STATE ESTIMATION OF SOFC/GT HYBRID SYSTEM USING UKF

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Abstract: A description of a Solid Oxide Fuel Cell (SOFC) combined Gas Turbine (GT) hybrid system is given. Modeling of all the components of the hybrid system is briefly presented. A decentralized control structure using PI controllers is designed and is considered as a part of the system. An Unscented Kalman Filter (UKF) is applied to estimate the state vector and the simulation results are presented.

Keywords: Fuel cell, Gas turbine, Unscented Kalman Filter

1. INTRODUCTION

In the foreseeable future, fossil fuels including natural gas will be a major source of energy. With today's increasing concern about global warming and climate change, there is an incentive to investigate natural gas power processes that operate efficiently, thus emitting less per kWh produced, and also power production processes with CO_2 capture capabilities. It is widely accepted that fuel cells are power sources that will become increasingly important, due to high efficiency, low levels of pollution and noise, and high reliability. One of the most promising fuel cell technologies is the Solid Oxide Fuel Cell (SOFC), due to its solid state design and internal reforming of gaseous fuels, in addition to its high efficiency. The SOFC converts the chemical energy of fuel directly to electrical energy. Since SOFCs operate at high temperatures (about 1000^0 C), natural gas can be used directly as fuel. The electrical efficiency of a SOFC can reach 55%. Another significant advantage of the SOFC is that since it operates at high temperature, its efficiency increases when pressurized, and it naturally lends itself as a heat source for a gas turbine (GT) cycle. The combined (hybrid) cycle can theoretically have an overall electrical efficiency of up to 70% with a power range from a few hundred kWs to a few MWs. The main applications of the hybrid system include remote area power supply and distributed power generation.

The hybrid system consists of tightly integrated dynamic subsystems with strict operating criteria making the control design more challenging in terms of disturbance rejection, part load operation and in particular start-up, shut down and load shedding. Suitable system actuation must be chosen, good control structures must be devised, and good controllers must be designed. As a basis for all these tasks, control relevant models must be developed for the subsystems, as well as for the total system. Such models should have limited complexity to allow for the necessary analysis, and at the same time should include the important dynamic interactions. In (Kandepu, *et al.,* 2006a), a control relevant model of the hybrid system integrated in an autonomous power system has been developed. Further, control design with PI controllers is proposed, which gives satisfactory results in terms of tracking. It is also concluded that there is a scope to improve the system efficiency by using an advanced control design, for example, Model Predictive Control (MPC).

State estimation plays an important role in developing the MPC and monitoring technologies. The hybrid system is highly nonlinear and it has to be operated under different load conditions, which makes it necessary to design a nonlinear estimator.

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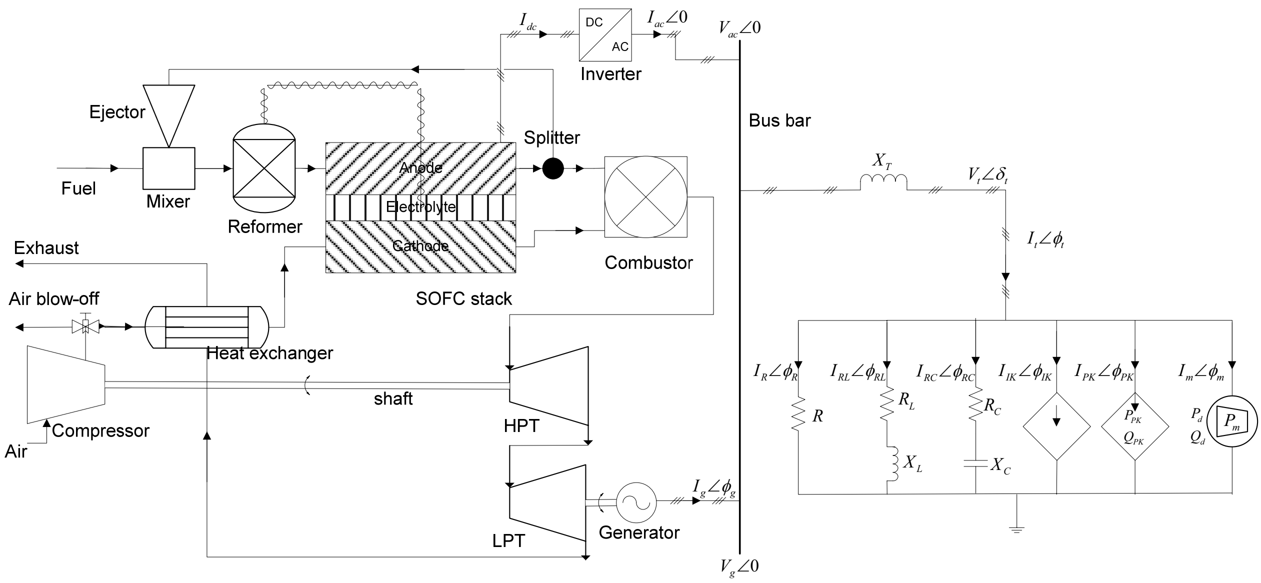

