

Receding horizon experiment design with application in SOFC parameter estimation^{*}

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Abstract: In this work the problem of optimal input design (OID) in a receding-horizon framework for online parameter estimation is solved. The designed optimum input is used for dynamic experiment and subsequent estimation of parameters. A fuel cell experiment design and parameter estimation problem is investigated through the proposed approach. Some of the issues related to the application of the proposed method are examined and guidelines for selecting appropriate experimental settings are provided.

Keywords: Identifiability, estimability, fuel cell, sensitivity, experiment design

1. INTRODUCTION

Optimal input design (OID) is an important part of the identification literature which seeks to address the issue of parameter estimation among model developers. The main focus of this work is to solve the receding horizon optimal input design method for parameter estimation and apply the method to solve a fuel cell experiment design and parameter estimation problem. A typical experiment design problem often involves minimizing or maximizing some a priori chosen norm of the Fisher information matrix (FIM) (Bates and Watts, 1988). The information matrix is a function of inputs and a carefully designed experiment is critical for obtaining good parameter estimates. Stigter et al. (2006) investigated the OID problem in tandem with a recursive parameter update scheme by minimizing the minimum eigenvalue of the FIM (E-optimum), which they called adaptive optimal input design and adaptive receding horizon optimal control problem for parameter estimation.

In this paper, we develop a receding horizon experiment design and parameter estimation approach with the following features: (1) A state estimation approach for parameter estimation is used in tandem with the receding-horizon experiment design, which is a natural extension of model predictive control (MPC). The state estimation used here is similar to that used in MPC while the experiment design is similar to the calculation of MPC control moves. (2) The D-optimal design which maximizes the determinant of the FIM is solved in tandem with parameter estimation. (3) To resolve a heavy computation issue encountered in the previous work, a prediction horizon is introduced, in analogy to model predictive control, so that the optimization horizon need not extend to the final point of the experiment. The effect of applying different prediction and control horizons is analyzed via studying the variance of obtained estimates. (4) The proposed method is used to

investigate an outstanding fuel cell parameter estimation and experiment design problem.

A fuel cell is an energy device that produces electrical energy from the electrochemical reaction that occurs at its electrode-electrolyte interface. Fuel cells are a promising source of electrical energy that can be used to supplement traditional energy sources in distributed energy systems. For the development of such systems it is imperative to understand and predict the behavior of fuel cells under various operating conditions. A number of mathematical models have been developed to this end. All of the models contain some parameters that are either unknown or must be estimated.

Through a solid oxide fuel cell (SOFC) model, we demonstrate feasibility of the proposed receding horizon experiment design and parameter estimation approach. We verify that the critical parameters of the SOFC can be estimated effectively through the proposed approach and this can be achieved when the true parameters are compared with the estimated ones. A number of static and dynamic SOFC models have been proposed in the literature. The model used in this work is described in (Qi *et al.*, 2005). This dynamic nonlinear model provides a detailed description of the diffusion process of different species and that of the inherent impedance in a single cell. The parameters of interest are the diffusion coefficients of the reacting species and the impedance elements, namely, charge transfer capacitance and resistance. While the model is continuous, the outputs are sampled at discrete instants in time. The estimation of parameters is carried out using a continuous-discrete extended Kalman filter.

The remainder of the paper is organized as follows. Section 2 describes the receding horizon experiment design and parameter estimation approach. Section 3 describes the fuel cell model used in this work. Section 4 discusses the simulation results, followed by conclusions in Section 5.

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2. RECEDING HORIZON EXPERIMENT DESIGN

Consider the model of a system having p parameters and n states.

$$\dot{x}(t) = f(x(t), u(t), t, \theta) \quad (1)$$

$$y(t) = g(x(t), u(t), t, \theta) \quad (2)$$

where $x(t) \in \mathbb{R}^m$ are the states and $\theta \in \mathbb{R}^p$ are the parameters. The objective of this work is to estimate the parameters in the system using a 'designed' input. The advantage of using a 'designed' input over a 'naive' random binary sequence in parameter estimation is highlighted in the work by Stigter et al. (2006). An adaptive 'designed' input increases the information content of the parameters in the output signal and hence increases the ability to estimate the parameters.

