State Estimation in Solid Oxide Fuel Cell(SOFC) system

V Goutham Polisetty

A Thesis Submitted to

Indian Institute of Technology Hyderabad

In Partial Fulfillment of the Requirements for

The Degree of Master of Technology

Department of Chemical Engineering

June 2013

Declaration

I declare that this written submission represents my ideas in my own words, and where ideas or words of others have been included, I have adequately cited and referenced the original sources. I also declare that I have adhered to all principles of academic honesty and integrity and have not misrepresented or fabricated or falsified any idea/data/fact/source in my submission. I understand that any violation of the above will be a cause for disciplinary action by the Institute and can also evoke penal action from the sources that have thus not been properly cited, or from whom proper permission has not been taken when needed.

P. V. Goutham

(Signature)

V. GOUTHAM POLISETTY

(V Goutham Polisetty)

CH11M15

(Roll No.)

Approval Sheet

This Thesis entitled State Estimation in Solid Oxide Fuel Cell(SOFC) system by V Goutham Polisetty is approved for the degree of Master of Technology from IIT Hyderabad

(Dr. Niket Kaisare) External Examiner
ABB

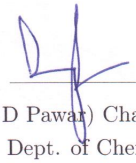
(Dr. Kamakshi Jagannathan)External Examiner
COMSOL

(Dr. Ketan P Detroja) Examiner
Dept. Electrical Engineering
IITH

(Dr. Vinod Janardhanan) Examiner
Dept.of Chem Eng
IITH

(Dr. Phanindra V Jampana) Adviser
Dept. of Chem Eng
IITH

(Dr. Dayadeep Monder) Co-Adviser
Dept. of Chem Eng
IITH



(Dr. Parag D Pawar) Chairman
Dept. of Chem Eng
IITH

iv

Acknowledgements

Firstly, I would like to express my sincere gratitude to my advisors Dr. Phanindra Jampana and Dr. Dayadeep Monder for their immense patience, motivation and guidance in doing this work.

I would like to thank my Thesis committee Dr. Parag D Pawar, Dr. Ketan P Detroja and Dr. Vinod Janarthanan for their patient listening, encouragement and reviews. I am also thankful to the Institute for providing the Teaching Assistantship during this two years.

I thank my friends Harish Ravikanth, Pinaki, Srinath, Prashil, Rakesh, Tejesh, Anup Patil, Paidi Naidu, Nanda Kumar, Sudhakar, Teja and all other batchmates for their support during these two years at IITH.

Last but not the least I would like to thank my parents and my sister for their constant source of love, concern, support, patience and strength during these two years.

Dedication

to my parents

Abstract

Solid oxide fuel cells (SOFCs) offer a clean, low pollution technology to electrochemically generate electricity at high efficiency. An SOFC consists of a dense solid electrolyte and two porous electrodes in contact with an interconnect on either side. The control of an SOFC stack becomes important in order to ensure adequate and disturbance free electric power. As several controlled/constrained variables are not directly measured in a stack, state estimators can be used in order to study the dynamic behaviour of SOFC stacks as well as to design effective SOFC controllers. In this thesis, A zero dimensional model represented by a set of ordinary differential equations is derived for dynamic modeling. The model consists of molar balances and an energy balance coupled with a simplified description of the fuel cell electrochemistry. The chemical species considered are H_2 and H_2O for fuel side (anode side) and O_2 and N_2 for air side (cathode side) and the electrochemical model accounts for ohmic, concentration and activation losses. Considering the estimation part, the state vector which is to be estimated consists of partial pressure of chemical species and temperature, with voltage as the measurement. Estimation of states for linear systems can be done by Kalman Filter. States of nonlinear systems can be estimated using Extended Kalman Filter(EKF), Unscented Kalman Filter (UKF). We choose UKF for non linear state estimation. UKF is a derivative free state estimator for non linear systems. This work investigates the use of non linear state estimator UKF to estimate the states of SOFC system. This method can be applied to estimate states in any type of fuel cells (PEMFC, AFC etc.) by very slight modifications.

Contents

List of Figures

Nomenclature

$\dot{n}_i^{in}$	inlet molar flow rate of species i (mols^{-1})
$\dot{n}_i^{out}$	outlet molar flow rate of species i (mols^{-1})
$\dot{n}_i^{r}$	reactive molar flow rate of species i (mols^{-1})
p_{H_2}	partial pressure of H_2 (atm)
p_{O_2}	partial pressure of O_2 (atm)
p_{H_2O}	partial pressure of H_2O (atm)
T_s	Temperature of stack (K)
R	Universal Gas Constant (J mol^{-1} K^{-1})
F	Faraday Constant (C mol^{-1})
V_{an}	Anode channel volume (m^3)
V_{cat}	Cathode channel volume (m^3)
K_{H_2}	Valve molar constant for H_2
K_{O_2}	Valve molar constant for O_2
K_{H_2O}	Valve molar constant for H_2O
V_s	Stack Voltage (V)
I	Stack Current (amp)
N_o	Number of Cells
η_{ohm}	Ohmic Loss (V)
η_{act}	Activation Loss (V)
η_{con}	Concentration Loss (V)
β	transfer coefficient
$\eta_{act,c}$	Cathodic Activation Loss (V)
$\eta_{act,a}$	Anodic Activation Loss (V)
$\eta_{con,c}$	Cathode Concentration Loss (V)
$\eta_{con,a}$	Anode Concentration Loss (V)
i_o	exchange current density (amp cm^{-2})
i_{as}	anode limiting current density (amp cm^{-2})
i_{cs}	cathode limiting current density (amp cm^{-2})

Nomenclature of state estimation

x	State Vector (States of system)
y	Measurement vector
t	time
Φ	State transition matrix
$\hat{x}(t)$	Estimate of state vector
$E[X]$	Expectation of random variable X
$E[X\|Y]$	Conditional Expectation
$\mathbb{R}$	set of Real numbers
$\mathbb{B}(\mathbb{R})$	Borel's set on $\mathbb{R}$
P	error covariance matrix
Q	state covariance matrix
R	measurement covariance matrix
W_i	Weight associated with i^{th} point
χ	Sigma points
f	process model
g	observation model

Abbreviations

EKF	Extended Kalman Filter
UKF	Unscented Kalman Filter

Chapter 1

Introduction

A futuristic view of energy supply is based on hydrogen rather than the fossil fuels . Also increasing demands on pollution reduction is driving innovation on clean energy sources. Among these Fuel Cells (FCs) are regarded as one of the most promising technologies, due to their efficiency, compactness and reliability. Though fuel cells are now commercially available , to make the technology cost effective research is still going throughout the world to deal with the engineering problems associated with them. Considering the wide availability of Hydrogen from many renewable sources fuel cells can be a feasible, attractive alternative to fossil fuels reducing the dependence on fossil fuels. Greenhouse gases like carbon monoxide are responsible for increasing temperature of planet leading to climate changes. In an attempt to slowdown the consequence of climate changes, many countries are serious about pollution reduction standards. The interest in hydrogen fuel is not just because of dependence on fossil fuels and green house gas effects, certain other factors like economic and political dependence on oil rich countries also account for this.

1.1 Fuel Cells

Fuel Cells are electrochemical devices that convert the chemical energy of a reaction directly into electrical energy . In a typical fuel cell, gaseous fuels are fed continuously to anode (negative electrode) compartment and an oxidant (i.e., oxygen from air) is fed continuously to the cathode (positive electrode) compartment, the electrochemical reactions take place at the electrode-electrolyte interface to produce an electric current. A fuel cell is a device that uses hydrogen as a fuel to produce electrons, protons, heat and water. Fuel Cell technology is based on simple combustion reaction given in Eq. (1.1)

$$H_2 + \frac{1}{2}O_2 \rightleftarrows H_2O \tag{1.1}$$

Fuel Cells are different types based on the type of electrolyte used for conducting the ions.[1] They are

1. Polymer Electrolyte Membrane Fuel Cell (PEMFC)
2. Alkaline Fuel Cell (AFC)
3. Phosphoric Acid Fuel Cell (PAFC)
4. Molten Carbonate Fuel Cell (MCFC)
5. Solid Oxide Fuel Cell (SOFC)

The electrochemical principle of operation is same for all the above fuel cells. Fuel is oxidized into electrons and protons at the anode and oxygen is reduced to oxide species at the cathode. The protons or the oxide ions are transported through the electrolyte and combines with oxide or protons to generate water and power. The major difference is they operate at different temperatures, employ different materials for construction and differ in fuel tolerance and performance.

1.2 Solid Oxide Fuel Cells

The Solid Oxide Fuel Cells (SOFC) are high temperature fuel cells with an operating temperature range of $600 - 1000°C$. SOFC like other fuel cells is an electrochemical device for the conversion of chemical energy of a fuel into electricity and heat. Now the oxide ions pass through the electrolyte to the fuel rich porous anode where oxide ions react with hydrogen, giving up electrons to external circuit. The reactions are as follows

$$H_2(g) + O^{2-} \rightarrow H_2O(g) + 2e^- \tag{1.2}$$

The liberated electrons pass through an external circuit to arrive at the cathode (air electrode) where they reduce oxygen (present in air) to oxide ions .

$$\frac{1}{2}O_2(g) + 2e^- \rightarrow O^{2-} \tag{1.3}$$

Water vapor is produced at the anode diluting the fuel. The hydrogen oxidation reaction and the oxygen reduction reaction occur at the triple phase boundary (TPB) where the electrode, electrolyte and the gas phase are in contact. The performance of the SOFC is highly dependent on the partial pressure of hydrogen, oxygen and the temperature of the cell. By stacking several cells in series or parallel, the voltage and power sought in an application can be attained. It requires another component, interconnect which is for electrical connection between the cells and gas separation within the cell stack. The

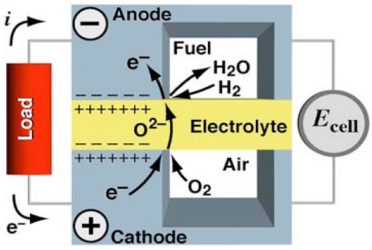


Figure 1.1: Solid Oxide Fuel Cell[17]

entire build up of individual cells and interconnect is called the stack. Insufficient supply of reactants results in starvation of the cell which leads to degradation of voltage , so to avoid this and to extend stack life , air and fuel flows , partial pressure of gases and temperature must be controlled properly.

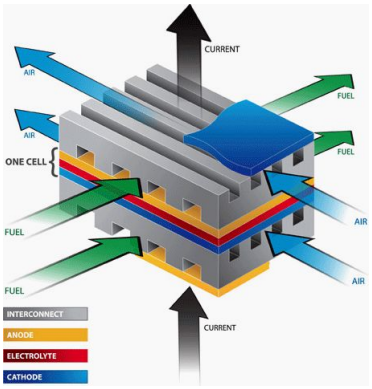


Figure 1.2: SOFC Stack (www.seca.doe.gov)

1.3 Motivation

Considering the control of fuel cells one major aspect is that we employ sensors to measure the partial pressures of reactants. Sensors are costly and sensitive in real applications. Constraints on usage of these sensors results in lack of reliable measurements of partial pressures. So, with consideration to the importance of these variables and difficulties in measuring these variables, interest in need of estimator design is encouraged. An active control model development of SOFCs to achieve satisfactory performance during load variations and also in meeting the dynamic constraints of operation is possible only when states of system are known. This motivates the use of estimators to find the partial pressures of hydrogen and oxygen at anode and cathode respectively. The estimators must be able to incorporate the non linear model, as fuel cell behavior is highly non linear and account for noise in the measurements.