Fig. 1. SOFC/GT hybrid system integrated in an autonomous power system

Extended Kalman Filter (EKF) is the most widely used estimation algorithm for nonlinear systems. There are some difficulties in applying the EKF such as difficult to implement, difficult to tune, and only reliable for systems that are almost linear on the time scale of updates (Julier and Uhlmann, 2004). Furthermore, it is accurate up to the first order in estimating mean and covariance for a nonlinear probability distribution (pdf) and Jacobian computation is necessary. (Julier and Uhlmann, 2004) developed Unscented Kalman Filter (UKF) as a novel extension of Kalman Filter. The UKF is based on the principle that propagation of a pdf through a nonlinear transformation is approximated by the propagation of a group of representative samples through the nonlinear transformation (van der Merwe, 2004; Huang and Wang, 2006). In EKF, the pdf propagation is approximated by a linear transformation obtained by the linearization of the nonlinear transformation at the present state. Compared to the EKF, the UKF approximates the pdf propagation for a nonlinear system in an efficient way, thus making the UKF estimation accurate up to the second order in estimating the mean and covariance. Furthermore, the computation of the Jacobian is not needed in implementing the UKF. This motivates us to apply the UKF for the state estimation of the hybrid system.

The paper is organized as follows: The SOFC/GT hybrid system is described at the system level. A brief description of modeling of all the components of the system is presented. The developed control structure with PI controllers and the need for MPC are presented. A brief description of UKF principle is explained and simulation results of state estimation are presented.

2. PROCESS DESCRIPTION

A schematic diagram of the integrated system where the hybrid system is connected to the load by a bus bar is shown in Figure 1. Methane (fuel) is mixed with a part of anode flue gas and is partially steam reformed in pre-reformer generating hydrogen. The heat required for endothermic reformation reactions in the pre-reformer is supplied from the SOFC stack through radiation. The gas mixture from the pre-reformer is fed to the anode volume of the SOFC, where the remaining part of the methane is reformed. Compressed atmospheric air is heated in a recuperative heat exchanger and is used as an oxygen source at the cathode side of the SOFC. In the SOFC, electrochemical reactions take place and DC voltage is produced. The rate of the electrochemical reactions depends on the current. A part of the anode flue gas is recycled to supply steam to the pre-reformer. The remaining part of the anode and cathode flue gases is supplied to a combustion chamber where the unused fuel is combusted. The hybrid system considered here uses a double shaft GT configuration. The combusted gas mixture is expanded in a high pressure turbine (HPT) with variable shaft speed driving the compressor. The HPT flue gas is further expanded to atmospheric pressure in a low pressure turbine (LPT) with constant shaft speed, which is coupled to a synchronous generator producing AC electric power. The expanded gas mixture is used to heat up the compressed air in a heat exchanger. The DC power from the SOFC stack is fed to an inverter which converts DC to AC with a fixed frequency. The inverter and the generator are connected to a local grid, which is connected to a six branch electric load. Both the SOFC stack and the generator supply the electric load demand on the grid. The load sharing between the SOFC stack and the generator cannot be controlled when there is a load change on the grid. Typically 60-70% of the total power is supplied by the SOFC stack.

3. MODELING

All the models of the system are developed in the modular modeling environment gPROMS (gPROMS, 2004). The detailed modeling of each component of the system can be found in (Kandepu, *et al., 2006a*; Kandepu, *et al.*, 2006b). A brief description of the each model is presented below.

3.1 SOFC stack

It is assumed that all the SOFCs in the stack operate at identical conditions along the fuel flow direction. A zero-dimensional SOFC model is developed with no regard to the geometry of the cell. The model developed is a lumped one, which includes dynamic molar balances of all the species both in anode and cathode volumes separately. It includes an energy balance treating the whole SOFC as a single volume to model the temperature dynamics of the SOFC solid phase mean temperature. There is a radiation from the SOFC to the pre-reformer. The voltage developed across the cell is modeled using Nernst equation, the operating cell voltage is calculated by considering both ohmic and activation losses.