The goal of this section is to develop a method for selecting an input trajectory that will maximize the ability to estimate the parameters. The sensitivity matrix based on derivative of dynamic response trajectory with respect to parameters has been given in Yao et al. (2003). With the previous estimate of parameter and state values, the values of the entries in the sensitivity matrix, called the sensitivity coefficients, will be predicted analytically n sampling steps ahead in time. An optimum input is selected which is the solution to

$$\arg \max_u \det(Z^T Z) \quad (3)$$

subject to

$$u_L < u < u_U \quad (4)$$

where u_L and u_U are the lower and upper bounds on the input. Z , the sensitivity matrix and for n steps ahead prediction it will include n rows corresponding to prediction of sensitivity function over n steps, and p columns corresponding to p parameters. The sensitivity coefficients, $(\frac{\partial y}{\partial \theta})$, can be derived from the model equations in a straightforward way. Predicting the values n step ahead in time will constitute the prediction horizon.

The optimal input trajectory can constitute any number of moves less than or equal to n . A control move is defined as changing the input from one level to another for the dynamic experiment. Let the number of control moves be denoted by c , with $c \leq n$. Control moves are made at the same discrete instants in time as the sensitivities are predicted, i.e., t_1, t_2, \dots, t_n . For $c < n$, the control moves are designed from the current instant until the time instant t_c ; from the time instant t_c to t_n , there are no more control moves, i.e., the input is held at the same level as that at the time instant t_c . The control move between two consecutive time instants can be parameterized as a piecewise constant, a sine wave or any other suitable function. The approach is similar to a receding horizon approach for control design as shown in Figure 1. The sensitivity value denoted by $s(t)$ in Figure 1 is predicted n steps ahead and an optimum input trajectory is chosen. The input trajectory is applied till the end of a window of n steps, when new estimates become available. The new input trajectory is then calculated and the sequence is repeated.

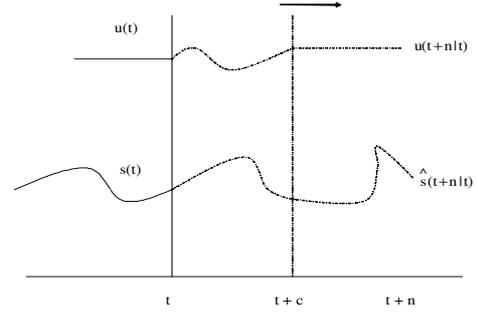


Fig. 1. Illustration of the Proposed Approach

To summarize, an optimum input trajectory consisting of c moves is selected which maximizes the objective function for the immediate n steps ahead in future.

For online estimation of parameters, the optimal input trajectory chosen is used in conjunction with extended Kalman filter. It is assumed that output measurements are available at the same instants as before, i.e., t_1, t_2, \dots, t_n . Once the first point of the optimal input trajectory has been applied, the parameter estimation algorithm will be used to update the estimates of parameters based on output measurements. The update continues for every sampling instant within the window of n prediction steps. Based on the most updated parameters at the end of n steps, the optimization is repeated for the subsequent window.

The EKF algorithm is a widely used method for estimating states and parameters from a nonlinear system. In this work, it is assumed that measurements from the system are available at discrete instants in time. Therefore a continuous-discrete formulation of the EKF is used for estimation. The detailed algorithm can be found in (Crassidis and Junkins, 2004).

With such a setup, it is important to realize how the choices of n and c would affect the experiment design. The value of n affects how frequent the optimization is carried out during the course of the entire experiment. Having too small a value of n increases the frequency to carry out the optimization of input design and hence increases the computational load. Recalling that the control moves for the next n steps within the prediction horizon is based on the parameter estimates available at the first point of the current prediction horizon, having a too large n might result in poor control moves due to possibly poor available values of the parameters at the beginning of the current horizon. The choice of c determines how many moves can be made within the entire prediction horizon. If c is too small then convergence of the estimates to true values might take longer time than having a larger value of c due to possibly poorer excitation of the signal. If a plant operator has to apply the control moves manually or physical constraints allow only certain number of moves possible within the period of time the prediction window operates, then having a smaller c may be necessary. A larger value of c increases the complexity of the optimization problem and hence increases the computational load.