1.4 Thesis Objective

The main focus of the thesis is to investigate the use of Unscented Kalman Filter to estimate the partial pressures of H_2, O_2 and H_2O and temperature of SOFC system considered.

Chapter 2

Literature Review

Given a physical system whether it may be an aircraft, chemical process an engineer first attempts to develop a mathematical model that represents the behavior of the system. Through physical insight, fundamental laws we can establish the interrelationship among the system variables i.e, inputs to system and outputs from system. To observe the actual system behavior, measurements and states of system are the important information available to study.

A great number of experimental and modeling studies have been carried out to explore the performance, problems and efficiency of fuel cells with ultimate goal of extensive commercialization of the fuel cells. By developing an accurate dynamic model of fuel cell system, one can understand the physics of the system and to control the system effectively and systematically. A comprehensive review of publications on mathematical modeling, steady state and dynamic behavior and control of PEMFC and SOFC is presented by [2]. Considering the control applications in mind and feasibility to implement the models in real time process control reduced order linear models for anode supported tubular SOFC are developed [4]. A linear parameter varying model structure is developed to obtain a control oriented dynamic model for SOFC stack and also a MPC controller is designed and implemented based on reduced order models [5]. A limited number of variables and parameters can be measured in a typical fuel cell, information on unmeasured variables can be obtained using an observer/estimator. SOFC systems are nonlinear systems, so the estimators that are to be used in SOFC state estimation are non linear.

A dynamic lumped model of a SOFC combined with a gas turbine to study the control of the system is developed by Kandepu et al [7], they implemented a PI controller and studied a comparision of implementation of Extended Kalman Filter (EKF) and Unscented Kalman Filter (UKF) on the SOFC-GT system in estimation of states. Murshed et al [8] [9] described the application of nonlinear model predictive control applied on fuel cell system by utilizing the estimated states from Unscented Kalman Filter (UKF). Vijay et al [10]

designed a non linear adaptive observer for estimating the temperature inside the hydrgoen fed planar SOFC. They designed an observer based on the lumped parameter model of the SOFC. They also reported that the developed observer could track the temperature and species concentration profiles in the planar SOFC during step changes in cell current.

Das and Mukherjee et.al [11], Lin and Hong et al [12], Mueller et al [13], are few other groups who worked on development of observers and estimators for control relevant models of SOFC.

Chapter 3

System Model

Knowledge of transient and steady state response of solid oxide fuel cell system is important for studying the fuel cell performance and also for designing the controller. A model can vary from a simple zero dimensional model to a 3-D model. Model should comprise a set of linear or nonlinear ODEs to predict the transient behavior of the fuel cell.It should be able to predict all the important variables like partial pressures and temperature. So we consider the electrochemical, thermal and reactant flow model to meet all the modeling characteristics in minimum. In this chapter we consider the derivation and development of lumped model in which we assume uniform temperature throughout the cell including both solid phase and gas phase. A detailed explanation of the derivation of equations of lumped model will be considered in the further sections of this chapter.

3.1 Introduction

A knowledge of mathematical modeling is necessary to study static and dynamic behavior of fuel cells,designing the cells, studying control strategies and designing experiments. In a fuel cell system many processes like heat and mass transfer take place. One should understand the physics of these processes to analyze and describe them in the form of mathematical equations.Fuel cell systems can be modeled by considering temporal effects and spatial changes. With respect to spatial changes it can be zero-dimensional (lumped model), 1-D, 2-D, 3-D. The simplest approach to dynamic modeling of fuel cells is to ignore spatial changes and to consider changes with time only. In lumped modeling we consider the study of transient behavior of system accounting for electrochemical processes, voltage losses caused by ohmic, activation, concentration and polarization, mass balance and energy balance of system.

The voltage output of a real fuel cell is less than thermodynamically predicted voltage output due to irreversible losses. The more current that is drawn from the cell, the greater are the losses. There are three major types of fuel cell losses. The losses are

1 Activation losses (losses due to electrochemical reaction)

2 Ohmic losses(losses due to ionic and electronic conduction)

3 Concentration losses (losses due to mass transport)

The real voltage output for a fuel cell can thus be written by subtracting the voltage drops due to various losses from the thermodynamically predicted voltage output.

$$V = E_{thermo} - \eta_{act} - \eta_{ohmic} - \eta_{conc} \tag{3.1}$$

We discuss in detail in the next section the lumped model considered in the modeling.

3.2 Lumped Model

The lumped model of the stack model solid oxide fuel cell which is fed with hydrogen and air is developed on the basis of the following assumptions.

1. The gases are ideal.
2. Channels that transport gases along the electrodes have a fixed volume , but their lengths are small , so that it is only necessary to assume pressure is constant in the channel.
3. The exhaust of each channel is via a single orifice. Ratio of pressures between the exterior of channel is large enough to consider orifice choking condition.
4. Uniform temperature distribution for the entire stack.
5. Ideal mixing of gas inside the channel so exit temperature of fuel and air are same as inside temperature.
6. Negligible heat losses to surroundings.
7. All the voltage losses are considered.

3.2.1 Material balance

Change in concentrations of each species that appears in SOFC can be written generally in terms of material balance equation.

$$Accumulation = Inflow + Generation - Consumption - Outflow \tag{3.2}$$

$$\frac{dn_i}{dt} = \dot{n}_i^{in} - \dot{n}_i^{out} + \dot{n}_i^{r} \tag{3.3}$$

where
$\dot{n}_i^{in}$ is inlet molar flow rate of i^{th} species.
$\dot{n}_i^{out}$ is outlet molar flow rate of i^{th} species.
$\dot{n}_i^{r}$ is reactive molar flow rate of i^{th} species.

3.2.2 Charcaterization of exhaust of channels

According to [14], an orifice that can be choked, when fed with a mixture of gases of average molar mass M and similar specific heat ratios, at a constant temperature, assumes the following form:

$$\frac{W}{P_u} = K\sqrt{M} \tag{3.4}$$

where, W is mass flow [kg/s], K is valve constant, and P_u is pressure upstream [atm] Now according to the above equation we can assume molar flow of any gas through the valve is proportional to its partial pressure inside the channel, then according to [**?**]

$$\frac{q_{H_2}}{P_{H_2}} = \frac{K_{an}}{\sqrt{M_{H_2}}} = K_{H_2} \tag{3.5}$$

$$\frac{q_{H_2O}}{P_{H_2O}} = \frac{K_{an}}{\sqrt{M_{H_2O}}} = K_{H_2O} \tag{3.6}$$

where q_{H_2O} are molar flow rates of hydrogen and water respectively, through anode valve. K_{H_2} and K_{H_2O} are valve molar constants for hydrogen and water respectively.

3.2.3 Species Balance

Let us consider the species balance for H_2 , Consider the equation of material balance (3.3)

$$\frac{dn_{H_2}}{dt} = \dot{n}_{H_2}^{in} - \dot{n}_{H_2}^{out} + \dot{n}_{H_2}^{r} \tag{3.7}$$

Since we assume ideal gas

$$n_{H_2} = \frac{p_{H_2} V_{an}}{RT_s} \tag{3.8}$$

where V_{an} is the volume of anode channel and $\dot{n}_{H_2}^{in}$, $\dot{n}_{H_2}^{out}$ and $\dot{n}_{H_2}^{r}$ are inlet, outlet and reactive molar flow rates of H_2 respectively, p_{H_2} is partial pressure of H_2 in the stack, T_s is temperature of the stack

$$\dot{n}_{H_2}^{r} = 2K_r I \tag{3.9}$$

$$\dot{n}_{H_2}^{out} = K_{H_2} p_{H_2} \tag{3.10}$$

where $K_r = \frac{N_o}{4F}$, I is stack current, N_o is number of cells associated in series in stack, K_{H_2} is valve molar constant.

Now we rewrite the species balance equation as

$$\frac{dp_{H_2}}{dt} = \frac{RT_s}{V_{an}}(\dot{n}^{in}_{H_2} - \dot{n}^{out}_{H_2} + \dot{n}^{r}_{H_2}) \tag{3.11}$$

$$\frac{dp_{H_2}}{dt} = \frac{RT_s}{V_{an}}(\dot{n}^{in}_{H_2} - K_{H_2}p_{H_2} - 2K_rI) \tag{3.12}$$

Similarly the species balance equations for O_2 and H_2O are

$$\frac{dp_{O_2}}{dt} = \frac{RT_s}{V_{cat}}(\dot{n}^{in}_{O_2} - K_{O_2}p_{O_2} - K_rI) \tag{3.13}$$

$$\frac{dp_{H_2O}}{dt} = \frac{RT_s}{V_{an}}(\dot{n}^{in}_{H_2O} - K_{H_2O}p_{H_2O} + 2K_rI) \tag{3.14}$$

3.2.4 Energy balance

According to assumptions mentioned for lumped modeling, there is no temperature variation inside stack all components possess same temperature at any instance. Also it is assumed that heat capacity of gases inside channels is assumed negligible compared to solid compartments of cell. then dynamic model of cell temperature, T_s is given by energy balance around entire stack

$$m_s\bar{C}_{ps}\frac{dT_s}{dt} = \Sigma\dot{n}^{in}_i\int_{T_{ref}}^{T_{in}} C_{p,i}(T)dT - \Sigma\dot{n}^{out}_i\int_{T_{ref}}^{T_s} C_{p,i}(T)dT - \dot{n}^{r}_{H_2}\Delta\hat{H}^0_r - V_sI \tag{3.15}$$

where m_s and $\bar{C}_{ps}$ are mass and average specific heat of fuel cell materials excluding gases, $C_{p,i}$ is specific heat of fuel or air gas , $\Delta\hat{H}^0_r$ is the specific heat of reaction and V_s is stack voltage.

3.2.5 Stack Voltage

Applying Nernst's equation and considering ohmic, activation and concentration losses, the stack voltage is given by

$$V_s = N_o\left(V_0 - \eta_{ohm} - \eta_{act} - \eta_{con}\right) \tag{3.16}$$

Open Circuit Voltage

Thermodynamic potential or the reversible cell voltage is the maximum voltage attained by fuel cell at thermal equilibrium . It is given by Nernst Equation as below

$$V_0 = N_0 \Delta E = N_0 \left[\Delta E_0 + \frac{RT_s}{2F} ln \frac{p_{H_2} p_{O_2}^{0.5}}{p_{H_2O}} \right] \tag{3.17}$$

where N_0 is Number of Cells, ΔE_0 is standard cell potential is given by

$$\Delta E_0 = -\frac{\Delta G_0}{2F} \tag{3.18}$$

where

$$\Delta G_0 = G_{H_2O} - 0.5 G_{O_2} - G_{H_2} \tag{3.19}$$

G_{H_2O}, G_{O_2}, G_{H_2} are Gibbs free energy of formation

Ohmic Loss

Voltage which is lost due to resistance to flow of electrons through electrodes and various interconnections and resistance to flow of ions through electrolyte is known as Ohmic Loss and is obtained by using the conductivity expression given by [15].

$$\sigma_{el} = \sigma_o exp\left(\frac{-E_{el}}{RT}\right) \tag{3.20}$$

where $E_{el} = 8 \times 10^4 J/mol$

$$R = \rho \frac{l}{A}$$
$$\sigma = \frac{1}{\rho}$$

$$R = R_o T exp\left(\frac{E_{el}}{RT}\right) \tag{3.21}$$

where $R_o = 0.02525\Omega$, Ohmic Loss is given by

$$V_{ohm} = I \times R \tag{3.22}$$

Activation Loss

Electrochemical reactions like chemical reactions involve energy barriers which must be overcome by the reacting species . This energy barrier is called the activation energy and results in activation or charge transfer polarization, which is due to transfer of charges between electronic and ionic conductors. It is the extra potential necessary to overcome the energy barrier of the rate determining step of the reaction to a value such that electrode reaction proceeds at desired reaction rate.

