A NONLINEAR PREDICTIVE CONTROL OF MICROSCOPIC PROCESSES USING A FUZZY SYSTEM IDENTIFICATION APPROACH

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Abstract

System identification and controller design for systems with atomic-scale dimensions is a challenging concept. In this work, the problem of model-based control of a microscopic process is investigated. The unavailability of closed-form models, as well as the ill-definition of variables to describe the process evolution, makes the controller design task challenging. We address this problem via a fuzzy system identification of the dominant process dynamics. The data required for the system identification of such processes is produced employing atomistic simulations. A methodology is developed in which fuzzy logic for nonlinear system identification is coupled with nonlinear model predictive control for regulation of microscopic processes. We illustrate the applicability of the proposed methodology on a Kinetic Monte Carlo (KMC) realization of a simplified surface reaction scheme that describes the dynamics of CO oxidation by O\textsubscript{2} on a Pt catalytic surface. The second case study on which this procedure performance will be evaluated is thin film deposition of silicon that has wide applicability in photovoltaic industry. Thin film deposition is of the most important manufacturing processes in the category of microscopic simulation and controller design. The quality of thin film which can be used in several different useful fields is highly dependent on the manipulated variables of the process which can be intentionally changed to achieve the highest quality. Using a lattice model of thin film evolution, the important characteristics of thin film, like thickness, roughness and porosity, can be simulated. The stochastic realization of this lattice model evolution is captured with KMC Simulation.
The nonlinear fuzzy model gives a reasonable approximation to the system even without using filter for the system and the proposed controller successfully forces the process from one stationary state to another state for the CO oxidation on Pt catalyst.

In the thin film deposition process, two important parameters are porosity and roughness of the film, which affect the quality of the thin film devices. The modeling and controller design approach is used for controlling porosity and roughness of thin film deposition process.
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1. Introduction

1.1. Modeling and control of thin film deposition

Modeling and control of thin film deposition, which is a process of delivering the precursor material on the substrate on which the precursor attaches to form the thin film, is becoming an important issue in various industries. Some of the most important applications include photovoltaics, microelectromechanical systems, memories and microprocessors.

One of the most important fields of thin film deposition usage is semiconductor manufacturing. For example, an integrated circuit consists of thin film layers with different patterns and chemical compositions (Automatic control in microelectronics manufacturing practices, challenges, and possibilities, 2000), (Modeling and control of microelectronics materials processing, 1995). The performance of semiconductors highly depends on thin film patterns and interfaces and microscopic structure of thin films (Thin films in the integrated circuit industry: Requirements and deposition methods, 1993).

The important factor in determining the quality of such materials is the microstructure of the product. Therefore, the precise control of microstructure during thin film production is of paramount importance. The most important microscopic parameters which should be controlled during thin film production are roughness of the film surface and porosity of the thin film. Many thin film deposition methods have been employed for
producing thin films, including chemical vapor deposition, evaporation, sputter deposition and electrochemical deposition.

Because of huge and increasing usage of thin film devices, there has been increasing research on modeling and control of thin film deposition for such devices with the main objectives of control the spatial uniformity and microstructure of thin films. The process models are generally derived from continuum conservation laws to describe the reactor scale process and for the atomistic scale models, approaches like Kinetic Monte Carlo (KMC) or Molecular Dynamics (MD) are used.

When the length scale of surface processes approaches the distance between atoms, continuum assumptions are no longer valid. In this situation, atom scale simulations like ab-initio, molecular dynamics or KMC are used for achieving the system approach. The high computational demands associated with ab-initio and molecular dynamics methods make their usage impractical in simulation of thin film growth.

Two determining variables affecting the quality of thin film deposition are deposition rate of precursor material and substrate temperature. The substrate temperature is more important in low rate growth thin film productions.

As mentioned, an important factor affecting the thin film quality is the change in deposition condition during thin film production. Therefore for online evaluation of the thin film production process, some sensors are used for online monitoring of the reactor condition or thin film properties.

If several layers are incorporated in thin film production, the need for more precise control on process would be increased because any defect in each layer can have considerable effect on the final product (Seshan, 2002).
As precursor atoms reach to the substrate, they may adsorb to the substrate or desorb to the reactor precursor area. Some of the atoms adsorbed would diffuse on the surface of the substrate and reorganize to reach to the lower levels of energy. The probability of desorption of an atom on the substrate surface depends on the number of bonds of that atom with the neighbor deposited atoms. The probability of diffusion decreases with increase in the number of bonds.

Detailed mathematical modeling for being used in the process optimization to minimize spatial nonuniformity of thin films has been the focus of significant research during recent years (A tailored optimization strategy for PDE-based design: application to a CVD reactor, 2004), (Thin Film Deposition, Patterning, and Printing in Organic Thin Film Transistors, 2004). However, the effect of macroscopic phenomena on the microstructure of thin films is not addressed in those studies. Therefore, the incorporation the macroscopic and microscopic phenomena into optimization through multiscale models for thin film growth is necessary. Recently, it has become possible to perform real-time measurements of microscopic properties of thin films by the techniques like scanning tunneling microscopy (Fundamental processes in Si/Si and Ge/Si studied by scanning tunneling microscopy during growth, 2001) or spectroscopic ellipsometry (Ultraviolet-extended real-time spectroscopic ellipsometry for characterization of phase evolution in BN thin films, 2001). Achieving to such abilities motivated more research in the field of real-time control of thin film deposition process.
1.2. Literature review

Unlike continuum models for reactor scale phenomena, the models that describe the evolution of microscopic state of thin film are not available in closed-form. Therefore, it is difficult to perform model-based controller design directly on the basis of microscopic simulation models. In (Estimation and control of surface roughness in thin film growth using kinetic Monte-Carlo methods, 2003), KMC simulations are employed as the underlying process model for control of the microstructure of thin film deposition. In (Multivariable predictive control of thin film deposition using a stochastic PDE model, 2005) the linear stochastic PDEs are employed as the underlying growth model to enable the use of PI and predictive controllers in thin film deposition. In (Reduction and identification methods for Markovian control systems, with application to thin film deposition, 2005), a methodology has been developed through statistical reduction of the master equation. The main limitation with these approaches is that they are not proper for complicated processes. It is important to consider the state and input constraints which are critical in thin film deposition in semiconductor production.

Multiscale models are used to quantify process evolution across all relevant length scales and model product behavior considering the current computational limitations. However, such models pose significant challenges, both from an analysis and control point of view (Control of Multiscale and Distributed process systems-preface, 2005). Such problems are attributed in part to the unavailability of closed-form models to describe the process evolution at molecular-level detail and also these modelings are computationally intensive where prevents their real-time implementation.
Because of the complex process dynamics and the precise quality requirements, a significant amount of research has focused on the design of control structures for such systems. In order to circumvent the mentioned limitations, one of the proposed approaches identifies stochastic partial differential equation models to design the controller (Nonlinear Feedback Control of Surface Roughness Using a Stochastic PDE: Design and Application to a Sputtering Process, 2006). This approach assumes specific structure to the nonlinear stochastic terms. In another approach, the off-line and subsequently the on-line identification of bilinear models for the process, which are then used for the controller synthesis (Multiscale Optimization using hybrid PDE /KMC process systems with applications to thin film growth, 2005). In order to improve on the linear controllers, an extension was proposed (Nonlinear feedback control of surface roughness using a stochastic PDE: Design and application to a sputtering process, 2006) in which a nonlinear feedback controller is designed to control the roughness of a one-dimensional surface using stochastic KSE as the underlying process growth model. The proposed approach assumed a specific structure to the nonlinear stochastic terms. In (Microscopic/stochastic timesteppers and coarse control: a kinetic Monte Carlo example, 2003), linear models were identified directly based on the output from KMC simulators. The linear controller, which is designed based on the identified model, is used to control the lower order statistical moments of microscopic distributions. In a different approach (Feedback control of surface roughness during thin-film growth using approximate low-order ODE model) the problem of non availability of closed-form models was addressed by deriving a low-order state space model through offline system identification, based on a finite set of “coarse” observables. The
identified state space model was used to design a model predictive controller to regulate the roughness, during thin film growth, at a particular setpoint. Although roughness is usually undesirable, it is difficult and expensive to control in manufacturing. Decreasing the roughness of a surface will usually increase its manufacturing costs exponentially. This often results in a trade-off between the manufacturing cost of a component and its performance in application. The coarse observables in this work were identified from spatial correlation functions of the thin film surface to represent the dominant traits of the microstructure during a deposition process. In (Identification of macroscopic variables for low-order modeling of thin-film growth, 2006), a minimum set of coarse spatially invariant parameters that accurately express the dominant behavior of the deposition surface during thin-film growth under adsorption and surface diffusion is identified and it is showed that different deposition surfaces constructed through a stochastic reconstruction procedure, with identical values for these parameters, exhibit approximately identical coarse dynamic behavior. In a different approach (Reduction and identification methods for Markovian control systems, with application to thin film deposition, 2004) a method is developed to reduce the dimension and complexity of a class of probabilistic systems that can be particularly useful when the number of inputs and outputs is small and in (A data-driven approach for reduction of molecular simulations, 2005), an approach is described in which targeted simulations are combined with systematic tools to describe the dynamics.

