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Estimation of internal fuel cell temperatures from surface temperature measurements

S. Bégot [a,*], J.M. Kauffmann [b]

[a] MESURTEK, Incubateur d'entreprises innovantes de Franche-Comté, Rue de Leupe, 90400 Sevenans, France
[b] Université de Franche-Comté, L2ES, Bât F, rue Thierry Mieg, 90010 Belfort Cedex, France

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Abstract

In this paper, a method to monitor PEM fuel cells internal temperature from surface measurements is presented. The aim of this work is to monitor fuel cells to prevent damages due to internal overheating. The measurements are taken at the side of the bipolar plate, and heat flux and temperature at the border of the active zone are estimated. The method is based on sensitivity analysis and inverse problem algorithms. The mathematical formulation and algorithm are described. The model is a transient heat conduction model in two dimensions, the inverse problem is solved with an optimization method using adjoint equation. Numerical test cases are presented for graphite and steel bipolar plates. The results show that internal temperature can be correctly estimated. The response time of the method is limited by the heat transfer rate in the material. Therefore, the method is particularly appropriate to fuel cells made of steel bipolar plates.

Keywords: PEM; Internal temperature; Inverse problem

1. Introduction

Internal temperature is one of the key parameters to monitor in proton exchange membrane fuel cells. The first reason is that the operating point efficiency depends on its value, the second is that a sharp raise in temperature can be an indication that direct combustion between air and hydrogen happens in the fuel cell. This combustion may cause important damages. Therefore, in this paper, a method based on inverse problem methodology to estimate internal temperatures from surface measurements is presented. The aim of the study is to investigate the capability of monitoring fuel cells with non-invasive temperature sensors. Inverse heat conduction problem is a topic that has been discussed by several authors [1–4]. In the field of fuel cells, only a few articles are published. In references [5,6] studies on steady state temperature distribution at the interface between the carbon plate and the membrane electrode assembly from measurements on the outer surface of the end plate are reported. The work presented here deals with the estimation of fuel cell transient internal temperature from surface temperature measurements taken at the side of bipolar plates. First, a mathematical method based on sensitivity analysis to estimate the possibilities of the inverse problem methodology is described, then the method to solve the inverse problem of 2D transient heat conduction is presented. The methodology relies on approaches developed in [1–3]. The paper is divided into three sections. In the first section, the heat conduction model in the fuel cell is formulated. The second section describes the mathematical formulation and method, the third part presents numerical results and summarizes the conclusions.

2. Model and formulation

2.1. General description

A proton exchange membrane (PEM) fuel cell is considered. Surface temperature measurements are assumed to be possible at the side of the bipolar plates. The aim of this work is to esti-

* Corresponding author. Tel.: +33 6 63 49 23 56; fax: +33 3 84 58 36 36.
E-mail addresses: sylvie.begot@mesurtek.com (S. Bégot), jean-marie.kauffmann@univ-fcomte.fr (J.M. Kauffmann).

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Nomenclature

D	descent direction
G	gradient
h	height of area under study (m)
i	iteration number
k	thermal conductivity ($W\,m^{-1}\,K^{-1}$)
l	length of the area under study (m)
L	objective function
S	objective function including the constraints
t	time variable
t_f	final time
T	temperature (°C)
T_0	initial temperature (°C)
u	heat flux ($W\,m^{-2}$)
x	horizontal coordinate
y	vertical coordinate

Greek symbols

α	thermal diffusivity ($m^2\,s^{-1}$)
β	conjugate direction coefficient
γ	descent step
δ	Dirac function
ΔT	temperature increment
Δu	heat flux increment
τ	reverse time variable
ψ	Lagrange multiplier

mate the internal temperatures of the plate in the active zone of the fuel cell (Fig. 1). The physical problem is formulated as a heat transfer problem. In the border zone of the bipolar plate, an unknown heat flux is considered to be flowing from the inside of the plate towards the outside. The purpose of this study is to estimate this heat flux and the internal temperature in order to monitor the fuel cell and prevent a destructive heat elevation.