In (Kandepu, *et al* 2005), the low complexity, control relevant SOFC model is evaluated against a detailed model developed in (Stiller, *et al.*, 2005a). The comparisons indicate that the low complexity model is sufficient to approximate the important dynamics of the SOFC and can hence be used for operability and control studies.

3.2 Pre-reformer

The pre-reformer is modeled as a Continuously Stirred Tank Reactor (CSTR). Mass balances of all the species are included dynamically and energy balance is implemented to model the pre-reformer temperature dynamics. The steam required for the steam-reforming is provided by the recycle flow of the anode flue gas. The heat required for the endothermic reforming reaction is obtained by the radiation heat from the SOFC stack.

3.3 Combustor

In the combustor, the unused fuel is burnt in presence of oxygen coming from the cathode outlet. The operating conditions will always be such that there is excess oxygen available for complete combustion due to the fact that air mass flow rate is much larger than the fuel mass flow rate. In the combustor, the fuel can be methane, hydrogen or carbon monoxide or a mixture of these fuels. As the combustion process is rapid it is modeled as a steady-state process.

3.4 Heat exchanger

A simple model of a counter-flow heat exchanger is used, in which the amount of the heat exchanged depends on the heat transfer coefficient of the exchanger wall and also on the average temperature difference between the hot and cold streams. A first order transfer function describes the dynamics of the temperatures of both the streams.

3.5 Gas turbine cycle

The compressor and turbine models are based on steady state performance map characteristics (Stiller, *et al.*, 2005b). The map is modeled using polynomials of 4th and 5th order for reduced mass flow, pressure and efficiency as functions of reduced shaft speed and operation line. A shaft model accounts for the dynamics of the rotating mass in the gas turbine system.

3.6 Electrical components

A simple model of the inverter is used to convert DC electric power from the SOFC stack to AC, which is given to an autonomous grid. The grid side voltage is maintained constant at 230V by using the inverter controllers and the dynamics of these controllers are neglected. An AC-AC frequency converter with 95% efficiency is assumed to be connected to the alternator to convert the varying frequency of the alternator to the grid frequency. The operating voltage of the alternator is controlled to the grid voltage by controlling the field current in the alternator. The electric load connected to the gird is represented by six parallel branches with different components in each branch. It is categorized into 4 types of loads: constant impedance, constant current, constant power and induction motor load. The constant impedance, constant current and constant power load represent the residential loads such as lights, water heaters, ovens etc. The induction motor load is considered to represent an industrial load. The constant impedance load is represented by the first three branches with resistive, inductive and capacitive loads. The fourth and fifth branches represent the constant current and constant power loads respectively. The sixth branch represents the induction motor load. The total load current is the sum of the currents from the inverter and the alternator.

4. REGULATORY CONTROLLER

Local regulatory control has been considered for the system, and the local control adds additional state to the system. Thus, to design state estimation of the complete system, the local control strategy has to be understood.

A control system is designed for the hybrid system to reject the disturbances; disturbances can be load changes, changes in fuel and air temperatures and pressures, fuel composition etc. Also during the disturbances, the SOFC temperature should also be controlled; otherwise it may lead to a cell break down. A decentralized control scheme with two PI controllers is proposed in [Kandepu, *et al.,* 2006a] to reject the disturbances and to control the SOFC temperature as shown in Figure 2.

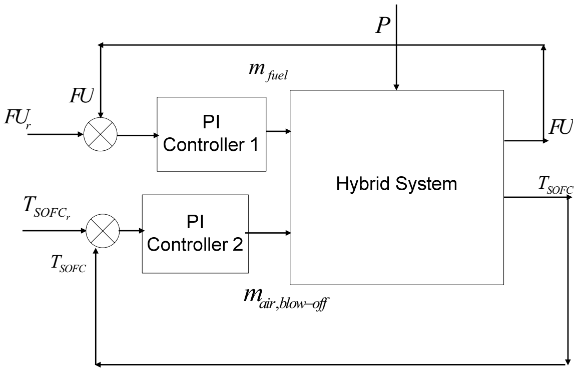

Fig. 2. De-centralized control structure using PI controllers

In Figure 2, FU refers to Fuel Utilization, which is defined as the ratio of fuel used in the SOFC and the fuel supplied to the SOFC. It is controlled to the reference value (0.85) by manipulating the fuel flow to the system. The air blow-off flow is manipulated to control the SOFC temperature to the reference value. The controller performs well in terms of tracking (Kandepu, *et al., 2006a*); the system efficiency can be improved by optimizing the reference values of the controlled variables. Also there are some constraints which are to be taken into account, for example, steam to carbon ratio at pre-reformer inlet, differential pressure across anode and cathode, compressor surge etc. To achieve this, MPC is necessary and overall control structure is as shown in Figure 3. As a basis to develop the MPC as well as monitoring of the hybrid system, the state estimator is to be designed.