Activation loss is normally expressed by the well known Butler Volmer equation

$$i = i_o \left\{ exp\left(\beta \frac{n_e F \eta_{act}}{2RT}\right) - exp\left(-(1-\beta)\frac{n_e F \eta_{act}}{2RT}\right)\right\} \tag{3.23}$$

where β is the transfer coefficient and i_o is the exchange current density . When $\beta = 0.5$

$$i = 2i_o sinh\left(\frac{n_e F \eta_{act}}{2RT}\right) \tag{3.24}$$

$$\eta_{act} = \frac{2RT}{n_e F} sinh^{-1}\left(\frac{i}{2i_o}\right) \tag{3.25}$$

Activation loss now for both anode and cathode is given by the following equations

$$\eta_{act,a} = \frac{2RT}{n_e F} sinh^{-1}\left(\frac{i}{2i_{oa}}\right) \tag{3.26}$$

$$\eta_{act,c} = \frac{2RT}{n_e F} sinh^{-1}\left(\frac{i}{2i_{oc}}\right) \tag{3.27}$$

Concentration Loss

In fuel cells reacting species are gaseous at anode and cathode. Hence, rate of mass transport to reaction sites in porous electrodes of a SOFC can be described by diffusion of gases in pores [**?**]. Gases have to diffuse through the gas filled pores of electrode in order to reach the reaction-sites. When the current is being drawn gas partial pressure at reaction site will be less than that in bulk of gas stream. So decrease of gas concentration in gas filled pores of electrode may result in voltage loss which is concentration loss.

The equations for concentration loss at both electrodes are given by the following.

Cathode concentration loss

$$\eta_{con,c} = \frac{RT}{4F} ln\left(1 - \frac{i}{i_{cs}}\right) \tag{3.28}$$

Anode concentration loss

$$\eta_{con,a} = \frac{RT}{4F} ln\left(1 - \frac{i}{i_{as}}\right) - \frac{RT}{2F} ln\left(1 + \frac{p_{H2} i}{p_{H_2O} i_{as}}\right) \tag{3.29}$$

where i_{as}, i_{cs} are anode and cathode limiting current densities respectively.

3.3 Lumped model with nonchoking assumption

We also considered the lumped model with non choking assumption for the flow gases through the orifice from the channel manifolds to the exhaust.

In this case we do not consider $\dot{n}_i^{out}$ directly proportional to the partial pressure of respective species in stack, Choked flow is a limiting condition which occurs when the mass flow rate will not increase with a further decrease in downstream pressure while upstream pressure is fixed.

Instead of choked flow if we consider normal flow through orifice, calculation of $\dot{n}_i^{out}$ is as follows.

$$\begin{aligned} \dot{n}_i^{out} &= y_i \dot{n}^{out} && (3.30)\\ &= \frac{P_i}{P}\dot{n}^{out} && (3.31)\\ &= \frac{P_i}{P}\frac{\dot{m}^{out}}{M_{avg}} && (3.32)\\ &= \frac{P_i}{\Sigma P_i M_i}\dot{m}^{out} && (3.33) \end{aligned}$$

The $\dot{m}^{out}$ is calculated by the equation of mass flowrate for flow of gases through orifice given by

$$\dot{m}^{out} = C A_2 Y \sqrt{2\rho(P_1 - P_2)} \tag{3.34}$$

where
C is Orifice flow coefficient, dimensionless
A_2 is Cross-section area of orifice hole, m^2
ρ is gas density, kg/m^3
P_1 is Upstream gas pressure, Pa
P_2 is Downstream gas presssure, Pa
Y is Expansion factor

3.4 Model Parameters

Table 3.1: Model Parameters and constants

Parameter	Value	Unit
Number of Cells, N_0	92	
Cell Area, A_c	0.055	m^2
r_0	0.02525	Ω
Activation energy for ion transport, E_{el}	8e4	J/mol
$\bar{C}_{ps}$	400	$J/kg/K$
Heat of Reaction, $\Delta\hat{H}_r^0$	-0.2418e-6	J/mol
Faraday Constant, F	96485.3365	As/mol
Anode thickness , l_a	500	μ
Electrolyte thickness	5	μ
Cathode thickness. l_c	50	μ
R, Universal Gas Constant	8.314	$J/K/mol$

3.5 Implementation of UKF

To implement the Unscented Kalman Filter in order to estimate the states for the lumped model, we consider the model in concise form as below

$$\dot{x} = f(x, I, V_s) \tag{3.35}$$

$$V_s = g(x, I) \tag{3.36}$$

where x is vector of states of SOFC system i.e, the partial pressures and temperature of the system. I is the current, V_s is the stack voltage. Using the voltage as measurement equation and set of derived ordinary differential equations in the earlier section as the state equations we investigate the implementation of UKF for this system.

Chapter 4

State Estimation

In general processes are accompanied with uncertainities like uncertainity in measurements and noise sources or unknown disturbances acting on the system. Information about the state variables and operating parameters must be available for control relevant model development for any model. State estimation plays an important role in reconstruction of important state variables which are not measurable.

Estimation problem can be formulated as follows , Current state x_k is determined using available measurements $y_{1:k}$, initial guess x_o in an optimal and recursive manner . The discrete time dynamic model of system can be formulated as

$$x_k = f(x_{k-1}, u_k, v_k) \tag{4.1}$$

$$y_k = g(x_k, w_k) \tag{4.2}$$

where $x_k \in \mathbb{R}^n$, where n is dimension of state vector. $y_k \in \mathbb{R}^m$, where m is dimension of measurement vector, $f : \mathbb{R}^n \to \mathbb{R}$, $g : \mathbb{R}^n \to \mathbb{R}^m$, $v_k \in \mathbb{R}^n$ represents state noise, $w_k \in \mathbb{R}^m$ represents measurement noise. In general any recursive estimation can be executed in two stages at any time instant as below

- Prediction: Given the previous estimate using the system model the next state is predicted.
- Updation: Given the current measurement , we estimate the current state

4.1 Kalman Filter

Kalman filter is optimal if the system is linear and the process noise is Gaussian . Kalman filter is executed in two steps , Prediction(Time update equation) where *apriori* estimates

for next step are calculated using the current state and error covariance and correction (measurement update equation) where an improved *aposteriori* estimate is obtained by incorporating new measurement into priori estimates. In state space form the linear model is represented as

$$x_{k+1} = Ax_k + v_k \tag{4.3}$$

$$y_k = Bx_k + w_k \tag{4.4}$$

*A*and B are the transition matrices for the system model and measurement model . The algorithm for Kalman filter is shown below in the figure.

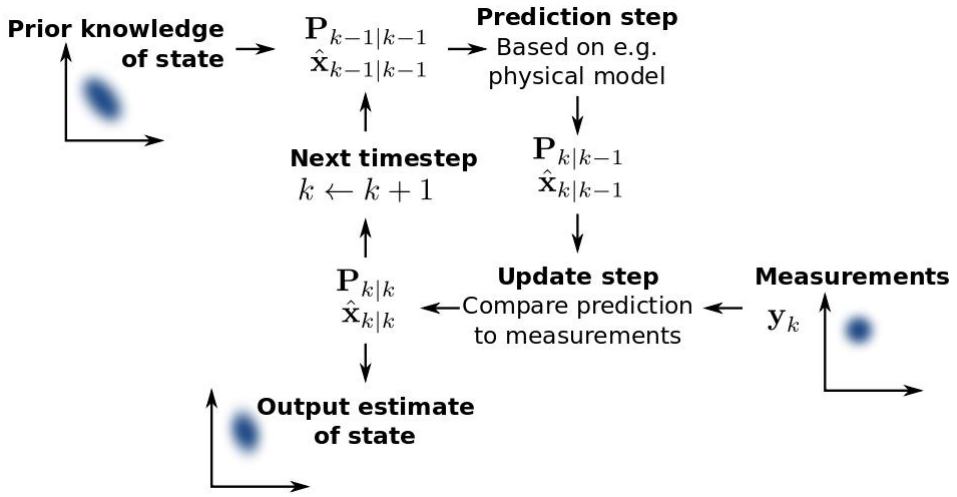


Figure 4.1: Kalman Filter Algorithm

4.1.1 Derivation for Kalman Filter

Introduction

Consider the dynamic model [21]

$$x(t+1)_{n\times 1} = \Phi(t+1;t)_{n\times n}x(t)_{n\times 1} + u(t)_{n\times 1} \tag{4.5}$$

$$y(t)_{p\times 1} = M(t)_{p\times n}x(t) \tag{4.6}$$

where u(t) is an independent Guassian random process of 'n' vectors with zero mean, $x(t)$ is an n-vector, $y(t)$ is a p- vector, $\Phi(t+1;t)$, $M(t)$ are $n \times n$ and $p \times n$ respectively whose elements are non random functions of time. Given the observed values of $y(t_0), ...y(t)$ find an estimate $X^*(t_1|t)$ of $X(t_1)$ which minimizes the expected loss

Optimal Estimate

Firstly, our idea is to get best estimate of $x(t)$ given all measurements $y(1), y(2).....y(t)$, which is Minimum Mean Squared Estimate. Let $\hat{x}(t)$ be the best estimate.

Theorem 4.1.1. *The best estimate is conditional expectation x(t) given Y(t) ie., $\hat{x}(t) = E[x(t)|\mathcal{Y}(t)]$*

Proof. The criterion that are to be satisfied are

(i) $\hat{x}(t)$ is $\sigma(y(1), y(2), ...y(t))$ measurable.

(ii) $E[(\hat{x}(t) - x(t))^2]$ should be minimum.