To test the receding horizon approach, Monte-Carlo simulations were conducted to investigate the variance property of the parameter estimation using the proposed method.

To illustrate the algorithm, the proposed approach is first applied to a simple circuit system whose dynamics is given by

$$\dot{x}(t) = \frac{-x(t)}{\theta_1 \times \theta_2} + \frac{u(t)}{\theta_2} \quad (5)$$

$$y(t) = x(t) \quad (6)$$

where the input term u in the model is the current i . The two parameters of interest are θ_1 and θ_2 . The estimates of the parameters are obtained from different experimental designs and compared below. The true values of parameters θ_1 and θ_2 are 1.2 and 1.5×10^{-3} respectively.

In the simulation, we assume there are both state and measurement noises. With a chosen value of n and c , the estimation is carried out sixty times with different noise seed in each run. These same noise elements are stored and used with other experiments having a different value of n and c . This allows comparison of two different tuning parameters n and c with the same noises. The initial guesses of the two parameters to be used in each of the sixty runs is drawn from a normal distribution with a suitable standard deviation. To compare the performance of two experiments having different values of n and c , the standard deviation of the sixty runs carried out for each setting of n and c are calculated. Since the objective function is to maximise the determinant of the FIM, the experiment that gives a better optimal solution will give a parameter estimate with less variance.

effect of c With a value of $n = 4$, different possible values of c are selected for estimation. For a given prediction horizon, an experiment with a higher value of c should be able to find a better optimum solution and thus should result in a better optimum input trajectory. Figure 2 shows the standard deviation of the sixty runs from each experiment. The initial standard deviation at sample point 0 should be equal to the standard deviation of the normal distribution from which the initial guesses were drawn. As the sample points increase, the estimates start to converge to the true value and each of the sixty runs form a tighter bundle. Hence the standard deviation lines shown in the Figure 2 gradually decrease. As expected, the experiment with $c = 4$ gives the lowest standard deviation (illustrated in θ_2 estimate). Figure 3 shows the value of the optimal objective function at each window. This confirms that the experiment with $c = 4$ gives a better optimal solution, i.e., higher determinant value of the FIM.

effect of n In this set of experiments, the value of n is varied and the effect of changing the window size on the estimation is analysed. Figure 4 compares the standard deviation lines obtained from experiments with $n = 2, 3$ and 4 similar to the previous case. In each case the value of c is maintained equal to the value of n . Under this condition having a larger window, n , helps in reducing the effect of noise on the estimation and a better estimate with less variance is obtained.

To summarize, the following points may be considered for selecting an appropriate experiment