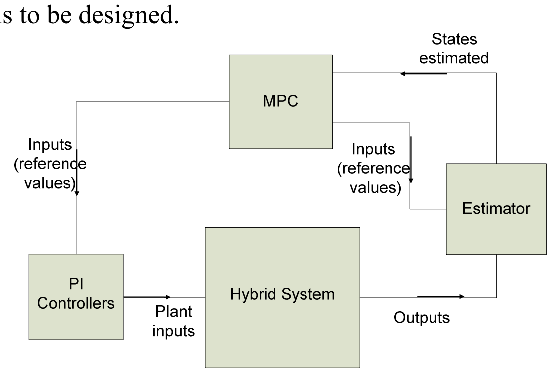

Fig. 3. Overall control structure

5. STATE ESTIMATION USING UKF

The principle of the UKF is explained with the following example: let x be a random variable and $y = f(x)$ be a nonlinear function. The question is how does the UKF approximate the propagation of pdf of x? In other words, how to calculate the mean ($\bar{y}$) and covariance ($\sum_y$) of y? Consider a set of sigma points $x^{(i)}$, (similar to the random samples of a specific distribution function in Monte Carlo simulations) with each point being associated with a weight $w^{(i)}$. Both the sigma points and the weights are computed deterministically through a set of conditions given in (Julier and Uhlmann, 2004). Then the following steps are involved in approximating the mean and covariance of y:

(I) Propagate each sigma point through the nonlinear function,

$$y^{(i)} = f(x^{(i)})$$

(II) Mean is the weighted average of the transformed points,

$$\bar{y} = \sum_{i=0}^{p} y^{(i)}$$

(III) The covariance is the weighted outer product of the transformed points,

$$\sum_y = \sum_{i=0}^{p} w^{(i)} \left(y^{(i)} - \bar{y}\right)\left(y^{(i)} - \bar{y}\right)^T$$

The UKF algorithm is presented below; for the fundamental theory, refer to (van der Merwe, 2004; Huang and Wang, 2006). Let the system be represented by the following standard discrete time equations:

$$\begin{aligned} x_k &= f(x_{k-1}, v_{k-1}, u_{1,k-1}) \\ y_k &= h(x_k, n_k, u_{2,k}) \end{aligned} \tag{1}$$

where x is the system state, v the process noise, n the observation noise, u_1 the exogenous input to the state transition function, u_2 the exogenous input to the state observation function and y the noisy observation of the system. An augmented state at time instant k,

$$x_k^a = \begin{bmatrix} x_k \\ v_k \\ n_k \end{bmatrix} \tag{2}$$

is defined. The augmented state variable dimension is,

$$L = L_x + L_v + L_n \tag{3}$$

where L_x is the original state dimension, L_v is the process noise dimension and L_n is the observation noise dimension. Similarly, the augmented state covariance matrix is built from the covariance matrices of x, v and n:

$$P^a = \begin{bmatrix} P_x & 0 & 0 \\ 0 & R_v & 0 \\ 0 & 0 & R_n \end{bmatrix} \tag{4}$$

where R_v and R_n are the process and observation noise covariance matrices.

5.1 Algorithm:

- *Initialization:*

$$\hat{x}_0 = E[x_0], \quad P_{x_0} = E\left[(x_0 - \hat{x}_0)(x_0 - \hat{x}_0)^T\right] \tag{5}$$

$$\hat{x}_0^a = E\left[x^a\right] = E\left[\hat{x}_0 \ 0 \ 0\right]^T,$$

$$P_0^a = E\left[(x_0^a - \hat{x}_0^a)(x_0^a - \hat{x}_0^a)^T\right] = \begin{bmatrix} P_x & 0 & 0 \\ 0 & R_v & 0 \\ 0 & 0 & R_n \end{bmatrix} \tag{6}$$

- *For* $k = 1, \ldots \infty$:

1. Calculate sigma-points (van der Merwe, 2006):

$$\chi_{k-1}^{a} = \left[\hat{x}_{k-1}^{a} \quad \hat{x}_{k-1}^{a} + \gamma\sqrt{P_{k-1}^{a}} \quad \hat{x}_{k-1}^{a} - \gamma\sqrt{P_{k-1}^{a}}\right] \quad (7)$$

2. Time-update equations:

$$\chi_{k/k-1}^{x} = f\left(\chi_{k-1}^{x}, \chi_{k-1}^{v}, u_{1,k-1}\right) \quad (8)$$

$$\hat{x}_{k}^{-} = \sum_{i=0}^{2L} w_i^{(m)} \chi_{i,k/k-1}^{x} \quad (9)$$

$$P_{x_k}^{-} = \sum_{i=0}^{2L} w_i^{(c)} \left(\chi_{i,k/k-1}^{x} - \hat{x}_k^{-}\right)\left(\chi_{i,k/k-1}^{x} - \hat{x}_k^{-}\right)^T \quad (10)$$

3. Measurement-update equations:

$$y_{k/k-1} = h\left(\chi_{k-1}^{x}, \chi_{k-1}^{n}, u_{2,k}\right) \quad (11)$$

$$\hat{y}_{k}^{-} = \sum_{i=0}^{2L} w_i^{(m)} y_{i,k/k-1} \quad (12)$$

$$P_{\bar{y}_k} = \sum_{i=0}^{2L} w_i^{(c)} \left(y_{i,k/k-1} - \hat{y}_k^{-}\right)\left(y_{i,k/k-1} - \hat{y}_k^{-}\right)^T \quad (13)$$

$$P_{x_k y_k} = \sum_{i=0}^{2L} w_i^{(c)} \left(\chi_{i,k/k-1}^{x} - \hat{x}_k^{-}\right)\left(y_{i,k/k-1} - \hat{y}_k^{-}\right)^T \quad (14)$$

$$K_k = P_{x_k y_k} P_{\bar{y}_k}^{-1} \quad (15)$$

$$\hat{x}_k = \hat{x}_k^{-} + K_k\left(y_k - \hat{y}_k^{-}\right) \quad (16)$$

$$P_{x_k} = P_{x_k}^{-} - K_k P_{\bar{y}_k} K_k^T \quad (17)$$

where γ is a scaling factor.

Table 1 Inputs

No.	Input
1	FU reference point
2	SOFC temperature reference point
3	electric load on the system (measured disturbance)

Table 2 Outputs

No.	Output
1	Pre-reformer temperature (K)
2	Shaft speed (rad/s)
3	Heat exchanger hot stream temperature (K)
4	Heat exchanger cold stream temperature (K)
5	SOFC temperature (K)
6	Combustor outlet temperature (K)
7	Fuel mass flow rate (kg/s)
8	Anode recycle flow rate (kg/s)
9	Flow to the combustion chamber (kg/s)
10	Air blow-off flow rate (kg/s)
11	Air mass flow rate (kg/s)
12	SOFC current (A)
13	SOFC voltage (V)
14	Generator power (kW)

Table 3 States

No.	State
1	Pre-reformer temperature (K)
2	H_2 concentration in pre-reformer (mol)
3	CH_4 concentration in pre-reformer (mol)
4	H_2O concentration in pre-reformer (mol)
5	CO concentration in pre-reformer (mol)
6	CO_2 concentration in pre-reformer (mol)
7	PI controller 1 integral term
8	Compressor shaft speed (rad/s)
9	PI controller 2 integral term
10	Heat exchanger hot stream temperature (K)
11	Heat exchanger cold stream temperature (K)
12	O_2 concentration in cathode (mol)
13	H_2 concentration in anode (mol)
14	CH_4 concentration in anode (mol)
15	H_2O concentration in anode (mol)
16	CO concentration in anode (mol)
17	CO_2 concentration in anode (mol)
18	SOFC temperature (K)

5.2 The SOFC/GT hybrid system description

The SOC/GT hybrid system is modeled in gPROMS (gPROMS, 2004) modeling environment. It has 3 inputs, 14 measured outputs and 18 states which are listed in Tables 1, 2, and 3 respectively. The hybrid system model in gPROMS is exported to matlab and can be used as function in matlab using the gO:MATLAB package (gPROMS, 2004).

5.3 Simulations and results

Process and observation noises that are applied to the system are white noise with Gaussian distribution. A simulation is done with disturbances in the load as shown in Figure 4. The initial state estimate is taken very near to the actual state and the initial state covariance matrix (P_x) is tuned in order to get a satisfactory predicted estimate. The simulation is performed online while applying the load disturbance, process noise and observation noise.