Our claim is that the best estimate satisfying the above is $\hat{x}(t)$.
This claim satisfies criteria (i) directly as it is one of the property by definition of conditional expectation. Now we have to check if the criterion (ii) is satisfied. By Tower Property of Conditional Expectation [22] we know that if H is a sub σ-algebra of Σ then

$$E[E(X|\Sigma)/H] = E[X|H]a.s$$

We can say $\sigma(y(1), y(2), ...y(t)) \in \Sigma$. By Double Expectation property we can write.

$$\begin{aligned} E[(\hat{x}(t) - x(t))^2] &= E[E[\hat{x}(t) - x(t))^2|\sigma(y(1), y(2), ...y(t))]]. \\ R.H.S &= E[E[(\hat{x}(t) - x(t))^2)|\sigma(y(1), y(2), ...y(t))]] \end{aligned}$$

In the inner term between $\hat{x}(t)$ and $x(t)$ we add and substract another term
$E[x(t)|y(1), y(2), ...y(t)]$ then

$$\begin{aligned} R.H.S = E[E[(\hat{x}(t) - E[x(t)|y(1), y(2), ...y(t)] \\ +E[x(t)|y(1), y(2), ...y(t)] - x(t))^2\sigma(y(1), y(2), ...y(t))]] \end{aligned}$$

Consider the inner part of the above expression in R.H.S

$$\begin{aligned} = E[(\hat{x}(t) - E[x(t)|y(1), y(2), ...y(t)] + E[x(t)|y(1), y(2), ...y(t)] \\ -x(t))^2|\sigma(y(1), y(2), ...y(t))] \end{aligned}$$

$$E[(\hat{x}(t) - E[x(t)|y(1), y(2), ...y(t)])^(2)|\Sigma_1] + E[E[(x(t) - E[x(t)|\Sigma_1])^2]/\Sigma_1] +$$

$$E[[(\hat{x}(t) - E[x(t)|\Sigma_1])(x(t) - E[x(t)|\Sigma_1])]/\Sigma_1]$$

where $\Sigma_1 = \sigma(y(1), y(2), ...y(t))$.We can observe that the third term in the summation

in L.H.S reducs to zero and the first two terms remain in the summation Now, the

$$E[Innerpart] = E[E[[\hat{x}(t) - E[x(t)|\Sigma_1]]^2|\Sigma_1] + E[E[[x(t) - E[x(t)|\Sigma_1]]^2|\Sigma_1]$$

By Double Expectation Property this further reduces to

$$R.H.S = E[[\hat{x}(t) - E[x(t)|\Sigma_1]]^2|\Sigma_1] + E[(x(t) - E[x(t)|\Sigma_1])^2|\Sigma_1]$$

$\hat{x}(t) = E[x(t)|\Sigma_1]$ minimizes the above.

Therefore, the MMSE condition is satisified i.e, $E[(\hat{x}(t) - x(t))^2] = 0$. □

Orthogonal Projection is Conditional Expectation

Suppose $x_n, y_1, y_2, ...y_n$ are Multivariate Gaussian and $x_n \in \mathcal{L}^2$
$\mathcal{Y} = span\,(y_1, y_2, ..., y_n) = \{\sum_{i=1}^{n} a_i y_i | \forall a_i \in \mathbb{R}$
$\mathcal{Y}$ is a Hilbert space.

Theorem 4.1.2. *The orthogonal projection of x_n on $\mathcal{Y}$ space is $\hat{E}[x_n|\mathcal{Y}] = E[x_n|\sigma(y_1, y_2, ...y_n)]$ is the optimal estimate and is the conditional expectation if the process is gaussian*

The above theorem can be proved if $\hat{E}[x_n|\mathcal{Y}]$ it satisfies all the three propeties below for it to be conditional expectation by definiton.

(i) $\hat{E}[x_n|\mathcal{Y}]$ should be $\sigma(y_1, y_2, ...y_n)$ measurable.

(ii) $E[|\hat{E}[x_n|\mathcal{Y}|]$ is finite.

(iii) $\int_B \hat{E}[x_n|\mathcal{Y}]dP = \int_B \mathrm{x}_n dP \; \forall \mathbb{B} \in \mathbb{B}(\mathbb{R})$.

Since the proof evolves to be another big section it is avoided presenting here.

One of the main ideas in the Kalman Filter is that geometric tools like orthogonal projection are used to solve Probabilistic problems. Random variables are thought of as points in an abstract Hilbert space. This is the core idea in derivation of Kalman filter which is discussed in detail in the paper by Kalman

4.1.2 Implementing Kalman Filter

We consider a stochastic linear system with some noise input. The state space form

$$x(t+1) = A(t)x(t) + w(t)y(t) = C(t)x(t) + v(t) \tag{4.7}$$

where $w(t)$ is state noise , $v(t)$ is measurement noise
We rewrite the above state space equation in discretized form as

$$X_k = AX_{K-1} + w_{k-1} \tag{4.8}$$

$$Y_k = CX_{k-1} + v_k \tag{4.9}$$

We will be given the observations $Y_1, Y_2, ...Y_k....$ and we implement the kalman filter in two steps

- Prediction step
- Updation step

First, Consider the Prediction step So from the knowledge of Kalman Filter derivation we know that

$$\begin{aligned} E[X_k|\sigma(Y_1, Y_2, ...Y_k)] &= \hat{E}[X_{k+1}|\mathcal{Y}_k] \\ &= \hat{E}[X_{k+1}|\mathcal{Y}_{k-1}] + \hat{E}[X_{k+1}|\mathcal{Z}_k] \\ &= A\hat{E}[X_k + \hat{E}[X_{k+1}|\mathcal{Z}_k] \end{aligned}$$

An important step here is $\hat{E}[X_{k+1}|\mathcal{Z}_k] = \Delta^*(\tilde{Y}_{k|k-1})$

from definiton of $\tilde{Y}_{k|k-1}$) we substitute the expression for it and we obtain the prediction step equations

$$\begin{aligned} \bar{X}_{k+1|k} &= A\bar{X}_{k|k-1} + \Delta^*[Y_k - \hat{E}[Y_k|\mathcal{Y}_{k-1}] \\ \bar{X}_{k+1|k} &= A\bar{X}_{k|k-1} + \Delta^*[Y_k - C\hat{E}[X_k|\mathcal{Y}_{k-1}] - 0] \\ \bar{X}_{k+1|k} &= (A - \Delta_k^* C)\bar{X}_{k|k-1} + \Delta_k^* Y_k \end{aligned}$$

where $\Delta_k^* = AP_{k|k-1}C^T(CP_{k|k-1}C^T)^{-1}$
and $P_{k+1|k} = (A - \Delta_k^* C)P_{k|k-1}(A - \Delta_k^* C)^T + Q + \Delta_k^* R\Delta_k^{*T}$
Here Q and R are state and measurement Covariance Matrices. Now, the equations for updation part

$$\bar{X}_{k|k} = \bar{X}_{k|k-1} + \hat{E}[X_k|\mathcal{Z}_k] \tag{4.10}$$

We know from kalman filter derivation that $\hat{E}[X_k|\mathcal{Z}_k] = \Lambda_k^* \ \tilde{Y}_{k|k-1}$ Now, considering the condition $E[(X_k - \Lambda_k^* \tilde{Y}_{k|k-1})\tilde{Y}_{k|k-1}^T = 0$ we solve for Λ_k^* In the above expression we substitute $X_k = X_{k|k-1} + \tilde{X}_{k|k-1}$ and also

$$\tilde{Y}_{k|k-1} = Y_k - \bar{Y}_{k|k-1} = CX_k + v_k - C\bar{X}_{k|k-1} - v_k = C\tilde{X}_{k|k-1} \tag{4.11}$$

Now we substitute expression for $\tilde{Y}_{k|k-1}$ then by further simplifying we get

$$\Lambda_k^* = P_{k|k-1}C^T[CP_{k|k-1}C^T]^{-1} \tag{4.12}$$

The final update equation is

$$\begin{aligned}
\bar{X}_{k|k} &= \bar{X}_{k|k-1} + \Lambda_k^*\tilde{Y}_{k|k-1} \\
&= \bar{X}_{k|k-1} + P_{k|k-1}C^T[CP_{k|k-1}C^T]^{-1}C\tilde{X}_{k|k-1} \\
&= \bar{X}_{k|k-1} + \Lambda^*[CX_{k|k-1} - C\bar{X}_{k|k-1}]
\end{aligned}$$

$$\bar{X}_{k|k} = \bar{X}_{k|k-1} + \Lambda^*[Y_k - v_k - C\bar{X}_{k|k-1}] \tag{4.13}$$

4.2 Simulation Results

A MATLAB program has been written to implement the KALMAN filter for a linear stochastic system, In this program , the input is

- No.of states ,n
- No. of Measurements, p
- State Noise covariance, q
- Measurement Noise Covariance, r
- Time, T