Another approach deals with the feedback linearization issue of nonlinear systems described by microscopic/stochastic simulators, where the lack of a closed-form model was circumvented by directly calculating the quantities needed for design of nonlinear controllers from appropriately initialized
microscopic simulations (An equation-free approach to nonlinear control: Coarse feedback linearization with pole-placement, 2006). However, the shortcoming of this method is that it is limited to stabilization and involves closed-loop eigenvalue assignment constraints. In two other works (Output feedback control of dissipative distributed process via microscopic simulations, 2005), (Multiscale optimization using hybrid PDE /KMC process systems with applications to thin film growth, 2005), hybrid multiscale process models were used, where the continuum laws which are applicable at the macroscopic level were combined with computationally expensive microscopic laws, Kinetic Monte-Carlo (KMC) or Molecular dynamics (MD) to get the “coarse” process behavior. Nonlinear process models were identified offline using the coarse variables through the solution of a series of nonlinear programs. Subsequently, the identified models were used to design output feedback controllers. The methodology used in this approach is computationally intensive and involves offline process identification.

To address the issues of both computational intensity and specific model structure, a methodology is demonstrated in (Online System-Identification Using Subspace algorithms for the control of Microscopic processes, 2008) where subspace algorithms for bilinear system identification were coupled with feedback linearization techniques for control of microscopic processes. Such models however are limited, since a one-to-one inputs-outputs map is necessary to ensure model convergence. Industrially relevant processes that exhibit complex behavior exist though such as those that have pitch-fork bifurcations. To ensure the accuracy of the identified stochastic models an approach based on a combination of Takagi-Sugeno (T-S) fuzzy system identification with locally linear models is evaluated in the present work and
nonlinear model predictive controllers are designed.

1.3. Applications and techniques

1.3.1. CO oxidation on Pt catalyst

The oxidation of CO by O$_2$ over Pt catalyst or other metal catalysts has been the subject of numerous studies, because of its importance in pollution control. This process has been traditionally used in the automotive industry for pollution control. During this process, the dangerous CO gas is converted to CO$_2$ on the Pt catalyst. There have been several studies on the kinetics of such process and identification of the parameters affecting this catalytic process.

The simplicity of this process was the main reason for its selection as the first case study in the simulation, system identification and controller design procedure in this study.

Each of the mechanistic steps in this process (adsorption, reaction and desorption) have been studied by surface science techniques (Oxygen inhibition of CO oxidation on polycrystalline Rh, 1980) (CO Oxidation on Pt(111): An Ab Initio Density Functional Theory Study, 1998) (CO Oxidation on Pt(110): Scanning Tunneling Microscopy Inside a High-Pressure Flow Reactor, 2002).

This reaction features most of the fundamental steps in a heterogeneous catalytic system:

1) molecular adsorption or desorption of the reactants ($CO \rightarrow CO_{ads}$)

2) dissociative adsorption of a reactant ($O_2 \rightarrow 2O_{ads}$)

3) surface reaction ($CO_{ads} + O_{ads} \rightarrow CO_2$)
Even it has been about 90 years since the classic investigations of CO oxidation on Pt catalyst by Langmuir (Langmuir, 1921), the CO oxidation reaction has remained as one of the most investigated reactions in heterogeneous catalysis (New insights into catalytic CO oxidation on Pt-group metals at elevated pressures, 2009).

1.3.2. Thin film deposition

As mentioned before, thin film products have found several different applications in different industries. Some examples of the usage of thin films are mentioned below:

- photovoltaic systems
- semiconductor industry (memories, microchips)
- corrosion resistant coatings
- jewelry and other decoration materials
- protective coatings and colors

Several methods for production of such devices have been used. These methods can be divided to two main categories: Physical Vapor Deposition (PVD) and Chemical Vapor Deposition (CVD).

In the PVD method, the thin film is formed by atoms directly transported from source to the substrate through gas phase. This method includes three main types (http://www.mrsec.harvard.edu):

- Evaporation
- Sputtering
- Reactive PVD
In the CVD method, the film is formed by chemical reaction on the surface of the substrate. This method includes four main types:

- Low Pressure CVD (LPCVD)
- Plasma Enhanced CVD (PECVD)
- Atmosphere Pressure CVD (APCVD)
- Metal Organic CVD (MOCVD)

For all those methods, the main parameters that should be controlled to be able to achieve the required quality are as follows:

- Substrate characteristics
- Material flux to the substrate
- Temperature
- Pressure
- Energy of the material deposited

The product of thin film deposition process should usually be uniform and free of voids and cracks. Much effort has been invested to enhance the manufacturing process to reach to the required quality with minimum use of time and material. The precise prediction of the shape of the deposited thin film based on the changes of the manipulated variables is so important in reaching to the required quality with acceptable cost.

In the reminder of this section, the most important thin film deposition techniques are briefly described.

**1.3.2.1. Evaporation**

In this method, the substrate is placed inside a vacuum chamber. The source of the material which should be deposited is put inside this vacuum chamber, as well. The source material is heated until the time that it starts to evaporate. The vacuum allows the evaporated materials to move freely in the
chamber towards the substrate. A schematic of this method is shown in figure 1 (http://ns.kopt.co.jp/English/ca_jou-gi/joutyaku.html). This technique is becoming the most important one in thin film deposition for high quality thin films like photovoltaic applications. The quality of the devices produced by this method has shown higher efficiency compared to other methods.

![Figure 1. Schematic of evaporation process](image)

1.3.2.2. Chemical Vapor Deposition (CVD)

In this technique, the substrate is exposed to one or more materials that react or decompose on the substrate. As mentioned before, this method is in different types that their difference is based on the chamber condition and material transport method to the substrate. Figure 2 depicts a schematic of a typical low-pressure hot wall CVD reactor used in coating silicon substrates (H.O.Pierson, 1992).

CVD owns some advantages over PVD techniques:

1. The pressure used in this method provides the condition for using this method for coating three-dimensional structures. Because in
PVD methods, the material has directional movements, complete coverage is not accessible for such structures.

2. The rate of material transport in this method is higher.

3. Because of simplicity of the reactor structure for such methods, changing the dimensions for fitting the required substrate would be easy.

4. Control of stochiometry is easy.

The main disadvantages of this method are as follows:

1. Lower efficiency for some products like photovoltaic devices
2. High temperature for some deposition cases which can be unfavorable for the structure
3. The materials used and by products in this method can be toxic
4. The amount of material used in this method can be much higher and this can increase the cost of the product considerably

![Figure 2. Schematic of a typical low pressure hot wall CVD reactor](image)

**1.3.2.3. Electrodeposition**

In the electrodeposition process, the substrate is placed in a liquid solution (electrolyte). When an electrical potential is applied between a counter electrode (anode) and the substrate or working electrode (cathode), a
chemical reaction takes place, resulting in the formation of a layer of material on the substrate. A schematic of this process is depicted in figure 3. The third electrode, that is, the reference electrode, is needed in potentiostatic electrodeposition where the potential of the working electrode is controlled in a predetermined manner. If materials are grown with the right conditions, electrodeposition is capable of producing high-quality materials for electronic device applications, but obtaining a uniform thickness with electrodeposition can be difficult depending on the geometry of the substrate.

