_f \rho_f h_f)}{\partial x} + \sum_{i=H_2,H_2o}^{ka} v_{i,(v)} R_{(v)} h_i \frac{1}{H_f} + k_{f,PEN}(T_{PEN} - T_f)\frac{1}{H_f} + k_{f,1}(T_1 - T_f)\frac{1}{H_f}, \quad (1)$$

$$x \in (0,L], t \in (0,t_H], T_f \;\Big|_{x=0} = T_f^{\;0}, t \in [0,t_H]$$

Air channel

$$\frac{\partial \rho_a e_a}{\partial t} = -\frac{\partial (u_a \rho_a h_a)}{\partial x} + \sum v_{O2,(v)} R_{(v)} h_i \frac{1}{H_a} + k_{a,PEN}(T_{PEN} - T_a)\frac{1}{H_a} + k_{a,1}(T_1 - T_a)\frac{1}{H_a},$$
$$x \in (0, L], t \in (0, t_H] \tag{2}$$
$$T_a \Big|_{x=0} = T_a^{\,0}, t \in [0, t_H]$$

PEN structure

$$\rho_{PEN} c_{p,PEN} \frac{\partial T_{PEN}}{\partial t} = \lambda_{PEN} \frac{\partial^2 (T_{PEN})}{\partial x^2} - k_{f,PEN}(T_{PEN} - T_f)\frac{1}{\tau_{PEN}} - k_{a,PEN}(T_{PEN} - T_f)\frac{1}{\tau_{PEN}} -$$
$$\sum_{i=H2,H2O} v_{i,(v)} R_{(v)} h_i \frac{1}{\tau_{PEN}} - v_{O2,(v)} R_{(v)} h_{O2} \frac{1}{\tau_{PEN}} - jU \frac{1}{\tau_{PEN}} + \left[\frac{\sigma (T_1^{\,4} - T_{PEN}^{\,4})}{\frac{1}{\varepsilon_1} + \frac{1}{\varepsilon_{PEN}} - 1} \right] \frac{1}{\tau_{PEN}}, \tag{3}$$
$$\frac{\partial T_{PEN}}{\partial x}\Big|_{x=0} = 0, \frac{\partial T_{PEN}}{\partial x}^{0}\Big|_{x=l} = 0, t \in [0, t_H]$$

The electrochemical reaction takes place in the PEN structure (anode/electrolyte interface), where hydrogen and oxygen migrate from the fuel and air channels and the water produced by the oxidation reaction diffuses back to the fuel channel. Therefore, the enthalpy fluxes associated with the flow of oxygen and hydrogen to the PEN structure and the flow of water from the PEN structure are taken into account in the PEN heat balance (fourth and fifth term on the right-hand side of Eq. (3)). Similarly, the second term on the right-hand side of Eqs (1) and (2) refers to the respective enthalpy fluxes to and from the fuel and air channels. The cell is taken to be placed in the central region of a stack, so that there is no heat flux through the external walls. The heat transfer coefficients between the gas channels and the solid parts are calculated using the channel hydraulic diameter and a constant Nusselt number. This is a common assumption given the laminar flow conditions.

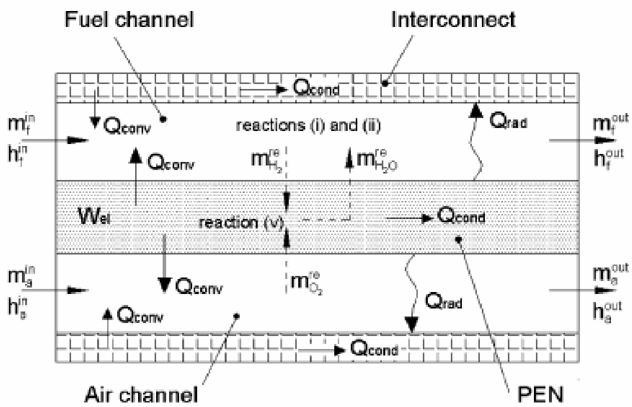

Figure.1. Mass transfer and heat exchange phenomena in a SOFC.