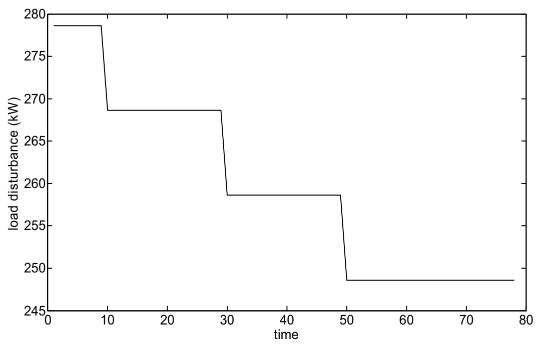

Fig. 4. Load perturbation on the hybrid system

The main challenge in designing the UKF is to tune the state covariance matrix P_x, to be able to get satisfactory results. The simulations results are presented in Figures 5, 6 and 7.

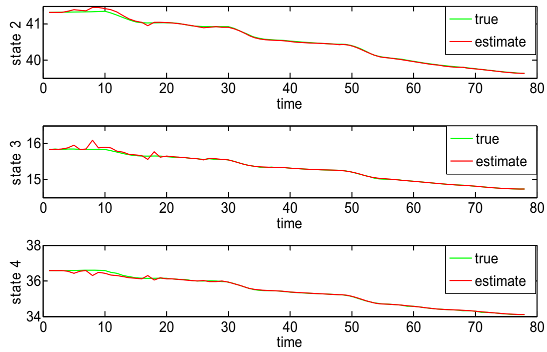

Fig.5. State estimation results showing the estimaed and actual states; concentrations of H_2, CH_4 and H_2O in pre-reformer

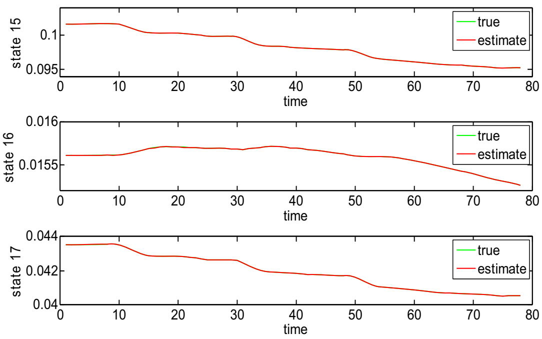

Fig.6. State estimation results showing the estimated and actual states; concentrations of H_2O, CO and CO_2 in SOFC anode.

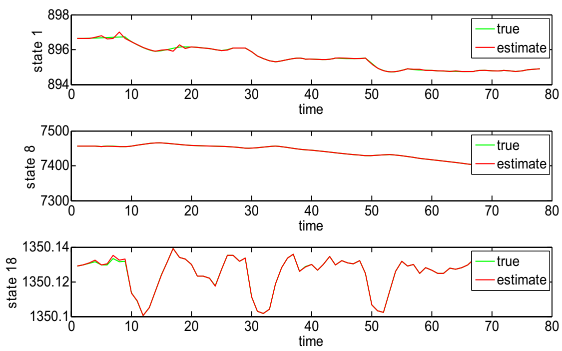

Fig.7. State estimation results showing the estimated and actual states; Pre-reformer, SOFC temperatures and compressor shaft speed

The simulation results (Fig. 5, 6 and 7) show that UKF is promising in tracking the actual state of the SOFC/GT hybrid system. The present results are with the assumption that the initial state estimate is very near to the actual state. This condition has to be met to avoid numerical problems in numerical solver for the nonlinear differential equations. The estimated state from UKF tracks actual state well even in the presence of significant load perturbations plus process and observation noise. Without the numerical issue in the nonlinear equation solution, we expect a good performance to be achieved, even if the initial state estimate is significantly different from the actual state, as the UKF estimate is able to converge in the presence of significant step perturbations in the load according to this simulation.

6. CONCLUSION AND FURTHER WORK

The state estimator is developed for SOFC/GT hybrid system using UKF. The results show that UKF is promising in the state estimation where the system is highly nonlinear with many sub-components being tightly integrated. The implementation of UKF is simpler compared to the EKF, as there is no need of Jacobian matrices.

Further work focuses on resolving numerical issue in the simulation, applying the EKF estimator for the same application and to compare it with the developed UKF estimator. Further, the developed UKF state estimator will be used in designing the MPC for the SOFC/GT hybrid system.

7. ACKNOWLEDGEMENTS

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