![Figure 3. Schematic of Electrodeposition process](image)

1.3.2.4. Sputtering

Sputtering is a process in which atoms are ejected with high momentum from the source (sputtering target) to substrate. The substrate is placed in a vacuum chamber with the source material and an inert gas (such as argon) is introduced at low pressure. Gas plasma is struck using a power source, causing the gas to become ionized. The ions are accelerated towards the substrate, causing atoms of the source material to break off from the source.
in vapor form and condense on the substrate. A schematic of this method is shown in figure 4 (http://www.reade.com)

![Figure 4. Schematic of Sputtering Process](http://www.reade.com)

The advantage of this method is that even materials with very high melting points are easily sputtered while evaporation of these materials is problematic or impossible. The main limitation of this method is that layer by layer control of material deposition is hard and preventing impurities in the deposited film is almost impossible.

### 1.4. Thesis overview

In this thesis, the issue of system identification and controller design for thin film deposition processes has been studied. For achieving simulation data of thin film deposition, the KMC simulation of this process is performed for two cases. The first and simpler case is CO oxidation on Pt catalyst and the second case is silicon thin film deposition which is use in photovoltaic production industry.

The data of KMC simulation is used for driving a fuzzy model of the system. Using an optimization algorithm, the parameters of such fuzzy model are
optimized. The procedure of this system identification is depicted in figure 5.

![Figure 5. Block Diagram of the System Identification](image)

The first block will be studied in chapter two and the second block will be studied in chapter 3.

For controlling the quality parameters of thin film deposition, like thickness, roughness and porosity, a Model Predictive Controller (MPC) is designed. This controller includes two main block boxes which are optimization block and the fuzzy model achieved from system identification (Figure 6). Based on the MPC controller parameters, like control and prediction horizons, the optimizer achieves the optimized manipulated control values that can drive the plant to the required set point. MPC control design is covered in chapter 4.

![Figure 6. Block Diagram of the MPC Controller](image)
2. Kinetic Monte Carlo Simulation

2.1. Introduction

When analytical formulation of thin film growth is not convenient, KMC simulation can be used as an appropriate simulation approach for such complicated processes. The name of this algorithm comes from the gambling at Monte Carlo, Monaco that implies the stochastic nature of this method. The KMC algorithm is also identified by other names, like n-fold algorithm or residence time algorithm. One of the most important attractive characteristics of KMC simulations is simplicity in building the basic film growth processes. Basically, the complex thin film growth process is reconstructed by a set of simple rules in KMC algorithm. Because the nature of these rules is stochastic, the results of multiple runs of KMC algorithm should be used for achieving an average approach of the system. Another benefit of this approach is the capability of choosing the film growth contributors in the overall growth process and observation of the results of such choosings. For example, if one wants to see the behavior of film growth in a situation where diffusion is negligible, experimentally one would have to ensure that the temperature during a deposition is low enough, or that non-diffusive materials are used in an experiment. In KMC simulation, one would simply turn off the diffusion effects in the simulation code to observe the effects of low diffusion, which can save time and effort as compared to an experimental investigation.

In KMC simulation of thin film deposition, the film thickness, roughness and porosity of the deposited film are two important parameters. In this study, the evolution of roughness and porosity in the thin film deposition
procedure are simulated by KMC simulation method. The popularity and applications of KMC for simulation in different areas has increased considerably.

### 2.2. Monte Carlo algorithm

KMC simulation of thin film growth evolves under simple rules defined to model particular growth effects. The general execution of such a model is as follows (Lu, 2007):

- Initialize a lattice on which the thin film growth processes will take place. This lattice can be of two or three dimensions. The lattice can have different shapes based on the type of the thin film growth case and the experimental evidences of crystal structure of thin film.
- Create the first particle on the lattice.
- Based on the process parameters, define the next process that can be deposition of the next particle or the diffusion of the current particle on the substrate.
- If the deposition of the new particle is the event that should take place, the probability of desorption of the particle after reaching to the substrate should be evaluated.
- Create a new particle and repeat the process.

Many KMC algorithms follow this process, but more complicated models allow for a parallel execution of the algorithm, which can then be run more efficiently under a parallel computation scheme. Ordinarily, the complexity of a KMC algorithm is simple enough that it can be run reasonably quickly on commercially available computers, and the resources of a supercomputing cluster are not needed. If computation power and resources
are an issue, choosing which growth effects to include in a model is often a trade-off between a more physical model and a more efficient model. A graphical representation of some of the growth processes for thin film deposition for a nanoscale mass sensor is depicted in figure 7 (http://blogs.physicstoday.org/update/microstructures-and-nanostruct/).

Figure 7. Adsorption, Desorption and Diffusion as some growth effects

Each site of the lattice is specified for one particle of the film material to occupy this site. This particle can be an atom or a molecule. For example, the particle can be silicon atom in physical vapor deposition or a molecule in chemical vapor deposition process.

KMC models often do not incorporate specifics of the deposition, such as the chemical nature of the deposition flux, but rather leave these effects to be modeled with more empirical parameters that can be easily implemented in the algorithm, such as the activation energy for diffusion or the sticking coefficient that determines the probability that a particle sticks to the substrate when it strikes.

After the particle is initialized, it should follow a trajectory. This trajectory can be deterministic or stochastic. In the deterministic trajectory a straight
line is determined for deposition of particle and only the angle of this straight line can be selected based on the probability assigned to the angles of deposition, which is based on the nature of the deposition process. In the stochastic trajectory, the motion of the particle is completely stochastic and actually, it would be a random walk.

One would expect that, under the conditions of high vacuum normally encountered in physical vapor deposition processes, the mean-free path of a particle is much longer than the distance it travels between the source and the substrate, and the assumption that it travels in a straight line is a valid assumption. Two main models that are based on this assumption are solid on solid and ballistic aggregation models. In the solid on solid model, the overhangs in the thin film deposition are not allowed, but in ballistic aggregation, overhangs can occur in the model.

On the other hand, in processes where the deposition pressure is high, diffusion is the primary transport mechanism, and the Brownian motion characteristic of diffusion is best modeled with a random walk. These types of simulations are commonly referred to as Diffusion-Limited Aggregation (DLA) and are often used to model transport phenomena in fluids.

The experiments of consideration in this study are performed under high vacuum and the deterministic trajectory assumption is used. In addition, periodic boundary conditions are imposed on the lattice, which means if the trajectory of a particle takes it off the edge of the lattice, it will reappear on the opposite side of the lattice with the same trajectory.

For KMC simulation, a set of transitions $w_i$ are considered from state $x_i$ to state $x_t$. For each transition there is a rate $r_i$ which should be determined based on the specific problem for which the simulation is performed. In this chapter, it will be explained how these rates are determined for CO oxidation
and thin film deposition examples. In KMC simulation, the process evolution is only dependent on the state of the system at the last step and the rates of different processes are independent.

The basic KMC algorithm includes the following steps (A general method for numerically simulating the stochastic time evolution of coupled chemical reactions, 1976):

1) Set the time at zero

2) Based on the current situation of the system and the formulas defined for determining different processes rates, form the list of the rates of all the possible events for the next step.

3) Calculate the cumulative rate value based on the following formula:

\[ R_i = \sum_{j=1}^{n} r_j \quad \text{for} \quad i = 1, \ldots, n \]  

(2-1)

Where \( n \) is the number of transitions and \( r_i \) is the rate of the event \( i \).

4) Calculate the total rate \( R = R_n \)

5) Create a uniform random number \( \mu \in [0,1] \)

6) Find the event that satisfies the following condition

\[ R_{i-1} < \mu R \leq R_i \]  

(2-2)

7) Event \( i \) should be considered as the event that should happen at this time stage

8) Determine the new possible transitions after the transition \( i \) in the step 7 has happened. That transition can affect the number of possible transitions for the next step

9) Create the uniform random variable \( \gamma \in [0,1] \) for the time

10) Update the time

\[ \tau = -\frac{\ln(\gamma)}{R} \]

\[ t = t + \tau \]  

(2-3)
11) Go to the step 2

Using the specified formulation in step 10 for calculating the time step allows scaling the time increment based on the random nature of the problem.