2.2. Problem formulation

2.2.1. Physical problem

The problem is a problem of transient heat conduction in two dimensions with no heat generation (Fig. 2).

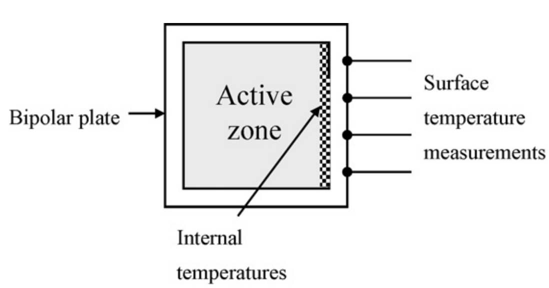

Fig. 1. Problem geometry.

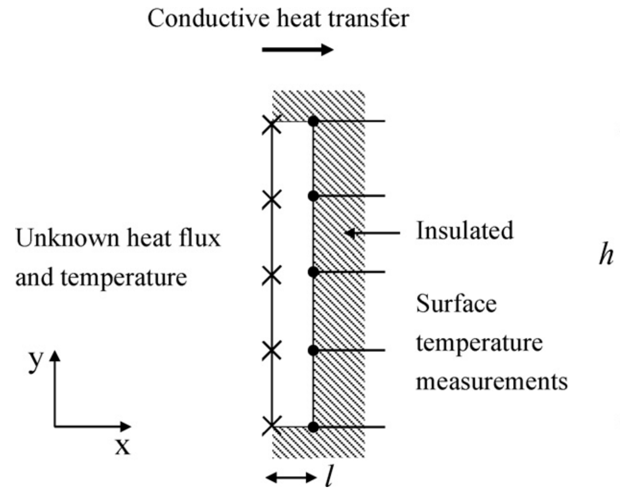

Fig. 2. Physical description.

The area under study is limited by:

$$0 \le x \le l$$
$$0 \le y \le h$$

It is considered that except on the left limit, the zone is thermally insulated.

2.2.2. Direct problem formulation

With the preceding assumptions, the direct problem formulation is [7]:

$$\begin{aligned} &\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = \frac{1}{\alpha}\frac{\partial T}{\partial t} \\ &-k\frac{\partial T}{\partial x} = u(x, y, t), \quad x = 0 \\ &k\frac{\partial T}{\partial x} = 0, \quad x = l \\ &-k\frac{\partial T}{\partial y} = 0, \quad y = 0 \\ &k\frac{\partial T}{\partial y} = 0, \quad y = h \\ &T(x, y, 0) = T_0 \end{aligned} \tag{1}$$

where α denotes diffusivity, k conductivity, u unknown heat flux, T_0 initial temperature that is supposed constant.

2.2.3. Sensitivity problem formulation

In order to be able to estimate what happens on the left side of the area, we have to check that the heat transfer produces a significant temperature elevation on the right side. This temperature evolution has to be measurable by the sensors used. If this is not the case, the estimation cannot be performed. This leads to sensitivity analysis [1].

The unknown heat flux u is perturbed by a small perturbation Δu in (1). Consequently, the temperature is perturbed by ΔT.

(1) is subtracted to the perturbed problem. This yields to the sensitivity problem:

$$\begin{aligned}
&\frac{\partial^2 \Delta T}{\partial x^2}+\frac{\partial^2 \Delta T}{\partial y^2}=\frac{1}{\alpha}\frac{\partial \Delta T}{\partial t}\\
&-k\frac{\partial \Delta T}{\partial x}=\Delta u(x,y,t), \quad x=0\\
&k\frac{\partial \Delta T}{\partial x}=0, \quad x=l\\
&-k\frac{\partial \Delta T}{\partial y}=0, \quad y=0\\
&k\frac{\partial \Delta T}{\partial y}=0, \quad y=h\\
&\Delta T(x,y,0)=0
\end{aligned} \tag{2}$$

With the results of the sensitivity analysis, it is possible to design an experiment that leads to a good inverse problem solution.