Here are a few results of the simulation

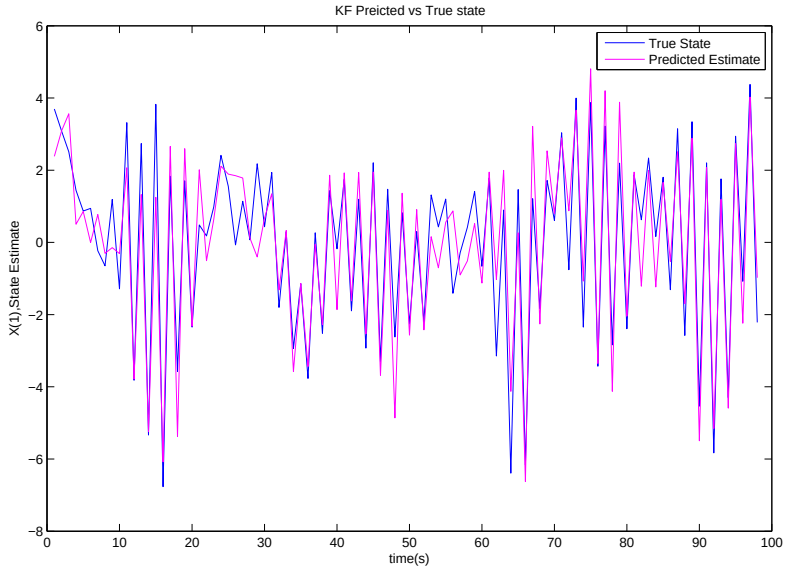


Figure 4.2: Predicted state vs True State

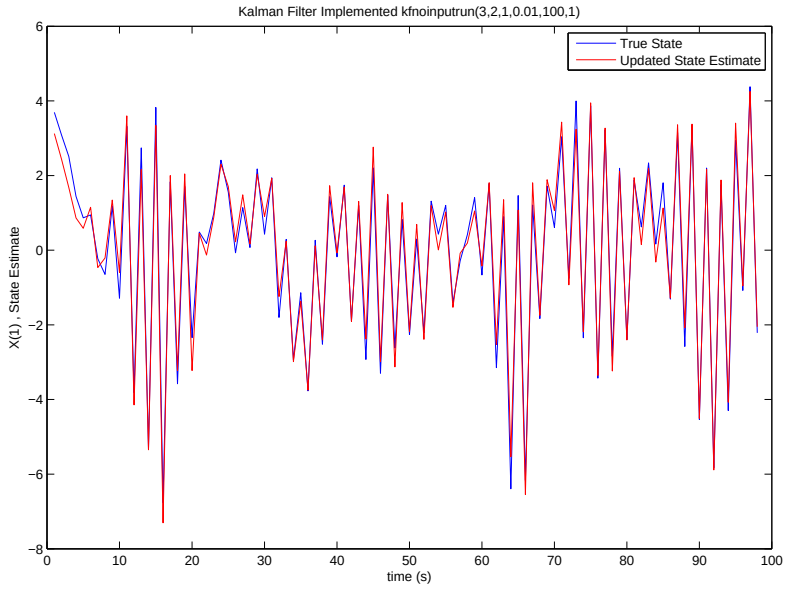


Figure 4.3: Updated State vs True State

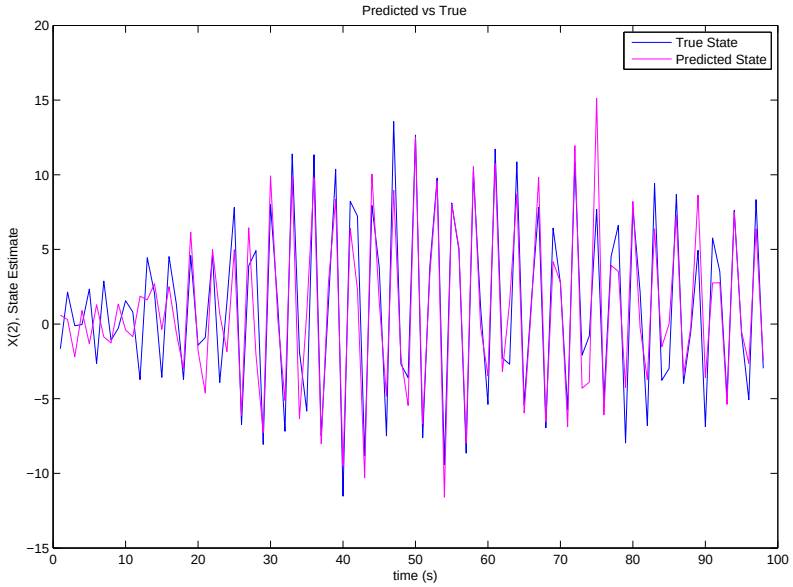


Figure 4.4: Predicted State vs True State

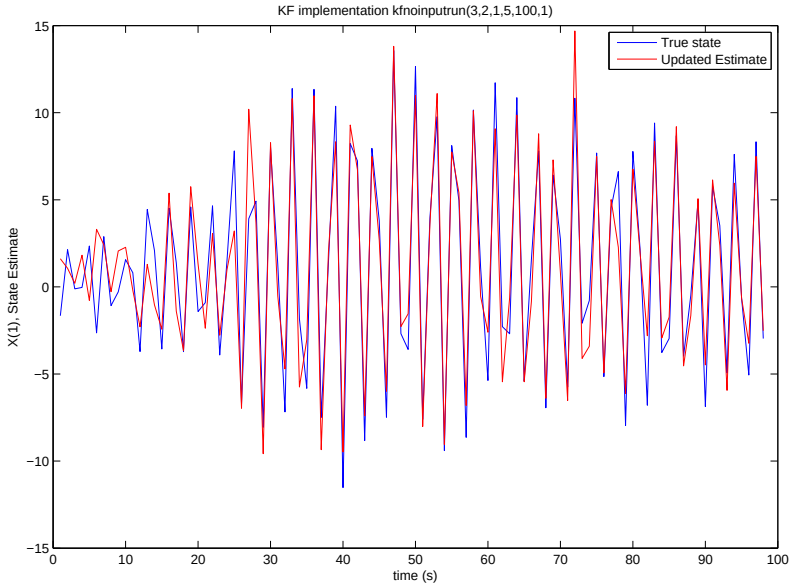


Figure 4.5: Updated State vs True State

4.3 Extended Kalman Filter

4.3.1 Introduction

In case of kalman filter we know it is applicable to the Linear systems in general, but if the system is non linear then we use the concept of extended kalman filter wher we linearize the non linear function value at an estimate Consider the non linear dynamics

$$X_{k+1} = f(X_k) + w_k \tag{4.14}$$

$$Y_k = g(X_k) + v_k \tag{4.15}$$

Here, $f(X_k)$, $g(X_k)$ are nonlinear functions. Also, $f : \mathbb{R}^n \to \mathbb{R}^n, g : \mathbb{R}^n \to \mathbb{R}^p$ where w_k,v_k are gaussian random processes with zero mean and covariance matrices Q and R respectively. As discussed in the Kalman filter here also we proceed with two steps Prediction and Updation. But in the prediction step we need to know about the linearization of non linear function at a point and also about the evaluation of the jacobian. The next section describes about these.

4.3.2 Linear Approximation and Multivariable function Derivates

$f : \mathbb{R}^n \to \mathbb{R}^m$ is a general multivariable function Derivative of such an $'f'$ at a point 'a' is defined as , Consider

$$\lim_{h \to 0} \frac{||f(a+h) - f(a) - Df(a)(h)||_2}{||h||_2} = 0 \tag{4.16}$$

Note here that $Df(a) : \mathbb{R}^n \to \mathbb{R}^m$ and is linear. Such $Df(a)$ is called the derivative of f at a. when h is very small, then

$$||f(a+h) - f(a) - Df(a)(h)|| = 0$$
$$f(a+h) \simeq f(a) + Df(a)(h)$$

Note that this is possible only if $Df(a)$ exists.

To ensure that these derivatives exist there are two theorems. [23]

Theorem 4.3.1. *If $f : \mathbb{R}^n \to \mathbb{R}^m$ is differentiable at a, then $D_j f^i(a)$ exists for $1 \leq i \leq m$, $1 \leq j \leq n$ and $Df(a)$ is the $m \times n$ matrix .Here,$D_j f^i(a)$ is the jth partial derivative of f^i at a .*

Theorem 4.3.2. *If $f : \mathbb{R}^n \to \mathbb{R}^m$ then $Df(a)$ exists if all $D_j f^i(a)$ exist in an open set containing 'a' and if each function $D_j f^i$ is continuous at a.*

So, if all $D_j f^i(x)$ exist in an open set containing 'a' and if each function $D_j f^i$ is continuous at a, then $Df(a)$ exists according to the above theorems.

4.3.3 Prediction step of EKF

We, first linearize f at the $\hat{X}_{k|k}$

$$\begin{aligned} f(X_k) &= f(\hat{X}_{k|k} + h) \\ f(\hat{X}_{k|k} + h) &= f(\hat{X}_{k|k}) + Df(\hat{X}_{k|k})h \\ f(X_k) &= f(\hat{X}_{k|k}) + +Df(\hat{X}_{k|k})[X_k - \hat{X}_{k|k}] \end{aligned}$$

Note that $Df(\hat{X}_{k|k})$ has to exist for this. Refer previous section on Linear Approximation.

$$\begin{aligned} f(X_k) &= [f(\hat{X}_{k|k}) - Df(\hat{X}_{k|k})\hat{X}_{k|k}] + Df(\hat{X}_{k|k})X_k \\ X_{k+1} &= [f(\hat{X}_{k|k}) - Df(\hat{X}_{k|k})\hat{X}_{k|k}] + Df(\hat{X}_{k|k})X_k + w_k \end{aligned}$$

Now, $\hat{X}_{k+1|k} = E[X_{k+1}/\mathcal{Y}_k]$

$$\begin{aligned} \hat{X}_{k+1|k} &= Df(\hat{X}_{k|k})E[X_k|\mathcal{Y}_k] + f(\hat{X}_{k|k}) - Df(\hat{X}_{k|k})\hat{X}_{k|k} + E[w_k|\mathcal{Y}_k] \\ &= f(\hat{X}_{k|k}) \end{aligned}$$

$$\begin{aligned} E[X_{k+1}|\mathcal{Y}_{k+1}] &= \hat{E}[X_{k+1}/\mathcal{Y}_k] + \hat{E}[X_{k+1}/\mathcal{Z}_{k+1}] \\ \hat{E}[X_{k+1}/\mathcal{Z}_{k+1}] &= \Delta_{k+1}[Y_{k+1} - C_{k+1}\hat{X}_{k+1|k} - G_{k+1}] \end{aligned}$$

we know the condition that

$$E[X_{k+1} - \hat{E}[X_{k+1}/\mathcal{Z}_{k+1}]]\tilde{Y}^T_{k+1|k} = 0 \tag{4.17}$$

$$E[X_{k+1}\tilde{Y}^T_{k+1|k}] = \Delta_{k+1}E[\ Y_{k+1|k}\ Y^T_{k+1|k}] \tag{4.18}$$

substitute $X_{k+1} = \hat{X}_{k+1|k} + \tilde{X}_{k+1|k}$ in the above equation where $\tilde{Y}_{k+1|k} = Y_{k+1} - C_{k+1}\hat{X}_{k+1|k} - G_{k+1}$, we solve for $\Delta_{k+1|k}$.

$$\Delta_{k+1|k} = (P_{k+1|k}C^T_{k+1})(C_{k+1}P_{k+1|k}C^T_{k+1} + R)^{-1}$$

where $P_{k+1|k} = E[\tilde{X}_{k+1|k}\tilde{X}^T_{k+1|k}]$ and to estimate $P_{k+1|k}$ we know $\tilde{X}_{k+1|k}$, $X_{k+1} - \hat{X}_{k+1|k}$ Substituting we get

$$P_{k+1|k} = A_k P_{k|k} A^T_k - F_k + Q \tag{4.19}$$

4.3.4 Updation step in EKF

The updation step is

$$\hat{X}_{k+1|k+1} = \hat{X}_{k+1|k} + \Delta_k(C_k\tilde{X}_{k+1|k}) + \Delta_k v_k)$$

$$\tilde{X}_{k+1|k} = (A_k - A_k\Delta_k C_k)\tilde{X}_{k|k-1} - A_k\Delta_k v_k$$
$$P_{k+1|k} = (A_k - A_k\Delta_k C_k)P_{k|k}(A_k - A_k\Delta_k C_k)^T + A_k\Delta_k R\Delta_k^T A_k^T$$

Finally the updation step would be

$$\hat{X}_{k+1|k+1} = f(\hat{X}_{k+1|k}) + \Delta_{k+1}(Y_{k+1} - C_{k+1}\hat{X}_{k+1} - G_{k+1}) \tag{4.20}$$

and also after obtaining the $\hat{X}_{k+1|k+1}$ we can get the updated estimate covariance as

$$P_{k+1|k+1} = A_k P_{k|k} A_k^T + Q + \Delta_{k+1}C_{k+1}P_{k+1}C_{k+1}^T\Delta_{k+1}^T + \Delta_{k+1}R\Delta_{k+1}^T. \tag{4.21}$$

4.3.5 Overall steps to Implement EKF

The following four steps are invovled in implementing Extended Kalman Filter
Overall steps to Implement EKF The following four steps are involved in implementing Extended Kalman Filter
Step1: Prediction Estimate

$$\hat{x}_{k+1|k} = f(\hat{x}_{k+1|k}) \tag{4.22}$$

Step 2: Predicted Estimate Covariance

$$P_{k+1|k} = A_k P_{k|k} A_k^T + Q \tag{4.23}$$

where

$$A_k = Df(\hat{x}_{k+1|k}) \tag{4.24}$$

where Df is the Jacobian
Step 3: Updated State Estimate

$$\hat{x}_{k+1|k+1} = f(\hat{x}_{k+1|k}) + \Delta_{k+1}(Y_{k+1} - C_{k+1}\hat{X}_{k+1} - G_{k+1}) \tag{4.25}$$

$$\Delta_{k+1|k} = (P_{k+1|k}C_{k+1}^T)(C_{k+1}P_{k+1|k}C_{k+1}^T + R)^{-1} \tag{4.26}$$

Step 4: Updated Estimate Covariance

$$P_{k+1|k+1} = A_k P_{k|k} A_k^T + Q + \Delta_{k+1}C_{k+1}P_{k+1}C_{k+1}^T\Delta_{k+1}^T + \Delta_{k+1}R\Delta_{k+1}^T \tag{4.27}$$

: Prediction Estimate

$$\hat{X}_{k+1|k} = f(\hat{X}_{k+1|k}) \tag{4.28}$$

Step 2: Predicted Estimate Covariance

$$P_{k+1|k} = A_k P_{k|k} A_k^T + Q \tag{4.29}$$

where

$$A_k = Df(\hat{X}_{k+1|k}) \tag{4.30}$$

Step 3: Updated State Estimate

$$\hat{X}_{k+1|k+1} = f(^{X}_{k+1|k}) + \Delta_{k+1}(Y_{k+1} - C_{k+1}\hat{X}_{k+1} - G_{k+1})\Delta_{k+1|k} = (P_{k+1|k}C_{k+1}^T)(C_{k+1}P_{k+1|k}C_{k+1}^T + R)^{-1} \tag{4.31}$$

Step 4: Updated Estimate Covariance

$$P_{k+1|k+1} = A_k P_{k|k} A_k^T + Q + \Delta_{k+1} C_{k+1} P_{k+1} C_{k+1}^T \Delta_{k+1}^T + \Delta_{k+1} R \Delta_{k+1}^T \tag{4.32}$$

4.3.6 Implementing EKF for Van Der Poll Oscillator

A MATLAB program is written to implement the Extended Kalman Filter for the Van Der Pol Oscillator.