For the problems where the amount of possible events is huge, for time efficiency in the implementation of KMC algorithm, some strategies for rate determining may be selected. In one of the most popular approaches, the events with the same rate are classified and the cumulative rate is calculated based on the rate of each group of events.

The probability of the lattice being in a specific configuration is given by the following master equation (Theoretical foundations of dynamical Monte Carlo simulation, 1991):

$$\frac{\partial P(\sigma,t)}{\partial t} = \sum_{\sigma'} W(\sigma',\sigma)P(\sigma',t) - W(\sigma,\sigma')P(\sigma,t)$$  \hspace{1cm} (2-4)

Where $P(\sigma,t)$ is the probability that the system is in state $\sigma$ at time $t$ and $W(\sigma,\sigma')$ is the probability per unit time of transition from configuration $\sigma$ to $\sigma'$. The KMC algorithm provides a numerical solution of the above master equation through Monte Carlo sampling (Low-order ODE approximations and model predictive control of surface roughness during thin-film growth, 2008). The solution of the master equation is achieved computationally by executing an event chosen randomly among various possible events (adsorption and desorption in the current case) based on the instantaneous event probabilities.
2.3. History of Kinetic Monte Carlo

The first issue of KMC was emerged in the middle of the 20th century, after the usage of computers in simulation was coming to play the important role which we see today. The most important Monte Carlo algorithm has been the Metropolis algorithm which is one of the most prominent algorithms of the 20th century (Equation of State Calculations by Fast Computing Machines, 1953). This algorithm was first proposed as the algorithm for the specific case of the Boltzmann distribution and after that was extended to the more general case (Monte Carlo sampling methods using Markov chains and their applications, 1970). The Metropolis algorithm and other algorithms based on that are the basis of most of the Monte Carlo simulations for study of systems at equilibrium.

In the 1960’s some other algorithms were developed for simulation of dynamic evolving of systems. This has been the start of creation of the algorithm known as KMC. Several simulations based on this algorithm have been done since those times. In one of these applications (Monte Carlo Calculation of the Order-Disorder Transformation in the Body-Centered Cubic Lattice, 1961), the transition probabilities and rates in vacancy motion are studied, but in this work time scale has not been drived and it can’t be considered as an KMC algorithm. The first work that contained the basics of KMC simulation and was done for study of vacancy migration was revealed by Young and Elcock (Monte Carlo studies of vacancy migration in binary ordered alloys, 1966).

Bortz, Kalos and Lebowitz developed a KMC algorithm for simulating an Ising Spin System. In their work, the algorithm is called n-fold
algorithm and the time increment $\tau = \frac{\ln(\gamma)}{R}$ was derived (A new algorithm for Monte Carlo simulation of Ising spin systems, 1975). Although the concept of KMC is not described in most Monte Carlo method textbooks compared to its importance in different applications, a good reference to the theory of KMC is the work by Fichthorn and Weinberg (Theoretical foundations of dynamical Monte Carlo simulations, 1991).

2.4. KMC in thin film deposition

In this study, thin film deposition is simulated by KMC and during film growth, the evolution of surface roughness and film porosity which are two important factors affecting thin film quality are evaluated. The triangular lattice is used for KMC simulation. The processes considered in KMC are adsorption and migration of particles on the lattice. The shadowing effect is considered in the simulation in which vacancies and overhangs are allowed to happen in simulation. The height of each column of particles on the substrate is considered as the distance of the last particle from the substrate in each column. This height also includes the vacancies in each column. The roughness parameter is evaluated as Root Mean Square (RMS) of surface height and porosity is evaluated as the ratio of vacancies to total number of deposited particles. For calculating the amount of vacancies in each time step, the number of vacant sites in each column, under the highest particles in that column, is calculated and the sum of these values would be the total vacancy number at each time step.
As mentioned before, surface roughness is measured by RMS of the surface height. It is quantified by the vertical deviations of the real surface of its ideal form (figure 8). If these deviations are large, the surface is rough; if they are small the surface is smooth. Roughness is typically considered to be the high frequency, short wavelength component of a measured surface.

![Figure 8. Surface Roughness (M.Pelliccione, 2007)](image)

The root mean square is defined based on the following formula:

\[
RMS = \sqrt{\frac{1}{n} \sum_{i=1}^{n} (h_i - \bar{h})^2}
\]  

(2-5)

Where \( h_i \) is the height of surface at column \( i \) and \( \bar{h} \) is the mean height.

As mentioned before, porosity which is the ratio of vacant sites to the total deposited particles is calculated according the following relation:

\[
Porosity = \frac{nvac}{ndep}
\]  

(2-6)

As mentioned, in KMC simulation different events like adsorption, desorption and diffusion can occur. If the event happening at a step of KMC is adsorption, the shadowing effect may be considered for achieving to more realistic simulation. Figure 9 depicts these events for KMC simulation on a cubic lattice (http://www.ualr.edu/txkarabacak/).
All particles in this simulation are considered as identical particles depositing on the lattice sites. The diameters of the particles are equal to the distance between two lattice sites. One dimensional triangular lattice is assumed and the dimension perpendicular to the lattice is the coordinate of film growth. The particles deposit from the top side of the lattice where the gas phase precursor is available. For implementing a KMC algorithm, the rates of adsorption and migration should be defined. The rate of adsorption is defined according to the following equation:

$$ ra = w \times \dim $$  \hspace{1cm} (2-7)

Where $w$ is the rate of deposition expressed as number of layers deposited per unit time. $w$ is dependent on the concentration of the precursor gas over the substrate and is a process dependent parameter. For the specific silicon thin film deposition in this study, the value of $w$ can change between 0.3 to 1. The parameter ‘dim’ is number of available sites per layer.
If based on the rate distribution, the deposition is the event that should occur at the current instant of simulation, a site on the surface is selected as the target deposition site randomly and also a random deposition angle between $-\frac{\pi}{2}$ and $-\frac{\pi}{2}$ based on a Gaussian distribution is selected for the direction of movement of the particle in the route between the source position and the target site. The source position is randomly selected in one column over the substrate dimension. During movement of the particle toward the target site from the source, when the particle is moving over each column, the position of the particle is compared to the height of surface at that column. If the height of surface is more than the height of the particle position, the particle sticks to the surface at that position and relaxes at the first position with more than one neighbor. This process is considered as shadowing effect during the deposition event. The shadowing effect and relaxation are happening in the time domain of deposition in the simulation and don’t have effect on the time evolution.

In the migration event, the particle overcomes the energy barrier of the site and migrates to a vacant neighbor site. The rate of migration for each particle is determined based on the number of neighbor particles for the specific particle. The number of neighbors can change between zero to six. With increasing the number of neighbor particles, the probability of migration of particle on the lattice decreases. The bottom layer of the lattice is assumed fully packed in the simulation. The migration rate is defined based on an Arrhenius-type equation which is stated as follows:

$$r_{m,i} = v_0 \exp\left(-\frac{n_i E_0}{k_B T}\right)$$

(2-8)
Where $v_0$ is the pre-exponential factor, $n_i$ is the number of neighbors of $i^{th}$ particle, $E_0$ is the activation energy barrier value, $K_B$ denotes Boltzmann’s constant and $T$ is the substrate temperature. In this work, the parameters are assigned to silicon thin film deposition in which the pre-exponential factor takes the value $v_0 = 10^{13}\text{ s}^{-1}$ and the activation energy barrier takes the value $E_0 = 0.6\text{ eV}$ (Monte Carlo simulation of growth and recovery of silicon, 1995). The Boltzmann’s constant value is $8.62 \times 10^{-5}$ and the temperature of the substrate changes between the values $100^\circ\text{C}$ to $600^\circ\text{C}$. After the rates of KMC events are determined, the simulations can be carried out. Because a limited size has been assumed for the lattice, periodic boundary conditions are considered for the model.