2.2.4. Inverse problem formulation

To estimate internal temperatures, computation of the heat flux at the plate left side is necessary. The internal temperature in $x=0$ is then computed by solving the direct problem. Thus, the inverse problem of estimating internal temperature is divided into two steps:

Step 1: Compute $u(0, y, t)$ from $T(l, y, t)$
Step 2: Compute $T(0, y, t)$ from $u(0, y, t)$

3. Numerical computations

3.1. Direct and sensitivity problems

The direct and sensitivity problem are classic heat transfer problems. For numerical heat transfer computations, we use a finite difference scheme in two dimensions [8].

3.2. Inverse problem

The inverse heat conduction problem (step 2) is iteratively solved by a gradient method. The gradient is computed using an adjoint problem. Among the various methods to derive the adjoint problem, the Lagrange multipliers are employed. The following paragraphs describe the method used. More details can be found in [1–3].

3.2.1. Objective function

The objective function is the quadratic residual between the computed temperatures and the measured temperatures:

$$S(u)=\frac{1}{2}\int_0^h\int_0^l\int_0^{t_f}(T_{\text{computed}}(u,x,y,t)-T_{\text{measured}}(x,y,t))^2 \times \delta(x-l)\delta(y-y_{\text{meas}})\,\mathrm{d}t\,\mathrm{d}x\,\mathrm{d}y$$

where T_{measured} denotes measured temperatures at the right side of the area, T_{computed} computed temperatures at the same points, δ Dirac delta function and y_{meas} coordinates of the measurements. The inverse problem is solved by minimizing this objective function under the constraint that the unknown function $u(x, y, t)$ verifies the direct problem (1).

3.2.2. Minimization algorithm

The conjugate gradient method [9] whose algorithm is as follows is employed:

$$\begin{aligned}
&D_0=-G_0\\
&\gamma_{i-1}=\operatorname{Arg\,min} J(U_{i-1}-\gamma D_{i-1})\\
&U_i=U_{i-1}+\gamma_{i-1}D_{i-1}\\
&\beta_{i-1}=\frac{\langle G_i^T, G_i-G_{i-1}\rangle}{||G_{i-1}||^2}\\
&D_i=-G_i+\beta_{i-1}D_{i-1}
\end{aligned}$$

where U denotes the unknown function, G gradient, D conjugate direction, γ step size, $\langle , \rangle$ scalar product, and subscript i is the iteration number.

3.2.3. Adjoint problem-gradient

The adjoint problem is derived by means of writing the minimization problem as an unconstrained one:

$$\begin{aligned}
L(u)=&\frac{1}{2}\int_0^h\int_0^l\int_0^{t_f}(T_{\text{computed}}(u,x,y,t)-T_{\text{measured}}(x,y,t))^2\\
&\times\delta(x-l)\delta(y-y_{\text{meas}})\,\mathrm{d}t\,\mathrm{d}x\,\mathrm{d}y\\
&+\int_0^{t_f}\int_0^l\int_0^h\psi(x,y,t)\left(\frac{\partial^2 T}{\partial x^2}+\frac{\partial^2 T}{\partial y^2}-\frac{1}{\alpha}\frac{\partial T}{\partial t}\right)\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}t
\end{aligned}$$

where ψ denotes a Lagrange multiplier that is solution of the adjoint problem.

The necessary conditions of stationarity for this functional lead to the following adjoint problem [3]:

$$\begin{aligned}
&\frac{\partial^2 \psi}{\partial x^2}+\frac{\partial^2 \psi}{\partial y^2}+(T_{\text{computed}}(l,y,t)\\
&-T_{\text{measured}}(l,y,t))\delta(y-y_{\text{meas}})\delta(x)=-\frac{1}{\alpha}\frac{\partial \psi}{\partial t}\\
&-k\frac{\partial \psi}{\partial x}=0, \quad x=0\\
&k\frac{\partial \psi}{\partial x}=0, \quad x=l\\
&-k\frac{\partial \psi}{\partial y}=0, \quad y=0\\
&k\frac{\partial \psi}{\partial y}=0, \quad y=h\\
&\psi(x,y,t_f)=0
\end{aligned} \tag{3}$$

By defining a new time variable $\tau=t_f-t$, the problem can be integrated.