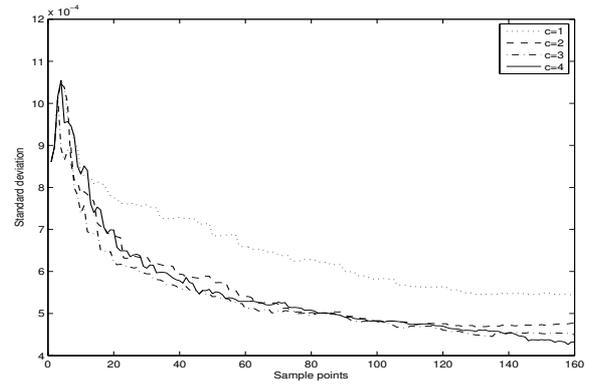


Fig. 2. Standard deviation for $n = 4$

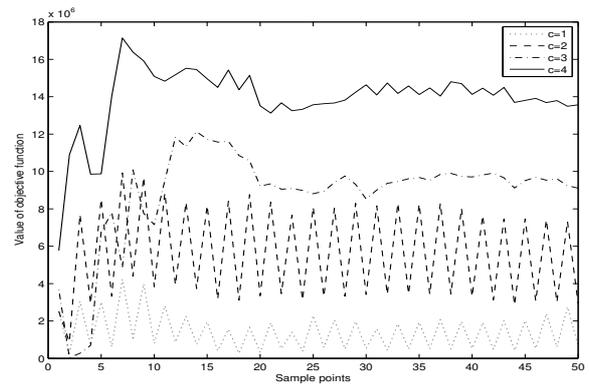


Fig. 3. Optimal objective function for $n = 4$

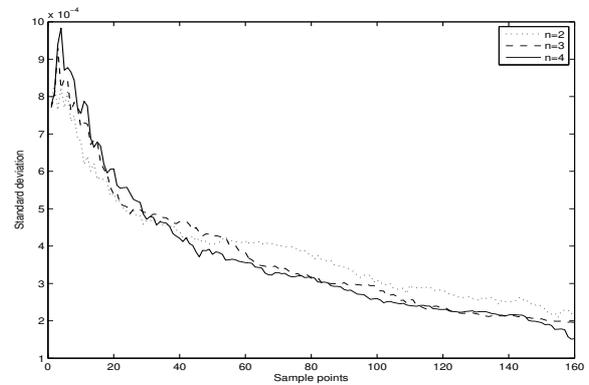


Fig. 4. Standard deviation for $c = n$

- (1) The upper bound of n is limited by the computational power and the complexity of a particular problem.
- (2) Having chosen n , the appropriate choice of c can be made from the following considerations. For example, if the duration of experiment is a fixed quantity, then it can be considered if increasing c improves the estimate in terms of rate of convergence, bias and standard deviation. It has been observed that the ratio c/n has an effect on variance of the estimates. A higher ratio helps reducing the variance of the estimates. A lower ratio helps in reducing the complexity of the optimisation problem.
- (3) Finally, the relative importance of different parameters in a system can be considered and an experiment suitable for estimating them can be chosen by suitably weighting the objective function $Z^T Z$.

Comparison of the EKF filter with prediction error approach One of the important components of the receding horizon estimation method is that a filter has to be employed as a predictor. So far EKF has been used as the filter in this work. Another approach to parameter estimation is the class of recursive parameter estimation algorithms called as the recursive prediction error method. This method of parameter estimation is based on adjusting the parameter estimates which minimise a cost functional of the prediction errors. To perform the minimisation, the gradient of the cost functional and consequently the gradient of the prediction errors are required. In this work, the gradients of the required quantities are obtained from a sensitivity model of the EKF equations based on the approach of (Bohn and Unbehauen, 2001). The features of using a sensitivity model of the EKF as a predictor/estimator are

- (1) It involves inherently the propagation of the model sensitivity equations which are used in the OID step in the proposed approach.
- (2) Since the optimal input for the next horizon is based on current estimates, once the parameter estimates are updated, it is logical to expect the predicted sensitivities to also be updated. The sensitivity model of the EKF derived in (Bohn and Unbehauen, 2001) accounts for this as well.

To compare the performance of the EKF filter against prediction error method (the sensitivity based filter), simulations were conducted with the prediction error method. Figure 5 compares the standard deviation curves obtained from simulations with $n = 4$. The curves are close to each other except for the case with $c = 1$. Note that the prediction error based method involve much more complicated procedure to derive the nonlinear predictor as demonstrated in (Bohn and Unbehauen, 2001).