2.5. Open loop simulation for CO oxidation on Pt catalyst

Using the KMC method, the stochastic simulation algorithm of a simplified reaction model of the form $A + \frac{1}{2}B_2 \rightarrow AB$ of CO oxidation by $O_2$ on Pt catalytic surface is performed. The process involves adsorption of $A$, dissociative adsorption of $B_2$, and a second-order surface reaction the products of which desorbs immediately (Online System-Identification Using Subspace algorithms for the control of microscopic processes, 2008). The mean-field Langmuir-Hinshelwood approximation equations for this process in the absence of adsorbate interaction would consist of a set of two ODES (Equation-free optimal switching policies for bistable reacting systems, 2005).
\[
\frac{d\theta_A}{dt} = \alpha(1 - \theta_A - \theta_B) - \gamma \theta_A - 4K_r \theta_A \theta_B \\
\frac{d\theta_B}{dt} = 2\beta(1 - \theta_A - \theta_B)^2 - 4K_r \theta_A \theta_B
\]  
(2-9)

where \( \theta_A, \theta_B \) represent the surface coverage of CO, and O\(_2\), respectively, \( \alpha, \beta \) are the rate constants for adsorption of CO and O\(_2\), respectively, \( \gamma \) is the rate constant for CO desorption and \( K_r \) is the reaction rate constant. We employed \( \beta \) as the manipulated input. The values of these parameters are taken to be \( \alpha = 1.6, \gamma = 0.04 \) and \( K_r = 1 \). Adsorption of molecules from the gas phase and desorption of molecules from the film surface are the dominant phenomena responsible for the evolution of the microstructure of the thin film.

For a range of values of \( \beta \), the system exhibits multiple steady states, where the first steady state (Table 1) and the third steady state are locally stable while the second steady state is unstable (Equation-free optimal switching policies for bistable reacting systems, 2005). These values are shown in Table I for value of \( \beta = 3.5 \).

<table>
<thead>
<tr>
<th>Table I. CO oxidation steady state values</th>
</tr>
</thead>
<tbody>
<tr>
<td>SS1</td>
</tr>
<tr>
<td>SS2</td>
</tr>
<tr>
<td>SS3</td>
</tr>
</tbody>
</table>

In the KMC simulation for this process, the values of \( \beta \) is changed smoothly between 3 and 5, as shown in figure 10. The reason for such input is to catch the system approach in both situations that the manipulated variable is increasing or decreasing.
The KMC simulation is performed ten times for different initial conditions and the evolution of the system is considered as the average of all the evolutions achieved from different KMC simulations. The simulation results for this process with three different initial conditions are depicted in the following figures.

Figure 10. The changes of manipulated variable $\beta$ in the KMC simulation

Figure 11. Evolution of $\theta_A$ and $\theta_B$, $\theta_{A0} = 0.4, \theta_{B0} = 0.3$
Figure 12. Evolution of $\theta_A$ and $\theta_B$, $\theta_{A0} = 0$, $\theta_{B0} = 0$

Figure 13. Evolution of $\theta_A$ and $\theta_B$, $\theta_{A0} = 0.85$, $\theta_{B0} = 0.1$
2.6. Open-loop simulations for thin film deposition
In this section, the KMC simulation results for silicon thin film deposition are presented. The input variables are substrate temperature and vapor flux. A Gaussian distribution is assumed for the deposition angles with zero mean. The standard deviation of the random angles can be considered as another input variable to the system, but for simplicity, this value is fed to the system as a constant.
Figure 14 shows the variation of the temperature and figure 15 depicts flux variations during KMC simulation.

Figure 14. Temperature Variation during KMC simulation
The reason for selecting such input is catching all the different changes depicted in table 2 in two inputs.

Table 2. Changes of temperature and flux during KMC simulation for thin film deposition

<table>
<thead>
<tr>
<th>Step</th>
<th>Input</th>
<th>Temperature</th>
<th>Flux</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Increase</td>
<td>Increase</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>Increase</td>
<td>Decrease</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>Decrease</td>
<td>Increase</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>Decrease</td>
<td>Decrease</td>
<td></td>
</tr>
</tbody>
</table>

The open-loop result of film deposition on a lattice with dimension 250 and the above input is shown in figure 16. A Gaussian angle distribution with zero mean and standard deviation 0.1 is selected for this KMC simulation.
The graphs of porosity and roughness, which are two outputs of the simulation, are shown in figures 17 and 18. As can be seen in these figures, the porosity and roughness evolution reach to a steady state by progress of film evolution. With increase of the lattice size, this steady state would be achieved at the longer times compared to the simulation results on the lattices with small size.
Figure 17. Porosity evolution in thin film deposition

Figure 18. Roughness evolution of thin film deposition
3. Fuzzy System Identification

3.1. Overview

System identification is a technique to achieve mathematical models for the systems based on the input-output data. In this chapter, the system identification using fuzzy models is studied. It covers the main aspects of fuzzy system identification including the structure, the membership functions and using optimization process to estimate system parameters.

There are several different nonlinear system identification methods, but the advantage of fuzzy system identification is that they can extract linguistic information from input-output data and the dynamics of the system can be described in local defined rules of the fuzzy system. The capability of fuzzy identification to identify the linguistic variables and local rules would be a considerable advantage over other black box system identification methods, because we can gain evaluation about what happens in the system based on quantitative input-output values.

Fuzzy controller design can be a strong alternative in challenging concept of nonlinear controller design. The main idea of fuzzy control comes from performance based on how human beings act for control of a system. Humans act based on uncertain or fuzzy ways, which are based mainly on the past experience, to decide how should change the manipulated variables to drive the system towards the desired situation. Using fuzzy control, we can impose intelligence to the control system to act based on a type of reasoning.

Fuzzy identification can be useful in the cases where creating a precise mathematical model for the system is impossible. In most dynamic systems,
there are lots of uncertainties that cannot be mathematically modeled. The basis of fuzzy identification is on logical rules in the shape of “If (premise) Then (Consequence)” in which the values are not strict numerical values, but they are fuzzy linguistic values. A good example for understanding the linguistic values is expressing the temperature of a material with expressions like hot, warm or cold. In these linguistic variables, there is not a strict value for hot, warm or cold, but they express a range of temperature values.

The amount of contribution of each fuzzy rule in the overall output of the system is determined by the values of membership functions. The membership functions can have different shapes like triangular or Gaussian, which are the most popular membership functions. The great effect of using these membership functions is that we can have a smooth transfer of each local rule contribution in the final result, instead of sharp transfer of the cases in which we use crisp numerical values.

In fuzzy system identification procedure, the numerical values are converted to linguistic values through the Fuzzification process. For performing this process, the membership functions are used. A simple membership function is shown in figure 19 which depicts the span of different linguistic variables in the temperature universe of discourse. As shown in figure 19, the temperature 30F is 80 percent freezing and 20 percent cool. The overlap of the membership functions provides the situation for smooth transition between local rules.
The output linguistic information should be transferred to a numerical value by defuzzification process. For performing the defuzzification process, different approaches may be selected.

The "centroid" method is one of the most popular methods used for defuzzification. In this method, "center of mass" of the result provides the crisp value. Another method is the "height" approach, which takes the value of the biggest contributor. The centroid method favors the rule with the output of greatest area, while the height method favors the rule with the greatest output value.

Figure 20 demonstrates max-min inferencing in which the output membership function is given the truth value generated by the premise and centroid defuzzification for a system with input variables “x”, “y”, and “z” and an output variable “n”. Note that “mu” is standard fuzzy-logic nomenclature for “truth value” (http://www.faqs.org).
Choosing the membership functions depends on different aspects. For example, if differentiability is important, using Gaussian membership functions is recommended. If the goal is to achieve simple linear interpolations, the triangular membership functions are favored. The most important factor determining the type of membership function is the application of the model (Jairo Espinosa, 2004).

In fuzzy identification, there are some different parameters which should be determined. The main issues are as follows:
1) To determine that the fuzzy identification should be based on model free or T-S fuzzy identification.
2) To determine the types of the membership functions used in the system.
3) To determine the local models used in the T-S fuzzy model
4) To determine the number of rules or local models
5) To determine the system coefficient

In the most popular approach, all the fuzzy sets are integrated with the corresponding weight. Other methods, like center of area or center of maximum, may be used for the defuzzification process.