The stationarity conditions lead to the gradient:

$$G(t)=-\psi(l,y,t)$$

Table 1
Properties of the bipolar plates

	Thermal conductivity ($W\,m^{-1}\,K^{-1}$)	Mass per unit volume ($kg\,m^{-3}$)	Heat capacity ($J\,kg^{-1}\,K^{-1}$)	Diffusivity ($m^2\,s^{-1}$)	Height h (m)	Length of the border zone l (m)
Graphite bipolar plate	1.68	2240	710	1.06e−6	0.2	0.02
Stainless steel bipolar plate	16.3	8027	502	4.05e−6	0.2	0.02

4. Results

4.1. General description of the numerical tests

In this section, the estimation of internal temperature of bipolar plates is numerically studied. The purpose of the numerical tests is to determine if it is possible to estimate an internal temperature raise due to faulty conditions from surface temperature measurements. Experimental data are simulated. An anomalous heat flux is supposed to happen inside the fuel cell at $x=0$. Solving the direct problem (1) leads to temperature values at $x=0$ and at $x=l$. Temperature values at $x=l$ are considered to be surface temperatures issued from temperature sensors. Temperature and heat flux data at $x=0$ are to be reconstructed, thus they are considered and denoted as the "exact values".

Using these simulated surface measurements at $x=l$, internal heat flux and temperature at $x=0$ are computed using the methodology described in Section 3.2. The results are referred as "computed values" in the following paragraphs.

The steel and graphite plates characteristics are displayed in Table 1. The anomalous heat flux applied at $x=0$ is 1e4 $W\,m^{-2}$. Nominal temperature operation is 80 °C. Thermocouples K of 0.3 °C accuracy are assumed to be used. Therefore, the measurement of a 2 °C-elevation is possible. Spatial discretization of the numerical scheme is 5×5.

4.2. Numerical test case 1: graphite bipolar plates

In this paragraph, estimation of internal temperature of a graphite plate is presented.

4.2.1. Sensitivity analysis

The influence of a flux variation at the point (O, $h/2$) on the temperature at the point (l, $h/2$) is computed using (2).

A numerical test case with 50 steps of 5 s each is considered. The results are plotted in Fig. 3. They show that a flux variation at the first time step produces a sensitivity coefficient that is maximal at the 20th time step. It means that in order

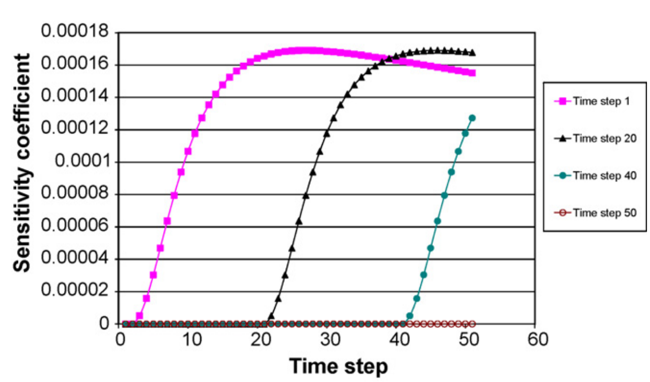

Fig. 3. Sensitivity coefficients for 50 time steps of 5 s, graphite plate.