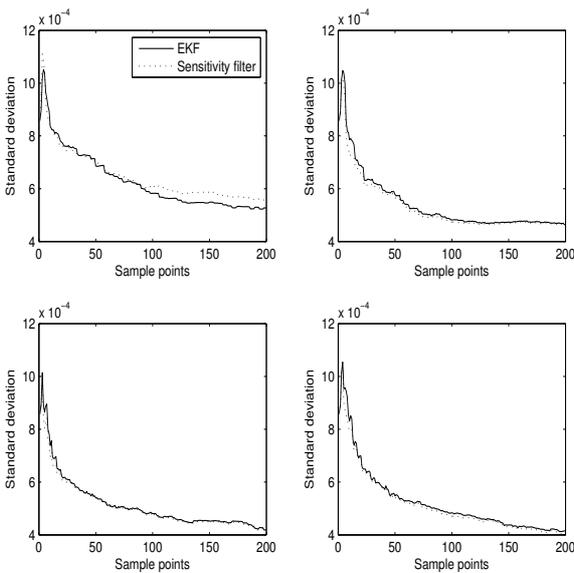


Fig. 5. Standard deviation comparison for $n = 4$ with $c = 1, 2, 3, 4$

3. A FUEL CELL EXPERIMENT DESIGN AND PARAMETER ESTIMATION PROBLEM

3.1 Solid Oxide Fuel Cell (SOFC) Model

A continuous time ODE model of the fuel cell (Qi *et al.*, 2005) is used to demonstrate the proposed receding horizon experiment design approach. The model equations are derived based on electrical energy and mass balances of the various reacting gases inside the cell. The definition of states, inputs, outputs and parameters are shown in Tables 1, 2, 3 and 4 respectively, where tpb refers to triple phase boundary in fuel cells.

Table 1. Inputs

Inputs	Description
u_1	External load
u_2	Bulk pressure of hydrogen
u_3	Bulk pressure of oxygen
u_4	Bulk pressure of water

Table 2. Outputs

Outputs	Description
y_1	External Voltage V_{out}
y_2	Current
y_3	Consumption rate of hydrogen
y_4	Consumption rate of oxygen
y_5	Production rate of water

Table 3. States

State	Description
x_1	Voltage V_{ct}
x_2	Consumption rate of hydrogen
x_3	Derivative of consumption rate of hydrogen
x_4	Intermediate variable
x_5	Consumption rate of oxygen
x_6	Derivative of consumption rate of oxygen
x_7	Intermediate variable
x_8	Production rate of water
x_9	Derivative of production rate of water
x_{10}	Intermediate variable
x_{11}	Concentration of hydrogen at tpb
x_{12}	Derivative of concentration of hydrogen at tpb
x_{13}	Concentration of oxygen at tpb
x_{14}	Derivative of concentration of oxygen at tpb
x_{15}	Concentration of water at tpb
x_{16}	Derivative of concentration of water at tpb
x_{17}	Intermediate variable

The overall model can be partitioned into subsystems describing the diffusion of hydrogen, oxygen and water species as shown below.

Hydrogen Diffusion The equations describing hydrogen diffusion are

Table 4. Parameters

Parameter	Description	Numerical value used in simulations
R_{ct}	Charge transfer resistance	0.9
C_{ct}	Charge transfer capacitance	300×10^{-6}
h_1, h_2, h_3, h_4	Functions only of diffusion coefficient of hydrogen D_{h_2}	1.041×10^{-4}
o_1, o_2, o_3, o_4	Functions only of diffusion coefficient of oxygen D_{o_2}	2.451×10^{-5}
w_1, w_2, w_3, w_4	Functions only of diffusion coefficient of water D_{h_2o}	1.041×10^{-4}

$$\dot{x}_2 = x_3 \tag{7}$$

$$\dot{x}_3 = -h_1 x_2 - h_2 x_3 + h_1 \frac{i}{2F} + \tag{8}$$

$$h_3 \frac{A}{RT} (K u_2 - x_4) \tag{9}$$

$$\dot{x}_4 = K^2 u_2 - K x_4 \tag{9}$$

$$y_3 = x_2 \tag{10}$$

where the substitution $i = \frac{x_1}{u_1 + R_o}$ has been made and the current i is treated as an input.

Oxygen Diffusion The above procedure adopted for oxygen diffusion gives the following equations.

$$\dot{x}_5 = x_6 \tag{11}$$

$$\dot{x}_6 = -o_1 x_5 - o_2 x_6 + o_1 \frac{i}{4F} + \tag{12}$$

$$o_3 \frac{A}{RT} (K u_3 - x_7) \tag{13}$$

$$\dot{x}_7 = K^2 u_3 - K x_7 \tag{13}$$

$$y_4 = x_5 \tag{14}$$

Water Diffusion Similarly for the diffusion of water species we have,

$$\dot{x}_8 = x_9 \tag{15}$$

$$\dot{x}_9 = -w_1 x_8 - w_2 x_9 + w_1 \frac{-i}{2F} + \tag{16}$$

$$w_3 \frac{A}{RT} (K u_4 - x_{10}) \tag{17}$$

$$\dot{x}_{10} = K^2 u_4 - K x_{10} \tag{17}$$

$$y_5 = x_8 \tag{18}$$

The fourth subsystem describes the voltage dynamics and is given by the remaining equations,