Initially, fuzzy modeling was based on considering expert knowledge using linguistic variables (Outline of a new approach to the analysis of complex systems and decision processes, 1973). Subsequently, the concept of Fuzzy system identification using the available data from the system became the focus of interest (H. Hellendoorn, 1997). Although the first fuzzy approaches were based on model-free designs (An experiment in linguistic synthesis with a fuzzy logic controller, 1975), gradually interest increased in model-based fuzzy identification (Fuzzy Identification of Systems and Its Applications to Modeling and Control, 1985). Once such models were developed, fuzzy model-based control approaches were investigated as an effective approach to address control design problems for nonlinear systems.

Recently, the Takagi-Sugeno fuzzy model-based identification became a widely used approach for nonlinear stochastic systems.
3.2. Mathematical formulation

3.2.1. Takagi Sugeno fuzzy identification

The T-S fuzzy structure is considered for identification of nonlinear models of the form (Perspectives of Fuzzy systems and control, 2005)

\[
\begin{align*}
  x(k+1) &= f(x(k), u(k)) \\
  y(k) &= g(x(k))
\end{align*}
\]  

(3-1)

where \( f \) is a nonlinear function of \( x(k) \) and \( u(k) \), \( x(k) \) is the state of the system at time step \( k \) and \( u(k) \) is the manipulated input variable exerted on the system which drives the states of the system until the next step \( k+1 \), \( y(k) \) is measurement vector, while \( g \) denotes a nonlinear function of \( x \). In several cases, it is assumed that complete state information is available \( y(k) = x(k+1) \); this assumption is also made in this work, since KMC simulation data will be used.

The rules defining fuzzy structure are defined according the following (K.M. Passino, 1998):

\[
\begin{align*}
  If \ z(k) \ is \ F_i \ then \ x(k+1) &= h_i(A, x(k) + B_iu(k)) \\
  i &= 1, 2, ..., r
\end{align*}
\]  

(3-2)

Where the premise variables \( z(k) \) can be defined from the states \( x(k) \) and the manipulated variable \( u(k) \) at each step \( k \). These parameters of \( z(k) \) are used for evaluating the membership functions for all rules in the fuzzy structure at each step (figure 21). \( F_i \) are the fuzzy sets that are the defining each rule. In each step, based on the information about the states and the manipulated
variable available in $z(k)$ and by evaluating the membership function values, the contribution of each rule is defined as $h_i$. The consequent parameters in this statement include the linear models for each rule.

![Figure 21. Fuzzy modeling structure](image-url)

The membership functions are chosen to have Gaussian distribution shapes (K.M. Passino, 1998) i.e.

$$h_i = \exp\left[-\frac{1}{2} \left(\frac{z_j - c_{j_i}}{\sigma_{j_i}}\right)^2\right]$$

(3-3)

where $i=\{1,\ldots,R\}$ defines the rule number $i$ and $j=\{1,\ldots,n\}$ defines the $j^{th}$ variable of the premise. Using this membership functions structure, the amount of the contribution of each rule in the overall output in each step will be determined.

The fuzzy system identification involves two main steps. The first step is the structure identification and the second step is parameter estimation.

In the structure identification step, after determining the number of rules considered in the fuzzy structure, the membership function structures will be determined, which has been supposed to be Gaussian.

After completing the two basic parts of the structure identification step, the overall output of the fuzzy model can be evaluated by the following equation:
\begin{equation}
\sum_{i=1}^{R} (A_i x(k) + B_i u(k)) \prod_{j=1}^{n} \exp\left[-\frac{1}{2} \left(\frac{z_j - c_j^i}{\sigma_j^i}\right)^2\right] 
\end{equation}

In order to perform the second step of the fuzzy identification (parameter estimation), an optimization problem should be solved to achieve the parameters that would give the minimum value of the following equation :

\begin{equation}
\phi^* = \arg \min \left( f(x(k)|\phi) - x(k+1) \right)^2
\end{equation}

In the presented work, a Newton-based search algorithm was employed to solve the constrained optimization problem. Specifically, the Levenberg-Marquardt algorithm was employed, within the computational environment of MATLAB. Global optimization search algorithms may also be employed (such as genetic algorithms) at the expense of slower convergence rate to an optimum point.

In T-S fuzzy identification, each local linear part acts as a rule and the overall output would be the result of union of local rule results.

### 3.2.2. Fuzzy system identification results

In order to perform the fuzzy system identification using the approach presented in this chapter, it is necessary to define the parameters that contribute to the definition of the centers of the Gaussian membership functions $c_j^i$, and the related spans $\sigma_j^i$. In this example, these values include the states of the system (concentrations of CO and O$_2$) and the manipulated input. To initialize the identification process, values are chosen for these parameters ($c_j^i$ and $\sigma_j^i$). The values of these parameters are part
of parameter vector $\Phi$ in equation (3.5). The remainder of $\phi$ includes the elements of the matrices $A_i$ and $B_i$ that are identified by solving the optimization problem.

After the fuzzy system identification phase, which is done based on the data from KMC simulation, a new data set is created using KMC with different initial conditions and a different manipulated variable. In this example, initial conditions include the concentrations of CO and $O_2$ and the manipulated variable is $\beta$, the rate constant for adsorption of $O_2$. The value of $\beta$ is changed smoothly between 3 and 5, as shown in figure 10. We have exerted this gradual change of manipulated variable to reach to the evolution of the reaction process without sudden big changes in the manipulated variable.

The evolution of the identified fuzzy model with the new initial condition and $\beta$ and the results of the KMC simulation are displayed in figures 23, 24, 25 for different initial values. The sampling step is every 4 seconds of the evolution of the process.
Figure 22. Evolution of $\theta_A$ and $\theta_B$, $\theta_A = 0.4, \theta_B = 0.3$

Figure 23. Evolution of $\theta_A$ and $\theta_B$, $\theta_A = 0.85, \theta_B = 0.1$
For fuzzy system identification of the thin film deposition process, the centers of the Gaussian membership functions \( c_j^i \), and the related spans \( \sigma_j^i \) include the states of the system (porosity and roughness of thin film) and the manipulated inputs (material flux and substrate temperature). To initialize the identification process, values are chosen for these parameters (\( c_j^i \) and \( \sigma_j^i \)). The values of these parameters are part of parameter vector \( \varphi \) in equation (3-5). The remainder of \( \varphi \) includes the elements of the matrices \( A_i \) and \( B_i \), that are identified by solving the optimization problem.

After the fuzzy system identification phase, which is done based on the data from KMC simulation, a new data set is created using KMC simulation. The values of flux and temperature are changed smoothly between 0.3 to 1 and...
100 to 500 degrees Centigrade’s respectively, and as shown in figures 14 and 15, We have exerted this gradually change of manipulated variable to reach to the evolution of the reaction process without sudden big changes in the manipulated variables.

There are two important issues in fuzzy system identification process in this study:

1) The number of rules or local linear models used in the T-S fuzzy structure.

2) The optimization procedure for achieving the fuzzy model parameters that predict the system evolution.

As depicted in figures 25-27, with increasing the number of rules in the fuzzy structure, more precise model can be achieved. However, with increasing the number of rules, the number of parameters which should be optimized increase and, as a result, the chance of optimization failure increases. For example, for the thin film deposition model with two state variables and two inputs, adding one rule to the fuzzy structure caused entering 16 more parameters which should be optimized. These parameters include the matrices of local linear models and centers and standard deviation parameters in the membership functions, which are used in anticipating the evolution of system in fuzzy structure.
Figure 25. Fuzzy system identification for thin film deposition with 5 rules

Figure 26. Fuzzy system identification for thin film deposition with 10 rules
As can be shown in the above figures, when the number of rules is increased, a better estimation of system performance is modeled, but a robust optimization procedure should be applied to the identification process to reach to correct parameters for the fuzzy system with higher number of rules.

3.3. Kalman filter in fuzzy identification

3.3.1. Covariance form of Kalman filter

In 1960, Rudolf E. Kalman developed a method named after him (Kalman Filter) for achieving values for the measures outputs of the systems in which the measurement contain noise (A new approach to linear filtering and prediction problems, 1960). After that, the Kalman filter has been used extensively in different areas. The basis of Kalman filter is developing
mathematical equations for recursive estimation of the states of the process based on considering the errors originated from the noise in measurements. The estimates produced by this method are closer to the true values than the original measurements. This method plays an important role in modeling the systems where the nature of the model is not exactly known. After introducing the Kalman filter, there have been several developments in this algorithm that have resulted in the development of the Kalman filter.