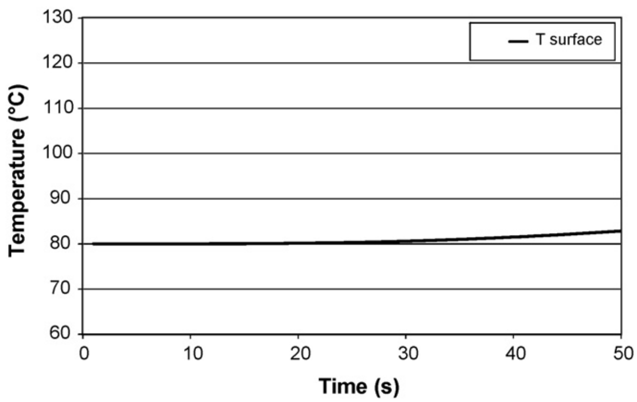

Fig. 4. Surface temperature (simulated measurements) for graphite bipolar plates.

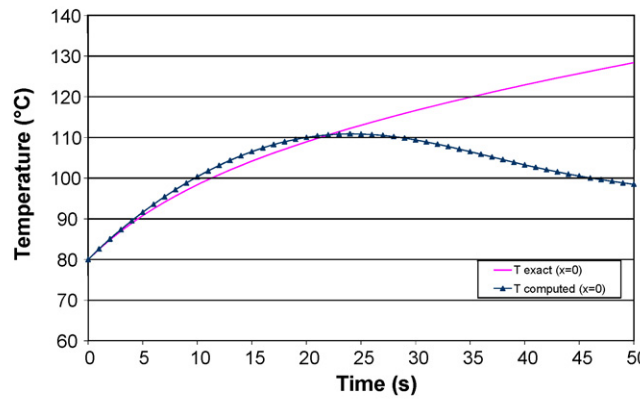

Fig. 6. Exact and estimated internal temperature for graphite bipolar plates.

to estimate the heat flux on one side of the plate at time step 1, the best measurement on the other side is the temperature at time step 20. For the next heat flux value (time step 20), the best measurement is the temperature at time step 40, and so forth. The sensitivity coefficient of the 40th time step is smaller. The heat flux value at this time step cannot be well estimated because the heat does not have the time to reach the temperature sensor. Of course, the heat flux at the last time step cannot be estimated at all, the sensitivity coefficient is zero.

So, this analysis shows that maximal sensitivity is achieved with a response time of about 100 s. This duration is too long to perform an efficient on-line monitoring of the fuel cell. If shorter duration is used, the temperature estimation is bounded to be less precise.

4.2.2. Inverse problem solution

In this paragraph, the inverse problem of estimating unknown heat flux and internal temperature values is solved by means of the methodology described in Section 3.2. The exact anomalous heat flux produces a temperature elevation of about 50 °C inside the plate and 3 °C at the surface in 50 s (Fig. 4). This simulated temperature surface is used to compute the internal heat flux and temperature. The computation lasts less than 2 s on an ordinary laptop computer.

Fig. 5 presents the exact and computed heat flux values at the point $x = 0$, $y = h/2$. The computed values are found to be accurately reconstructed in the first 20 s of the measurement interval. The relative error is less than 15%. After that, while the exact heat flux remains constant, the computed heat flux strongly decreases. Heat transfer in graphite is too slow to produce significant surface temperature elevation in less than 30 s. Therefore, the algorithm lacks information and is not able to reconstruct heat flux values in the last part of the interval. The accuracy decreases. This result is in accordance with the sensitivity analysis. Fig. 6 presents the exact and computed internal temperature. As before, the values are accurately computed in the first half of the time interval. The maximum relative error between the exact and computed values remains under 5% for 28 s. This accuracy is better than the accuracy obtained for the heat flux. It is due to the smoothing effect of the heat equation [1–4].