2. Identification of Solid Oxide fuel cell inverse heat transfer problem and presentation of solution

For simplifying we neglected the radiation heat transfer .Below equation with 4 boundary conditions for solution the equation considering the structure of cell are presented .Temperature and heat flux on the interconnect wall(and also temperature on the time=0) are taken T_0, Q .These are the unknown parameters.

$$\rho c_{p,}\frac{\partial T_I}{\partial t}=\lambda\frac{\partial^2(T_I)}{\partial x^2}-k_{f,I}(T_I-T_f)\frac{1}{\tau_I}-k_{a,I}(T_I-T_f)\frac{1}{\tau_I}$$
$$\frac{\partial T_I}{\partial x}\Big|_{x=0}=Q,\frac{\partial T_I}{\partial x}\Big|_{x=L}=Q,T_I\Big|_{x=0}=T_0,T_I\Big|_{t=0}=T_0 \qquad (4)$$

For subsisting of parameters in the top equations, we need the below identifications:

$$\rho_{H2]T=900}=0.02723kg/m^3,\rho_{air]T=900}=0.3925kg/m^3 ,$$
$$Cp_{air]T=900}=1.1212kj/kg ,Cp_{H2]T=900}=14.821kj/kg$$
$$\lambda_{H2]T=900}=0.412w/m^oc \; Nu=3.09 ,\lambda_{air]T=900}=0.068w/m^oc$$
$$H_f=H_a=0.001\ m ,L=0.4m ,w=0.1m$$

The first step is solution of the direct problem with known initial conditions; the equation is a non-homogeneous partial differential equation. A fully numerical scheme by Mathematica Software is employed to solve the equation .To find the solution distribute from the direct problem we determine the inverse algorithm for finding the unknown derivative conditions. It is solved as an optimization problem which minimizes the summation of the square of the differences between the estimated dimensionless solutions $T(X_i,Y_1,\tau_k)$ and the measured dimensionless solution $Z(X_i,Y_1,\tau_k)$. The last term is a range of temperature over the surface which are obtained from sensors .The objective function J is given by[Hung-Yi Li, 2003]

$$J=\sum_{i=1}^{M}\sum_{j=1}^{N}\left(T_{(I)i,k}-Z_{i,k}\right) \qquad (5)$$

M is the number of the sensors; N is the number of the data sampled for each sensor. The minimization of the objective function is obtained by the conjugate gradient method determined by differentiating equation once with respect to $Q_{m,n}$ and another time respect to $T_{m,n}$

$$\frac{\partial J}{\partial T_{m,n}} = 2\sum_{i=1}^{M}\sum_{j=1}^{N}\left(T_{(I)i,k} - Z_{i,k}\right)\frac{\partial T_{(I)i,k}}{\partial T_{m,n}} \tag{6}$$

$$\frac{\partial J}{\partial Q_{m,n}} = 2\sum_{i=1}^{M}\sum_{j=1}^{N}\left(T_{(I)i,k} - Z_{i,k}\right)\frac{\partial T_{(I)i,k}}{\partial Q_{m,n}} \tag{7}$$

Where T_I is known from the solution of direct problem and Z is known from sensors. For finding the last terms of right hand of equations requires the sensitivity problem which is obtained by differentiating the direct problem given by equation series (4) with respect to Q and T from which, we can show that

$$\Delta T_I = \frac{\partial T_{(I)i,k}}{\partial Q_{m,n}} \quad , \quad \Delta T_I = \frac{\partial T_{(I)i,k}}{\partial T_{m,n}}$$

$$\rho c_{p,P}\frac{\partial \Delta T_I}{\partial t} = \lambda\frac{\partial^2(\Delta T_I)}{\partial x^2} - k_{f,I}(\Delta T_I - T_f)\frac{1}{\tau_I} - k_{a,I}(\Delta T_I - T_f)\frac{1}{\tau_I} \tag{8}$$