In this study, the standard Kalman filter which is applied to a discrete state space model is briefly introduced and after that an idea has been developed to use this type of Kalman filter in the identified nonlinear fuzzy model.

In the Kalman filter, the discrete state $x \in \mathbb{R}^n$ is estimated in each step. This state evolves based on the following equation:

$$
\begin{align*}
x_i &= A_i x_{i-1} + B_i u_{i-1} + w_{i-1} \\
z_i &= H_i x_i + v_i
\end{align*}
$$

Where $A$, $B$, and $H$ are the matrices of the system parameters which have been determined by system identification process. The variables $w_k$ and $v_k$ are the process and measurement noises, respectively.

The processes $w_k$ and $v_k$ are considered to be $p \times 1$ and $m \times 1$ zero mean white noise processes. Their covariance and cross-covariance are defined by

$$
E \left[ \begin{bmatrix} w_i & w_j \\ v_i & v_j \end{bmatrix} \right]^T = \begin{bmatrix} Q_i & S_i \\
S_i^T & R_i \end{bmatrix} \delta_{ij}
$$

The Kalman filter formulation for achieving the state estimates described in equation (3-8). Given the observations $\{z_i\}$ that satisfy the state space model
(3-8), the innovation process \( \{e_i\} \) can be recursively computed as follows.

\[
\begin{align*}
\hat{x}_{i|i-1} &= 0, \quad P_{o|l-1} = \Pi_0 \\
\text{Start with} & \quad x_{o|l-1} = 0, \quad P_{o|l-1} = \Pi_0 \
\text{and repeat for} & \quad i \geq 0 :
\end{align*}
\]

\[
\begin{align*}
R_{e_i} &= R_i + CP_{(i-1)} C' \\
K_{p,j} &= (AP_{(i-1)} C' + GS_j) \frac{1}{R_i} \\
e_i &= y_i - C \hat{x}_{i|i-1} \\
x_{i+1|i+1} &= A \hat{x}_{i|i-1} + K_{p,j} e_i \\
P_{i+1|i+1} &= AP_{(i-1)} A' + G Q G' - K_{p,j} R_{e_i} K_{p,j}
\end{align*}
\]

The procedure of applying this type of Kalman filter to a linear system is depicted in figure 28.

Figure 28. Covariance form Kalman Filter block diagram

For more information about the details of derivation of above formulation, the “Adaptive Filters” book (Sayed, 2008) is recommended.
3.3.2. Fuzzy-Kalman
For applying the propose Kalman filter on the identified fuzzy model, the Kalman filter formulation is used for each local linear model. The measurement at each sampling instant is divided based on the membership value of each rule at that time instant. Using these divided measurements, the Kalman filter is applied for each local linear model and the state estimates of these models are combined to achieve the total state estimate for the whole system at that special time instant. The procedure of this fuzzy-Kalman approach is depicted in figure 29.

![Figure 29. Fuzzy-Kalman block diagram](image)

The result of applying the Kalman filter to the fuzzy model identified for a KMC realization of CO oxidation on Pt catalyst is displayed in figure 30. It is clear from this figure that applying the Kalman filter has a considerable effect of taking into account the noises of the system.
Figure 30. Kalman filter application to an identified fuzzy model of CO oxidation on Pt catalyst
4. Model Predictive Control

4.1. Overview

Model Predictive Control (MPC) contains a class of controller design in which the model of the process is used for prediction of the control action. One of the most important characteristics of MPC is the ease of applying the necessary constraints in the controller design. During last decades, the use of MPC in different fields of industry has increased enormously. This type of controller design has been known by other names like receding horizon control or moving horizon control. The main issues which should be addressed in MPC include:

1) The model for the system to be controlled.
2) The cost function including the prediction error cost and change in manipulated control cost. This cost can contain the final state cost as well.
3) The optimization algorithm to find the optimum change in manipulated variable for achieving the minimum cost.
4) The prediction and control horizon applied to MPC design.

At each step, the current time state is assumed as the initial condition and the optimal control problem is solved over the prediction horizon. The result of the optimization problem would be a sequence of optimal manipulated variables over the control horizon. The first control action is applied and the other actions are discarded and at the next step, the same procedure will be repeated with the current state as the new initial state. The procedure of MPC is shown in Figure 31 (http://www.kxcad.net). The sampling instants are the times at which the controller acts.
Integer $k$ represents the current instant. The latest measured output, $y_k$, and previous measurements, $y_{k-1}, y_{k-2}, \ldots$, are known and are the filled circles in Figure 31(a). Figure 31(b) shows the controller's previous moves, $u_{k-4}, \ldots, u_{k-1}$ as filled circles. Each manipulated variable value is received from the controller and is held constant until the next sampling instant, causing the step-wise variations shown in Figure 31 (b).
Based on the type of the model used in MPC design (linear or nonlinear), the MPC would be linear or nonlinear. Although the first MPC designs were majorly linear, because most of the systems are nonlinear, most of these types of controller design have been based on NMPC in recent years. Apparently, there are more complicated issues like optimization and stability with such designs. For the purpose of stability analysis of MPC, the Lyapunov function is considered as the cost function.

The other important issue is the robustness of the MPC, meaning how the controller will perform in the presence of uncertainties and disturbances. One of the main reasons for using fuzzy modeling in the MPC was evaluating the capability of such type of modeling in improving the robustness of MPC.

Based on a survey by Mayne et al. (2000), the literature on MPC is divided in three categories:

1) The theoretical foundation that includes optimal control literature. These theoretical concepts cover dynamic programming and maximum principle.

2) “Process control” literature including MPC applications in industry. The literature about improvements in MPC applications in different industries.

3) Theoretical improvements in MPC design including stability and robustness of MPC designs.

One of the important constraints for applications of MPC is that because the optimization problem is solved online over a finite horizon, the application can be constrained by the time constant of the system. For systems with fast time constant, the optimization time in MPC makes this type of controller
difficult to apply to the system. There have been several improvements in application of MPC in fast systems.

4.2. Model predictive controller principles

If the control design problem is considered with fixed horizon optimization, it leads to a control sequence \{u_k, \ldots ,u_{k+N-1}\} which begins at the current time \(k\) and ends at the future time \(k+N-1\). This fixed horizon solution has the important drawbacks that with passing of time, something unpredicted could happen that the designed control sequence would not be appropriate for the new condition. If there is such possibility, the fixed control sequence won’t be appropriate. This drawback can be addressed by the idea of model predictive controller. This approach can be summarized in the following steps:

1) At time \(k\) and with the current state \(x_k\), an optimal control problem is solved over a fixed interval \([k, k+N-1]\) with considering the current and future constraints.

2) Choose the first time instant optimal manipulated control values and ignore the optimal manipulated control values at next time instants.

3) Measure the state at the next time instant \(k+1\).

4) Repeat the optimization process considering the measures state \(x_{k+1}\) as the new initial state.

If the assumption in the problem is a system without disturbances, the state measured in step 3 would be the same as the state predicted by the model. Otherwise, for better results, the system should be considered with disturbances and an observer should be designed for the system.

The overall formulation for model predictive control will be as follows:
The sets \( U \subset \mathbb{R}^m, X \subset \mathbb{R}^n, X_f \subset \mathbb{R}^n \) are the input, state and terminal constraint set, respectively.

The solution of the above formulation would be the feasible sequences \( \{x_0, \ldots, x_N\} \) and \( \{u_0, \ldots, u_{N-1}\} \) that satisfy all the constraints. The functions \( F \) and \( L \) in the cost function (7) respectively are the terminal cost and running cost.