These observations led to the fact that it is necessary to take into account the duration of the heat transfer process to achieve accurate estimation of internal values. In this example, if the temperature measurements interval is of 50 s, the estimation of the internal values is accurate only for the 20 first seconds. So, the proposed method produces 5% accurate temperature

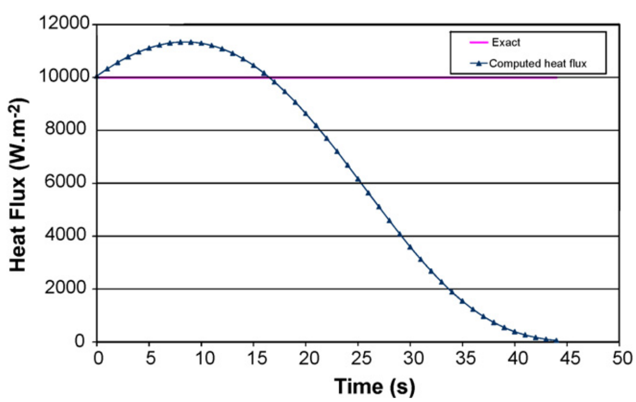

Fig. 5. Exact and estimated heat flux for graphite bipolar plates.

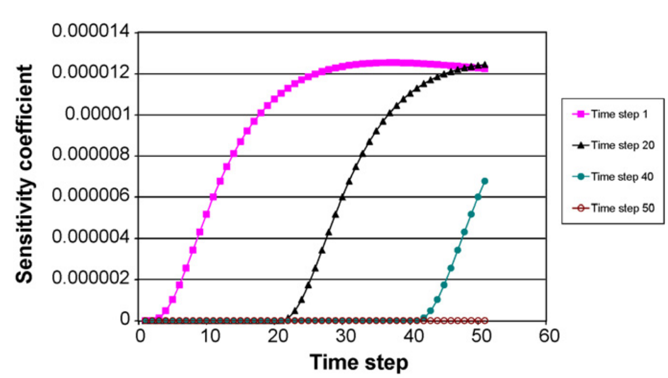

Fig. 7. Sensitivity coefficients: 50 time steps of 1 s, steel plate.

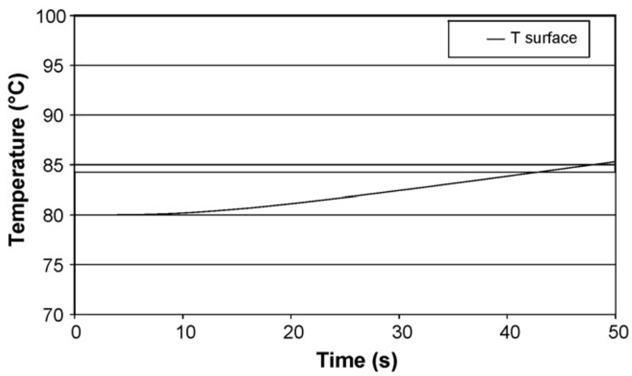

Fig. 8. Surface temperature (simulated measurements) for steel bipolar plates.

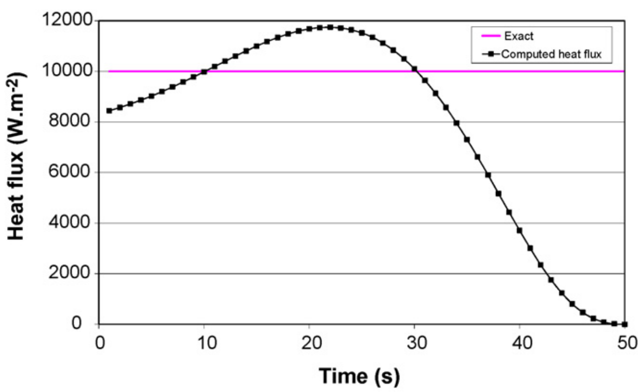

Fig. 9. Exact and estimated heat flux for steel bipolar plates.

values with a 50-s measurement duration and a 30-s response time.

4.3. Numerical test case 2: stainless steel bipolar plates

In this paragraph, the bipolar plates are now supposed to be made of stainless steel. The steel characteristics are presented in Table 1. As the thermal conductivity of steel is much higher, an improvement in the response time of the temperature estimation is expected.

4.3.1. Sensitivity analysis

Fig. 7 presents the sensitivity coefficients for steel plates. The coefficients are higher than those for graphite plates. Only the coefficient of the 40th time step is strongly smaller.