$$\dot{x}_1 = \frac{E}{R_{ct} C_{ct}} - \frac{x_1}{R_{ct} C_{ct}} - \frac{x_1}{C_{ct}(u_1 + R_o)} \tag{19}$$

$$\dot{x}_{11} = x_{12} \tag{20}$$

$$\dot{x}_{12} = -h_1 x_{11} - h_2 x_{12} - h_4 \frac{RT}{A} \frac{x_1}{2F(u_1 + R_o)} \tag{21}$$

$$- \frac{RT}{A} \frac{4}{l_a} \frac{1}{2F} \left(\frac{\dot{x}_1}{u_1 + R_o} - \frac{x_1}{(u_1 + R_o)^2} (K u_1 - x_{17}) \right) + h_1 u_2 \tag{22}$$

$$\dot{x}_{13} = x_{14} \tag{22}$$

$$\dot{x}_{14} = -o_1 x_{13} - o_2 x_{14} - o_4 \frac{RT}{A} \frac{x_1}{4F(u_1 + R_o)} \tag{23}$$

$$- \frac{RT}{A} \frac{4}{l_c} \frac{1}{4F} \left(\frac{\dot{x}_1}{u_1 + R_o} - \frac{x_1}{(u_1 + R_o)^2} (K u_1 - x_{17}) \right) + o_1 u_3 \tag{24}$$

$$\dot{x}_{15} = x_{16} \tag{24}$$

$$\dot{x}_{16} = -w_1 x_{15} - w_2 x_{16} - w_4 \frac{RT}{A} \frac{-x_1}{2F(u_1 + R_o)} \tag{25}$$

$$+ \frac{RT}{A} \frac{4}{l_a} \frac{1}{2F} \left(\frac{\dot{x}_1}{u_1 + R_o} - \frac{x_1}{(u_1 + R_o)^2} (K u_1 - x_{17}) \right) + w_1 u_4 \tag{26}$$

$$\dot{x}_{17} = K^2 u_1 - K x_{17} \tag{26}$$

The objective of this work is to design optimal inputs to estimate the parameters associated with each of the subsystems, taking one subsystem at a time. Table 5 lists the parameters and outputs involved in each of the subsystems. Note that the model assumes the diffusion coefficient of hydrogen to be equal in magnitude to the diffusion coefficient of water. Therefore the water diffusion subsystem has not been listed. It has been shown that all parameters are estimable by manipulating external load input u_1 (Jayasankar *et al.*, 2008). The input u_1 is the external load on the fuel cell.

4. SIMULATION OF RECEDING HORIZON EXPERIMENT DESIGN AND PARAMETER ESTIMATION FOR THE FUEL CELL MODEL

4.1 Subsystem 1

Parameter estimation of fuel cells particularly SOFC has been considered as a difficult task, and almost all existing methods are based on electrochemical impedance spectroscopy (EIS) method (Barbucci *et al.*, 2002). In this section, we will demonstrate that it is possible to effectively estimate critical parameters of SOFC through direct time-domain experiment and estimation methods. The input function used, the parameters to be estimated and the output observed for estimation of this subsystem are given in Table 5 in the row corresponding to impedance dynamics. Using the method developed above, the parameter estimates are determined in the presence of both observation and state noises. The following section presents the results obtained for an experiment design with $n = 2$.

Experiment design with $n = 2$ The choice of $n = 2$ was made for this simulation.