Van Der Pol Oscillator is a non conservative oscillator with non linear damping. The system is described by the following second order differential equation.

$$\frac{d^2x}{dt^2} - \mu(1 - x^2)\frac{dx}{dt} + x = 0 \tag{4.33}$$

x is position coordinate , μ is scalar parameter indicating non linearity

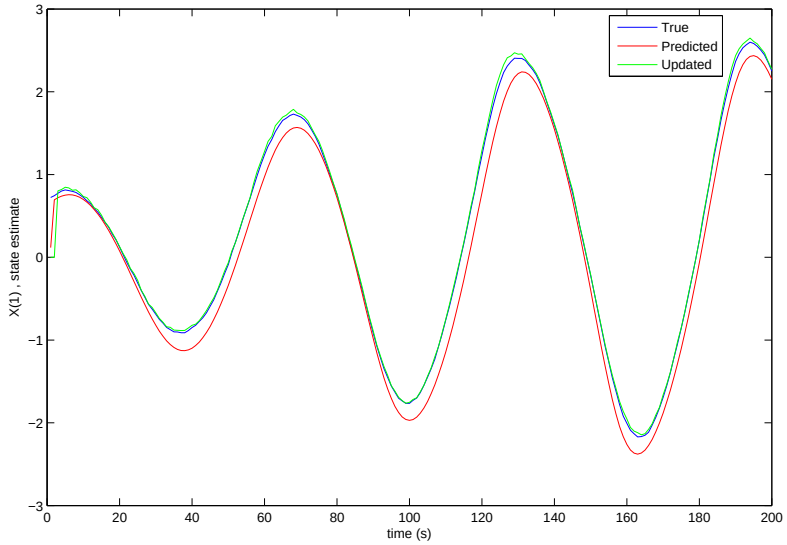


Figure 4.6: Van Der Pol Oscillator State Estimates by Implementing Extended Kalman Filter

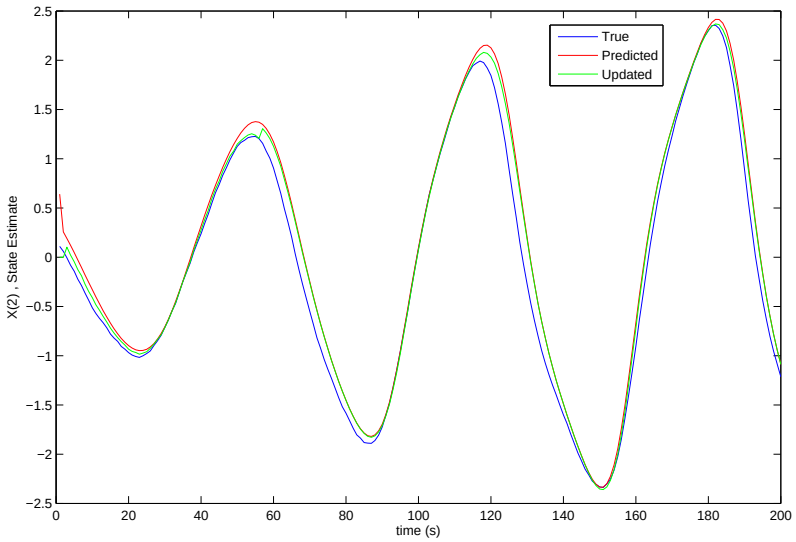


Figure 4.7: Van Der Pol Oscillator State Estimates by Implementing Extended Kalman Filter

4.4 Unscented Kalman Filter

Extended Kalman Filters are widely used for non linear systems where the non linear states are linearized and calculated Jacobian matrices are substituted in Kalman filter equations. Extended Kalman Filter (EKF) has some limitations

- If the error propagation is approximated by a linear function then only the linear transformations are reliable. If this is not followed linearization approximation will be poor and results in estimate divergence.
- Linearization can be applied only if Jacobian matrix exists. Some systems contain singularities and discontinuties.
- Calculating jacobian matrices can be difficult and also error prone process.

So overcome the limitations of implementing EKF for non linear systems, Julier et.al [17] developed a new linear estimator which yields performance equivalent to Kalman filter for linear systems, yet generalizes elegantly to non linear systems without linearization steps required by EKF.

The principle of unscented transformation as illustrated below in figure

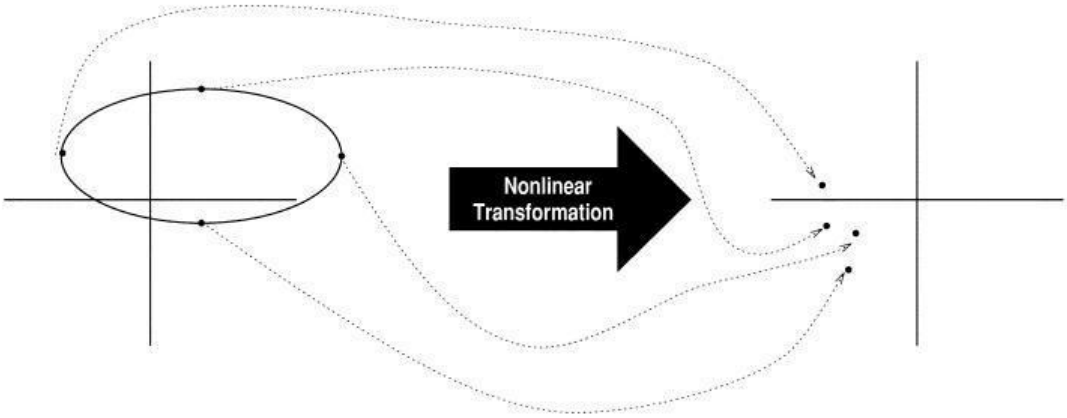


Figure 4.8: The principle of the Unscented Transformation [16]

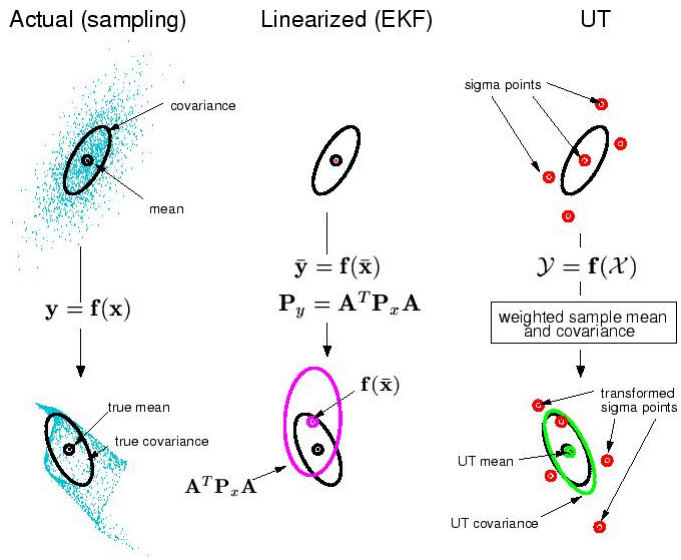


Figure 4.9: EKF and UKF (www.azimuthproject.org)

We generate a set of points whose sample mean and sample covariance are $\hat{\mathbf{x}}(k|k)$ and covariance $\mathbf{\Sigma}(k|k)$ respectively. The non linear function is applied to each of these points in turn to yield a sample and predicted mean and covariance are calculated from the transformed sample. Though it resembles a Monte Carlo method samples are not drawn at random.

The n-dimensional random variable $\mathbf{x}(k)$ with mean $\hat{\mathbf{x}}(k|k)$ and covariance $\mathbf{\Sigma}(k|k)$ is approximated by 2n+1 weighted samples or Sigma points selected by the algorithm

$$\begin{aligned}
\chi_o(k|k) &= \hat{\mathbf{x}}(k|k) i = 0 && (4.34)\\
W_o &= \kappa/(n+\kappa) && (4.35)\\
\chi_i(k|k) &= \hat{\mathbf{x}}(k|k) + \left(\sqrt{(n+\kappa)\mathbf{\Sigma}(k|k)}\right)_i \; i = 1, 2, ..n && (4.36)\\
W_i &= 1/2(n+\kappa) && (4.37)\\
\chi_{i+n}(k|k) &= \hat{\mathbf{x}}(k|k) + \left(\sqrt{(n+\kappa)\mathbf{\Sigma}(k|k)}\right)_i \; i = 1, 2, ..n && (4.38)\\
& && (4.39)
\end{aligned}$$

where $\kappa \in \mathbb{R}$, $\left(\sqrt{(n+\kappa)\mathbf{\Sigma}(k|k)}\right)_i$ is the i^{th} row or column of the matrix square root of $(n+\kappa)\mathbf{\Sigma}(k|k)$, W_i is the weight associated with i^{th} point.

4.5 Applying the Unscented Transformation

As discussed in the paper [16] , The UKF consists of the following steps

1 Predict the new state of the system $\hat{\mu}_n$ and its associated covariance $\hat{K}_n$. This

prediction must take into account the effects of process noise.

2 Predict the expected observation $\hat{y}_n$ and the innovation covariance $\hat{S}_n$. This prediction should include effects of observation noise.