$$\frac{\partial \Delta T_I}{\partial x}\Big|_{x=0} = \delta_{i.j}\Delta Q, \frac{\partial \Delta T_I}{\partial x}^0\Big|_{x=L} = 0, \Delta T_I\Big|_{x=0} = 0, \Delta T_I\Big|_{t=0} = 0, \delta_{i,j} = \begin{cases} 0, for i \neq j \\ 1, for i = j \end{cases}$$

$$\frac{\partial \Delta T_I}{\partial x}\Big|_{x=0} = 0, \frac{\partial \Delta T_I}{\partial x}^0\Big|_{x=L} = \delta_{i,j}\Delta Q, \Delta T_I\Big|_{x=0} = 0, \Delta T_I\Big|_{t=0} = 0, \delta_{i,j} = \begin{cases} 0, for i \neq j \\ 1, for i = j \end{cases}$$

$$\frac{\partial \Delta T_I}{\partial x}\Big|_{x=0} = 0, \frac{\partial \Delta T_I}{\partial x}^0\Big|_{x=L} = 0, \Delta T_I\Big|_{x=0} = \delta_{i.j}\Delta T_0, \Delta T_I\Big|_{t=0} = \delta_{i.j}\Delta T_0, \delta_{i,j} = \begin{cases} 0, for i \neq j \\ 1, for i = j \end{cases}$$

Now we consider the next iteration value solution and derivative, the iterative procedure of the conjugate gradient method is given by

$$T_{m,n}^{p+1} = T_{m,n}^{p} - \beta_T{}^p d_{Tm,n}^{p} \tag{9}$$

$$Q_{m,n}^{p+1} = Q_{m,n}^{p} - \beta_Q{}^p d_{Qm,n}^{p} \tag{10}$$

Where $Q,(T)_{m,n}$=$Q,(T)(X_m,\tau_n)$ and $\beta_Q,(\beta_T)^p$ are the step sizes, $d_Q,(d_T)_{m,n}{}^p$ are the directions of descent which are:

$$d_{Qm,n}^{p} = \left(\frac{\partial J}{\partial Q_{m,n}}\right)^p + \gamma_Q{}^p d_{Qm,n}^{p-1} \tag{11}$$

$$d_{Tm,n}^{p} = \left(\frac{\partial J}{\partial T_{m,n}}\right)^p + \gamma_T{}^p d_{Tm,n}^{p-1} \tag{12}$$

And the conjugate coefficients $\gamma_Q, (\gamma_T)^p$ are computed from the below equations:

$$\delta_T^p = \frac{\sum_{m=1}^{M}\sum_{n=1}^{N}\left(\left(\frac{\partial J}{\partial T_{m,n}}\right)^p\right)^2}{\sum_{m=1}^{M}\sum_{n=1}^{N}\left(\left(\frac{\partial J}{\partial T_{m,n}}\right)^{p-1}\right)^2} \tag{13}$$

$$\delta_Q^p = \frac{\sum_{m=1}^{M}\sum_{n=1}^{N}\left(\left(\frac{\partial J}{\partial Q_{m,n}}\right)^p\right)^2}{\sum_{m=1}^{M}\sum_{n=1}^{N}\left(\left(\frac{\partial J}{\partial Q_{m,n}}\right)^{p-1}\right)^2} \tag{14}$$

Two last parameters would be zero for the iteration $p=0$. The step sizes are determined from

$$\beta_T^p = \frac{\sum_{i=1}^{M}\sum_{k=1}^{N}\left(T_{(I)i,k}^p - Z_{i,k}\right)\sum_{m=1}^{M}\sum_{n=1}^{N}\left(\frac{\partial T_{(I)i,k}}{\partial T_{m,n}}\right)^p d_{Tm,n}^p}{\sum_{i=1}^{M}\sum_{k=1}^{N}\left[\sum_{m=1}^{M}\sum_{n=1}^{N}\left(\frac{\partial T_{(I)i,k}}{\partial T_{m,n}}\right)^p d_{Tm,n}^p\right]} \tag{15}$$

$$\beta_Q^p = \frac{\sum_{i=1}^{M}\sum_{k=1}^{N}\left(T_{(I)i,k}^p - Z_{i,k}\right)\sum_{m=1}^{M}\sum_{n=1}^{N}\left(\frac{\partial T_{(I)i,k}}{\partial Q_{m,n}}\right)^p d_{Qm,n}^p}{\sum_{i=1}^{M}\sum_{k=1}^{N}\left[\sum_{m=1}^{M}\sum_{n=1}^{N}\left(\frac{\partial T_{(I)i,k}}{\partial Q_{m,n}}\right)^p d_{Qm,n}^p\right]} \tag{16}$$