Table 5. Subsystems

Subsystem	Parameter(s)	Output	Input	Bounds
Impedance	C_{ct} and R_{ct}	y_1	$u_1 = a$	$1 < a < 4$
H_2 diffusion	D_{h_2}	y_3	$u_1 = a$	$1 < a < 4$
O_2 diffusion	D_{o_2}	y_4	$u_1 = a$	$1 < a < 4$

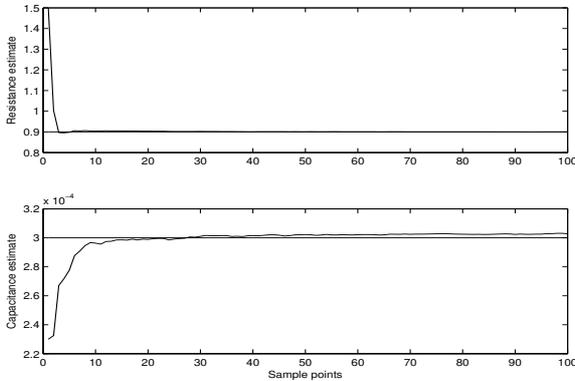


Fig. 6. Resistance and Capacitance estimates

Two different setups are possible in this case, i.e. with $c = 1$ and 2 . However a value of $c = 2$ was chosen as it has been shown that a higher value of c for a given n gives a better estimate with less variance. With observation noise, the estimates for parameters R_{ct} and C_{ct} are shown in Figure 6. The curves represent the mean of fifty runs and the standard deviation for the estimate of R_{ct} converges to 6.8×10^{-4} and for the estimate of C_{ct} converges to 3.7×10^{-6} . The true values of the parameters used in the simulation are $R_{ct} = 0.9$ and $C_{ct} = 300 \times 10^{-6}$. It can be seen that parameter convergence is arrived within about 10 seconds.

4.2 Subsystem 2 and Subsystem 3

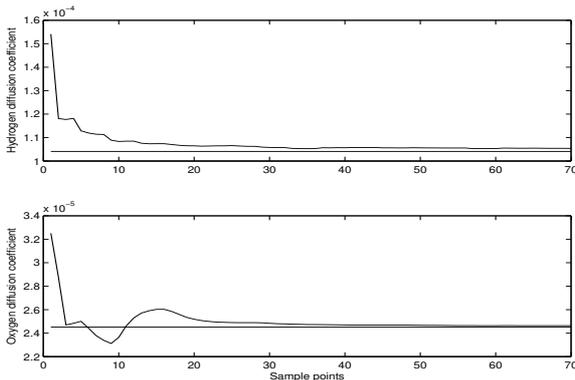


Fig. 7. Hydrogen diffusion coefficient and Oxygen diffusion coefficient estimates

The input function used, the parameters to be estimated and the output observed for estimation for these subsystems are given in Table 5 in the rows corresponding to Hydrogen diffusion and Oxygen diffusion. Since the subsystem consists of one output and one parameter, the sensitivity matrix Z reduces to a scalar value for $n = 1$ and the optimum input is the one which maximizes the scalar sensitivity value. For $n > 1$, Z is a column vector and the

optimum input is based on the objective function defined in Equation 27. The mean estimates for the Hydrogen and Oxygen diffusion coefficients obtained with $n = 2, c = 2$ based on Monte-carlo simulations are shown in figure 7 and the standard deviation for the estimate of D_{h_2} converges to 0.02×10^{-4} and for the estimate of D_{o_2} converges to 1.03×10^{-8} . The true values of the parameters used in the simulation are $D_{h_2} = 1.041 \times 10^{-4} \text{ m}^2\text{s}^{-1}$ and $D_{o_2} = 2.451 \times 10^{-5} \text{ m}^2\text{s}^{-1}$. Parameter convergence is arrived within about 30 seconds.

$$\arg \max_u \sum_{j=1}^n (Z(j)^2) \quad (27)$$

5. CONCLUSIONS

A method for on-line receding-horizon experiment design and estimation of parameters for dynamic systems was developed. It was based on designing experiments by choosing a specific input trajectory which maximised the sensitivity of the parameters. More specifically the design of experiments was based on maximising the determinant of $Z^T Z$, where the matrix Z is the sensitivity matrix of the outputs with respect to parameters. Such a design allows for the effect of parameters on outputs to be more pronounced which in turn helps in estimating the parameters. Several practical issues regarding the choice of experimental settings were raised and a guideline was provided to help choosing them. The proposed method is demonstrated through a simulation on SOFC experiment design and parameter estimation.

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