3 Predict the cross covariance matrix $\hat{K}_n^{xy}$.

In the Unscented Kalman filter these states are augmented with the process and noise terms to give an augmented vector and that augmented vector is used in the algorithm of filter. The process model is given by

$$X_k = f(X_{k-1}) + v_k \tag{4.40}$$

The observation model is given by

$$Y_k = g(X_k) + w_k \tag{4.41}$$

The augmented vector is

$$\bar{X}_{n-1}^a = \begin{bmatrix} X_{n-1} \\ v_k \\ w_k \end{bmatrix} \tag{4.42}$$

The process and observation models are written as functions of $\bar{X}_n^a$

$$\begin{aligned} \bar{X}_n^a &= f^a[\bar{X}_n^a] \\ Y_n &= g^a[\bar{X}_n^a] \end{aligned}$$

But the unscented transformation actually uses the Sigma Points that are computed from the augmented mean and covariance as below

$$\mu_{a,n} = \begin{pmatrix} \mu_n \\ 0 \\ 0 \end{pmatrix} \tag{4.43}$$

and

$$K_{a,n} = \begin{bmatrix} K_n & 0 & 0 \\ 0 & Q & 0 \\ 0 & 0 & R \end{bmatrix} \tag{4.44}$$

4.5.1 General formulation of KF using Unscented Transformation

As discussed in the paper by Simon Julier et. al it involves the following 9 steps.

1 The set of sigma points are generated by the Sigma Point Algorithm as discussed in earlier section to the augmented system .

2 Instantiation of each point through the process model gives the transformed set of points

$$\hat{X}_{a,n}^{(i)} = f[\hat{X}_{a,n}]$$

3 Predicted mean is computed as

$$\hat{\mu}_{a,n} = \sum_{i=0}^{p} W^{(i)} \hat{X}_{a,n}^{(i)}$$

4 Predicted Covariance is computed as

$$\hat{K}_{a,n} = \sum_{i=0}^{p} W^{(i)} \left(\hat{X}_{a,n}^{(i)} - \hat{\mu}_{a,n}\right) \left(\hat{X}_{a,n}^{(i)} - \hat{\mu}_{a,n}\right)^T$$

5 Instantiation of each of the prediction point through the observation model.

$$\hat{Y}_{a,n}^{(i)} = g[\hat{X}_{a,n}^{(i)}]$$

6 Predicted Observation is calculated by

$$\hat{Y}_{a,n} = \sum_{i=0}^{p} W^{(i)} \hat{Y}_{a,n}^{(i)} \tag{4.45}$$

7 The innovation covariance is calculated by

$$\hat{S}_n = \sum_{i=0}^{p} W^{(i)} \left(\hat{Y}_n^{(i)} - \hat{Y}_n\right) \left(\hat{Y}_{a,n}^{i} - \hat{Y}_n\right)^T \tag{4.46}$$

8 Cross Covariance matrix is determined by

$$\hat{K}_n^{xy} = \sum_{i=0}^{p} W^{(i)} \left(\hat{X}_n^{(i)} - \hat{\mu}_n\right) \left(\hat{Y}_n^{(i)} - \hat{Y}_n\right)^T \tag{4.47}$$

9 Finally the update can be performed using the normal Kalman filter equations

$$\mu_n = \hat{\mu} + W_n \nu_n \tag{4.48}$$
$$K_n = \hat{K}_n^{xy} - W_n \hat{S}_n W_n^T \tag{4.49}$$
$$\nu_n = Y_n - \hat{Y}_n \tag{4.50}$$
$$W_n = \hat{K}_n^{xy} \hat{S}_n^{-1} \tag{4.51}$$

At the end of step 9 when the updated mean and covariance are obtained the steps 1 to 9 are executed again in the loop for next time steps. This completes the algorithm for the

Unscented Kalman Filter.

4.5.2 Implementing Unscented Kalman Filter

A MATLAB program is written to implement the unscented kalman filter . The problem is A vehicle enters the atmosphere at high altitude and at a very high speed [17]. The position of the body is tracked by a radar which measures the range. The vehicle state dynamics are given by the following equations.This is a higly non linear system.

$$\begin{aligned}
\dot{x}_1(k) &= x_3(k) \\
\dot{x}_2(k) &= x_4(k) \\
\dot{x}_3(k) &= D(k)x_3(k) + G(k)x_1(k) + v_1(k) \\
\dot{x}_4(k) &= D(k)x_4(k) + G(k)x_2(k) + v_2(k) \\
\dot{x}_5(k) &= v_3(k)
\end{aligned}$$

where

$$\begin{aligned}
D(k) &= -\beta(k)exp\left(\frac{R_0 - R(k)}{H_0}\right)V(k) \\
G(k) &= -\frac{Gm_0}{r^3(k)} \\
\beta(k) &= \beta_0 exp\left(x_5(k)\right) \\
R(k) &= \sqrt{x_1^2(k) + x_2^2(k)} \\
V(k) &= \sqrt{x_3^2(k) + x_4^2(k)}
\end{aligned}$$

Here is a result of simulation ,

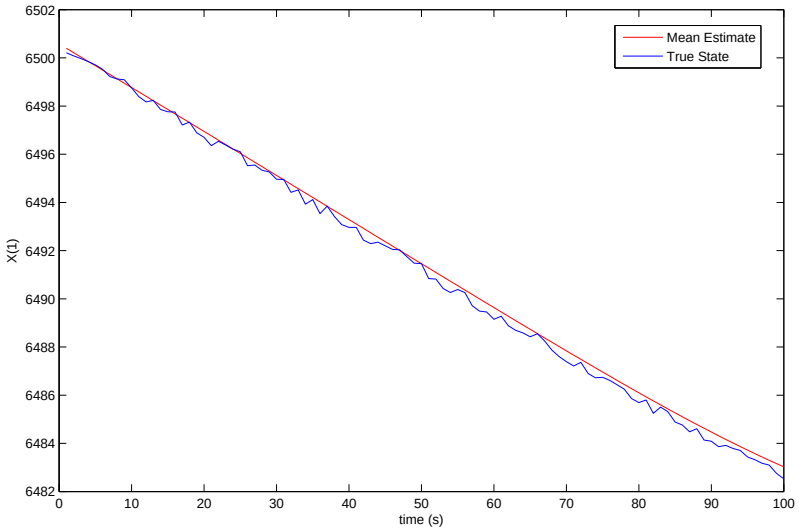


Figure 4.10: The reentry problem implemented by UKF, result showing state x(1)

Chapter 5

Results

5.1 Implementation of UKF for SOFC system

In the earlier two chapters the model development is explained and the theory and derivation of KF, EKF algorithms are discussed with some examples. Also the Unscented Kalman Filter (UKF) algorithm is discussed in detail in the Chapter 4 last section which with an example. We now implemented the UKF algorithm in estimating the states for SOFC system. The lumped model with choked flow assumption is simulated and we implemented UKF to estimate the states of the system. It is observed that UKF estimates the states of system only with very low covariance values. The estimates of states and the polarization loss are shown in this section. It is observed that UKF is able to estimate the states for lumped model of SOFC . For the modified lumped model with non-choked flow the estimation by UKF is to be investigated. In the lumped model we considered the feed in anode side with fuel composition as 97.5% H_2 and 2.5% H_2O and cathode side is air. We assumed that anode and cathode channel pressures to be 3 atm and inlet temperature is 1073 K and draw current value as input. The dynamics of the system is obtained by solving using ode solver in MATLAB and then that model is simulated by writing a program to simulate the system in MATLAB for time of 300 sec. The time step considered is 0.01. A program in MATLAB has been written to obtain the estimates by using Unscented Kalman Filter (UKF) with an input of initial state conditions as mean. The initial error covariance for first three states (partial pressures) is 0.00000001 and fourth state (temperature) is 0.01 . Similar values are considered for State noise covariance. The measurement noise covariance is considered to be 0.0001. It is observed that if the noise covariance are increased than the earlier mentioned values UKF is not able to estimate the states because the states (i.e. the partial pressures) can become negative. So this limitation brings into picture the use of constraints in implementation of UKF to be able to estimate states.