After solving the equation (4) and Knowing $\partial J/\partial Q_{m,n}$, $\partial J/\partial T_{m,n}$ from the equations (6),(7) for the last and present step the equation (13),(14)are computed for finding γ^p , γt^p then $d_{m,n}{}^p$, $dt_{m,n}{}^p$ compute from (11),(12). Next step is computing the step size β^p ,$\beta^p{}_T$ where T is known from the solution of direct problem and Z is known from sensors and $\partial T_I/\partial Q_{m,n}$,$\partial T_I/\partial T_{m,n}$ from solving the equation (8)and d , d_T from (11),(12) and the final step is , computation Q and T for the new iteration from equations (9),(10)and Set $p=p+1$, Calculate the objective function. Terminate the iteration process if the specified stopping criterion is satisfied. Otherwise continue the algorithm, If the problem contains no measurement errors, the condition $J(T,Q) < MN\sigma^2$ can be used for terminated the iterative process, where σ is a small specified positive number. However, the measured temperature data contain measurement errors. Below algorithm is written and run by MATLAB software. [Gholami, 2006]

Set the error limit

1. Identification of the iteration loop σ
2. Input the initial value of T(Temperature) and Q(heat flux)
3. Calculate the p^{th} iteration of T from direct problem
4. Calculate the p^{th} iteration of J
5. If J is less than σ, stop and set Q ant T are finals otherwise continue
6. Calculate the p^{th} iteration of $\partial T_I / \partial Q_{m,n}$, $\partial T_I / \partial T_{m,n}$
7. Calculate the p^{th} iteration of $\partial J / \partial Q_{m,n}$, $\partial J / \partial T_{m,n}$
8. Calculate the p^{th} iteration of β_Q, β_T ,d_Q, d_T and γ_Q, γ_T
9. Calculate the $p+1^{th}$ iteration of T,Q
10. Set $p=p+1$ and start from first

3. Results

For the results presented below, we considered a range of 10 values of solution that the presented method optimizes them. The iterative procedure $J(Q_{m,n}^{p})<MN\sigma^2$ $(\sigma=0.01)$as the stopped criterion, for both unknown parameters ,T and Q is determined. Ten iterations are required to get the inverse problem solutions for the cases considered in this paper. Stop criteria was located in $j=0.009$.

Table1.Results

Iteration	Temperature	Heat flux
P=1	900	160000
P=2	901.897	160800
P=3	906.948	161400
P=4	914.28	162300
P=5	923.139	164100
P=6	932.881	165400
P=7	942.963	166200
P=8	952.939	167500
P=9	962.451	168400
P=10	971.224	169000

symbols	
$\rho_{e,f,PEN,I}$	density of the gas streams, PEN structure, and interconnect, kgm−3
e	specific internal energy, kJ kg−1
u	velocity, ms−1
h	specific enthalpy, kJ kg−1
v_{ik}	stoichiometric coefficient of component *i* in reaction *k*
Rk	rate of reaction *k*, molm−2 s−1
H	channel height, m
k	heat transfer coefficient, kJm−2 s−1 K−1
Q	heat flux, W/m2
T	temperature, K
c_p	specific heat capacity of the gas streams, PEN structure, and interconnect,kJ kg−1 K−1
λ	thermal conductivity of the gas streams, PEN structure, and interconnect,kJm−1 s−1 K−1
τ	thickness of electrolyte, PEN structure and interconnect, m
p	iteration number
j	Objective function
M	Number of sensors
N	Number of data
β	Step size
d	Direction of descent
γ	Conjugate coefficient

4. REFERENCES

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