4.3.2. Inverse problem solution

The internal heat flux and temperature are estimated from surface simulated measurements. The exact heat flux is 1e4 W m^{-2} as in the preceding test case. As the thermophysical properties of steel and graphite are different, temperature evolution in the two cases differs. Globally, the increase in temperature for steel plates is less important, but the heat transfer is quicker. Fig. 8 presents the simulated surface temperature of the bipolar plate. The estimated heat flux and temperature are plotted in Figs. 9 and 10.

As expected, a clear improvement in heat flux and temperature estimation is observed. For a 50-s measurement, the heat flux estimation is accurate for 70% of the measurement interval. The internal temperature is computed with an accuracy better than 5% for 48 s. Before 35 s, the accuracy of the temperature estimation is even better (2%). This result is in accordance with the sensitivity analysis. Heat transfer in the steel is fast enough to produce a significant surface temperature elevation in about 15 s. Therefore, the algorithm has sufficient data to produce accurate results. An accurate estimation of internal temperature can be carried out with a 2% accuracy and a 15-s response time.

So, the proposed method enables us to estimate internal temperature with a predicted accuracy and response time. The performance of the method is linked to the thermophysical properties of the material, so it is particularly appropriate for fuel cells made of steel bipolar plates.

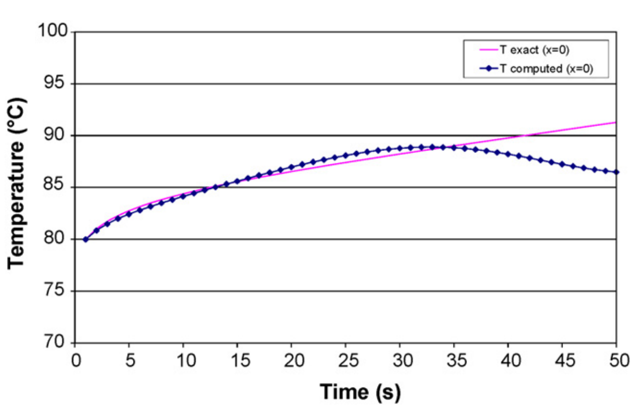

Fig. 10. Exact and estimated internal temperature for stainless steel bipolar plates.

5. Conclusion

In this paper, a method to estimate internal fuel cell internal temperature from surface measurements is presented. The aim is to monitor fuel cells to prevent damages due to internal overheating. The measurements are taken on the side of the bipolar plate, and the heat flux and the temperature at the border of the active zone are estimated. The method is based on sensitivity analysis and inverse problem algorithms. Numerical results show that internal temperature can be correctly estimated. The response time of the method is limited by the heat transfer rate in the material. Therefore, the method is particularly appropriate to fuel cells made of steel bipolar plates.

References

[1] O.M. Alifanov, E.A. Artyukhin, S.V. Rumyantsev, Extreme Methods for Solving Ill-posed Problems with Applications to Inverse Heat Transfer Problems, Begell House, 1995.

[2] O.M. Alifanov, Inverse Heat Transfer Problems, Springer-Verlag, 1994.
[3] M.N. Ozisik, H.R.B. Orlande, Inverse Heat Transfer, Fundamentals and Applications, Taylor and Francis, 2000.
[4] J.V. Beck, B. Blackwell, C.R.St. Clair, Inverse Heat Conduction, Wiley, 1985.
[5] M.-H. Chang, C.-H. Cheng, J. Power Sources 142 (2005) 200–210.
[6] C.-H. Cheng, M.-H. Chang, J. Power Sources 139 (2005) 115–125.
[7] M.N. Ozisik, Heat Conduction, Wiley, 1993.
[8] D.R. Croft, D.G. Lilley, Heat Transfer Calculations using Finite Differences Equations, Applied Science Publishers, 1977.
[9] P.E. Gill, W. Murray, M.H Wright, Practical Optimization, Academic Press, New York, 1981.