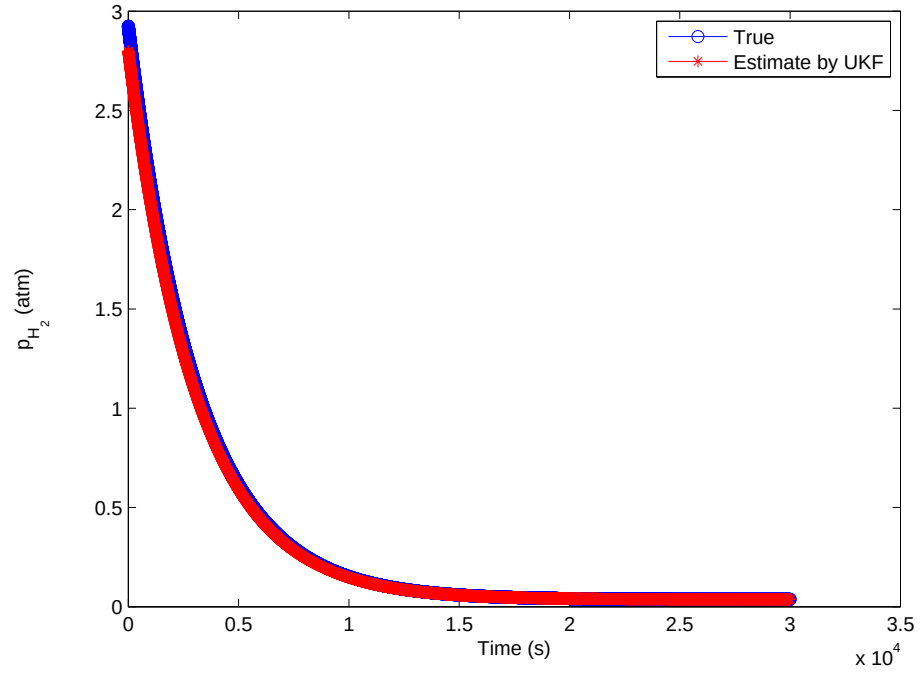


Figure 5.1: Estimate of p_{H_2} by UKF

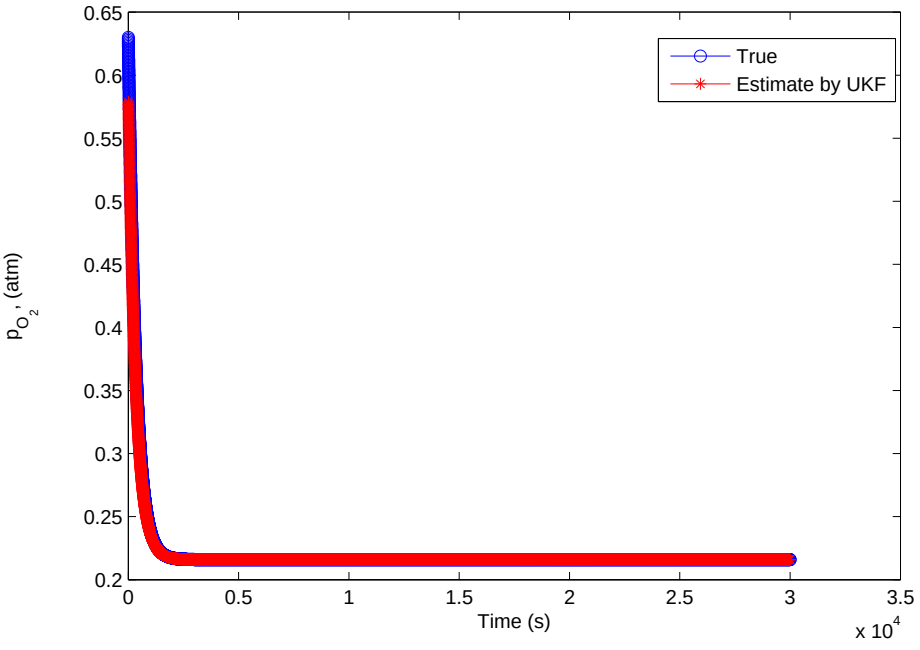


Figure 5.2: Estimate of p_{O_2} by UKF

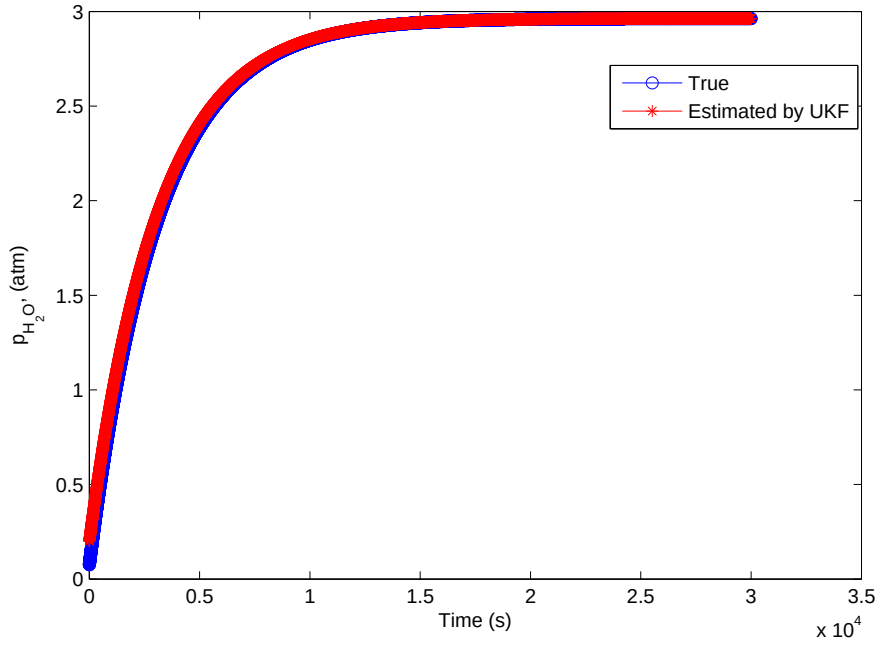


Figure 5.3: Estimate of p_{H_2O} by UKF

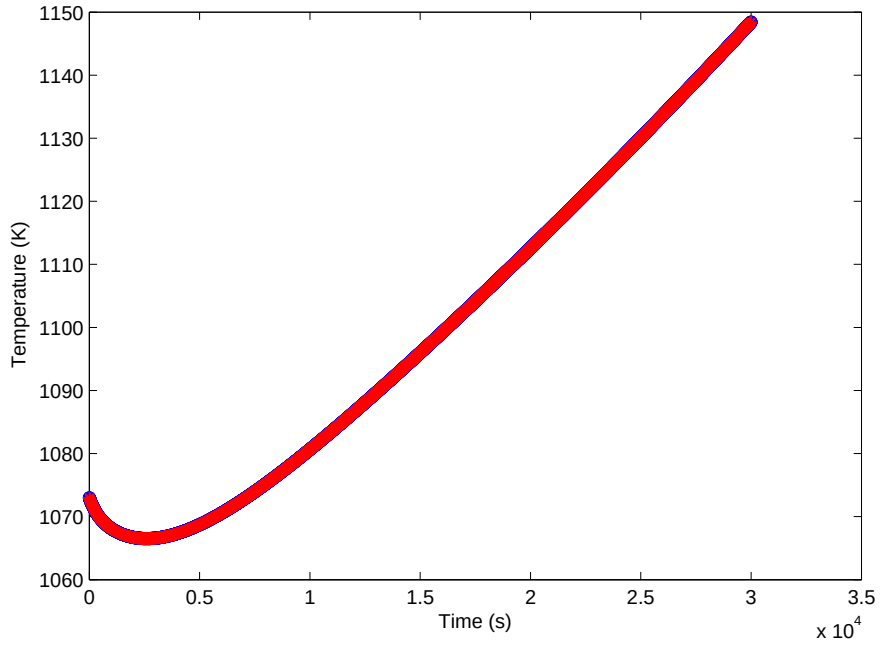


Figure 5.4: Estimate of T_s by UKF

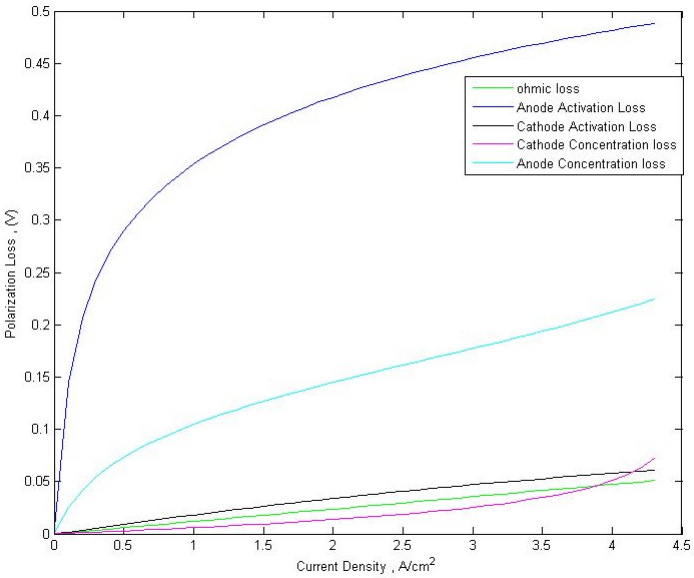


Figure 5.5: Polarization Loss-Cell

Chapter 6

Conclusion and Future Work

Considering the practical benefits of fuel cells, it is important to develop control models for SOFC which will benifical to the commercialization of this technology. The performance if the cell depends on the partial pressures and temperature of the stack which must be properly controlled. So this motivated to work on the Implementation of Unscented Kalman Filter(UKF) on SOFC system. As it is good to start the model development with less complex model like lumped model and to employ it in state estimation, we proceeded this way. It is observed that UKF with proper initialization is able to estimate the states of system.

In the lumped model, by modifying few assumptions a much better model can be developed and that mathematical model coupled with other models can be used to design control relevant models for SOFC systems. A more sophisticated method of estimation using Particle filters, which are alternative to UKF can be considered for estimation of states in systems like SOFC. Application of Particle filters with constraints for non linear state estimation in systems like SOFC is one which can be further investigated.

References

[1] Ryan O'Hayre, Suk Won Cha, Whitney Colella, Fritz B. Prinz. *Fuel Cell Fundamentals, John Wiley Sons* 2nd edition, 2009

[2] Mona Bavarian and Masod Soroush, Mathematical Modeling, Steady State and Dynamic Behavior, and Control of Fuel Cells: A Review, *Ind. Eng. Chem. Res* **49**, 7922-7950, 2010

[3] Debangsu Bhattacharyya and Raghunathan Rengaswamy, A Review of Solid Oxide Fuel Cell (SOFC) Dynamic Models *Ind. Eng. Chem. Res* **48**, 6068–6086, 2009.

[4] Andrew M. Colclasure, Borhan M. Sanandaji, Tyrone L. Vincent , Robert J. Kee, Modeling and control of tubular solid-oxide fuel cell systems. I: Physical models and linear model reduction *Journal of Power Sources* **196**,197-207, 2011

[5] Borhan M. Sanandaji, Tyrone L. Vincent ,Andrew M. Colclasure and Robert J. Kee, Modeling and control of tubular solid-oxide fuel cell systems: II. Nonlinear model reduction and model predictive control *Journal of Power Sources* **196**,208-217, 2011

[6] M. Secanell , J. Wishart , P. Dobson, Computational design and optimization of fuel cells and fuel cell systems:A review *Journal of Power Sources* **196**, 3690-3704, 2011

[7] M. Kandepu R, Imsland L, Foss B, Stiller C, Thorud B, Bolland O. Modeling and Control of a SOFC-GT-based autonomous power system. *Energy* **32(4)**, 406-417, 2007

[8] A K M Murshed, Biao Huang, K Nandakumar. Control relevant modeling of planar solid oxide fuel cell system. *Journal of Power Sources* **163**, 830-845, 2007

[9] A K M Murshed, Biao Huang, K Nandakumar. Estimation and control of solid oxide fuel cell system. *Computers and Chemical Engineering* **34**, 96-111, 2010

[10] Periasamy Vijay, Moses O tade. An adaptive non linear observer for the estimation of temperature distribution in the planar solid oxide fuel cell. *Journal of Process Control* **xxx**, xxx-xxx, 2012 (Article in Press)

[11] Das, T.; Mukherjee, R. Observer design for a steam reformer based solid oxide fuel cell system with anode recirculation. Proceedings of the ASME, IMECE; Seattle, WA, 2007; American Society of Mechanical Engineers: New York, 2007

[12] Lin, P.-H.; Hong, C.-W. Cold start dynamics and temperature sliding observer design of an automotive SOFC APU. *J. Power Sources* **187 (2)**, 517–526. 2009

[13] Mueller, F.; Jabbari, F.; Brouwer, J.; Junker, S.; Ghezel-Ayagh,H. Linear quadratic regulator for a bottoming solid oxide fuel cell gas turbine hybrid system. *J. Dyn. Syst., Meas., Control* **131**,051002, 2009

[14] J. Padulles, G.W. Ault , J.R. McDonald . An integrated SOFC plant dynamic model for power systems simulation. *Journal of Process Sources* **86**, 495–500, 2000.

[15] Huayang Zhu, Robert J. Kee, Vinod M. Janardhanan,Olaf Deutschmann and David G. Goodwin,An integrated SOFC plant dynamic model for power systems simulation. *Journal of The Electrochemical Society* **152(12)**, A2427-A2440, 2005.

[16] Simon J Julier and Jeffrey K Uhlmann, Unscented filtering and nonlinear state estimation. *Proceesings of IEEE* **92(3)**, 401-422, 2004.

[17] Simon Julier, Jeffrey Uhlmann and Hugh F Durrant Whyte. A New method for nonlinear transformation of means and covariances in filters and estimators. *IEEE transactions on Automatic Control* **45(3)**, 477-482, 2000.

[18] Robert J. Kee,Huayang Zhu and D. G. Goodwin, *International Symposium* on Combustion july 2004

[19] Huayang Zhu, Robert J. Kee, Vinod M. Janardhanan, Olaf Deutschmann, and David G. Goodwin, Modeling Elementary Heterogeneous Chemistry and Electrochemistry in Solid-Oxide Fuel Cells, *Journal of The Electrochemical Society* **152** (12), A2427-A2440, 200

[20] S.H. Chan , K.A. Khor, Z.T. Xia, A complete polarization model of a solid oxide fuel cell and its sensitivity to the change of cell component thickness *Journal of Process Sources* **93**, 130–140, 2001.

[21] R.E.Kalman , A New Approach to Linear Filtering and prediction Problems, Transactions of ASME *Journal Of Basic Engineering* **82**, 35-45, 1960.

[22] Probability With Martingales by David Williams, Cambrige University Press, 1991.

[23] Calculus on Manifolds by Michael Spivak, Perseus Book Publishing, 1965.

[24] www.seca.doe.gov