Typical choices for the terminal cost and running cost are quadratic functions of the form

\[
F(x) = x^T P x \quad \text{and} \quad L(x, u) = x^T Q x + u^T R u
\]

where

\[
P = P^T \geq 0, \quad Q = Q^T \geq 0 \quad \text{and} \quad R = R^T \succ 0
\]  

(4-2)

Based on the type of system, other cost functions that can be more complicated would be used.
The most popular cost function which should be used in the optimization process in MPC is Linear Quadratic Regulator (LQR) form:

\[
V_N(x_k, u_k) = x_N^T P x_N + \frac{1}{2} \sum_{k=0}^{N-1} (x_k^T Q x_k + u_k^T R u_k)
\]  

\[(4-3)\]

Where \(x_k\) denotes the state at time instant \(k\), \(u_k\) denotes the input at time instant \(k\) and \(x_N\) denotes the final state of the system. The states and control inputs are related based on the following equation:

\[
X_{k+1} = A x_k + B u_k, \quad k = 0, 1, ..., N - 1
\]  

\[(4-4)\]

The initial condition \(x_0\) of the system is known and by this initial condition, the system evolves based on the above formula.

The problem involves three different weighting matrices:

- The state weighting matrix \(Q\)
- The control weighting matrix \(R\)
- The final state weighting matrix \(P\)

Changing the values of these matrices can considerably affect the approach of the controller. For example, if the limitation on the amount of change in manipulated control value is not the primary importance and the important output is that the controller drives the system towards the set point, the weight of the state matrix should be bigger. If there are limitation in the actuator and the changes in the manipulated control is important, we can increase the weight of the control matrix. With increasing the weight of this matrix, the manipulated control variables change more smoothly.
Besides the weighting matrices, the performance of MPC is affected by other variables like prediction and control horizon. The minimizing control sequence which is a function of the current state $x_k$, would be:

$$u_{x_k}^{\text{opt}} = \{u_0^{\text{opt}}, u_1^{\text{opt}}, \ldots, u_{N-1}^{\text{opt}}\} \quad (4-5)$$

The control applied to the system at time instant $k$ is the first element of the above optimized control sequence:

$$U_k = u_0^{\text{opt}}$$

In the next step, the time is stepped forward one instant and the above procedure is repeated for all steps until reaching to the optimization horizon. The procedure of model predictive controller is depicted in figure 32 (http://www.newcastle.edu.au/research-centre/cdsc/).
Figure 32 shows the model predictive control for horizon N=5. Each plot shows the optimal control sequence $u^{opt}_{x_i}$ computed at time instants $k=0,1,2$. Only the shaded control inputs are actually applied to the system. The model predictive control in closed loop is depicted in figure 33 (http://www.newcastle.edu.au/research-centre/cdsc/).
4.3. MPC design for CO oxidation on Pt catalyst process

4.3.1. Controller structure design

A model predictive controller design is combined to the identified fuzzy model to regulate the surface reaction at a desired level during the reaction process. In the design of the model predictive controller, the objective is to dynamically force the system from an initial stationary state to a desired stationary state.

As mentioned before, model predictive control is based on the recursive solution of finite-horizon optimization problems with a receding final time, where the surface reaction model is now a constraint. In this approach, in each step of evolution of the reaction process, the states of the system in the next $N_p$ steps under the effect of the optimized manipulated variable in the next $N_c$ steps are anticipated.
The model predictive control objective is to minimize a cost function $J$:

$$J = \sum_{i=1}^{N_p} R_s (S - x_i)^2 + \sum_{i=1}^{N_c} R_\beta \Delta \beta_i^2$$

(4-6)

where $S$ is the set point, $x_i$ is i-th controlled state variable, $\Delta \beta_i$ is the i-th change in the manipulated variable $\beta$, $N_p$ is the prediction horizon, $N_c$ is the control horizon, $R_s$ is the weighting coefficient for minimizing the first term in equation (4-6) and $R_\beta$ is the weighting coefficient for minimizing the second term in equation (4-6). Note that in the specific formulation there is no final time penalty, employing large enough prediction horizons to ensure stability of the controller (E.E. Camacho, 2004), while also $N_p > N_c$.

The problem is subject to the following inequality constraints:

$$0 \leq \beta(t + j) \leq 5 \quad j = \{1,...,N_c - 1\}$$
$$-5 \leq \Delta \beta(t + j) \leq 5 \quad j = \{1,...,N_c - 1\}$$

(4-7)

As well as the fuzzy model predictions of the state evolution as equality constraints. Because of the nonlinear nature of the identified fuzzy model, the related model predictive controller design is a nonlinear model predictive control (NMPC).

In the model predictive procedure, by having the current information about the state of the system and the value of manipulated variable and using the nonlinear model for the system, the next states of the system within the prediction horizon are estimated using the manipulated variables within the control horizon. Considering these prediction and control horizons, an optimization problem is solved to reach to the minimum of the cost function.
J in equation (4-6). After this optimization, the first value for the change in the manipulated variable $\Delta \beta_i$ is applied to the system and the same procedure is repeated to complete the next step.

Depending on the desire to control the system to reach the set point as close as possible or the desire of having a smooth change in the manipulated variable, we can put more weight on the first term or second term in the cost function defined in equation (4-6) by changing the values of $R_s$ and $R_\beta$. For example, if the value of $R_\beta$ is increased, there is more weight for changing the manipulated variable on the cost function $J$, so we can achieve a more gradual change in the manipulated variable $\beta$ by increasing $R_\beta$.

**4.3.2. Closed Loop simulation results**

The obtained data set is used to construct a model of T-S structure. Note that the T-S model is able to accurately capture the system evolution in all the presented cases, starting from different initial conditions as presented in figures 34, 35 and 36. Based on this model, an NMPC structure is designed where the prediction horizon, $N_p$, is set to 20 steps and the control horizon, $N_c$, is set to 6 steps. The weighting coefficient for difference between state and the set point is set to 2 and the weighting coefficient for manipulated variable change is set to 1.

In our example, the objective is to decrease the surface coverage $\theta_A$ of CO on the catalytic surface from the steady state 0.97 to the desired steady state 0.67. As shown in the figure 34, by using this controller, we successfully drive the system to the desired value. Note that this value is at an open-loop
unstable steady-state, which defines the separatrix between two steady-states.

![Figure 34](image1.png)

**Figure 34.** The evolution of $\theta_A$ from initial steady state $\theta_A = 0.97$ to set point $\theta_A = 0.67$

The temporal profile of the manipulated variable $\beta$ that was employed for achieving this goal is displayed in the figure 35. We observe that the manipulated variable $\beta$ attains values close to zero to drive the system to reducing the coverage and then $\beta$ increases again. It is important to note that no chattering in $\beta$ is observed once the states reach the desired, open-loop unstable, steady state, even though the process is in itself fluctuating around the desired steady state, due to stochastic noise.
Figure 35. Manipulated variable $\beta$ for driving the CO coverage from initial steady state $\theta_A = 0.97$ to the set point $\theta_A = 0.67$

To evaluate the capability of the controller, which is designed based on our nonlinear model to traverse bifurcation points, we also investigated cases where the objective was to drive the system to the lower, open-loop stable, steady state point.

In figure 36, we present the temporal profiles of the system states, while the manipulated variable temporal profile is shown in the figure 37. It is observed in figure 36 that the controller can successfully drive the system from one open-loop stable steady-state to the other one in a smooth fashion, and the separatrix point is passed successfully during the process evolution.
Figure 36. The evolution of $\theta_A$ from initial steady state $\theta_A = 0.97$ to set point $\theta_A = 0.13$

Figure 37. Manipulated variable $\theta_A$ for driving the CO coverage from initial steady state $\theta_A = 0.97$ to the set point $\theta_A = 0.13$
4.4. MPC design for thin film deposition process

4.4.1. Controller structure design

A model predictive controller design is combined to the identified fuzzy model to regulate the porosity and roughness of the film around a desired level during the thin film deposition process.

The model predictive control objective is to minimize a cost function $J$:

$$J = \sum_{i=1}^{N_p} R_s (S_p - x_{pi})^2 + \sum_{i=1}^{N_p} R_s (S_R - x_{R_i})^2 + \sum_{i=1}^{N_c} R_T \Delta T_i^2$$

where $S_p$ is the set point for porosity, $x_{pi}$ is i-th controlled porosity state variable, $x_{Ri}$ is i-th controlled roughness state variable, $\Delta T_i$ is the i-th change in the temperature as the manipulated variable, $N_p$ is the prediction horizon, $N_c$ is the control horizon, $R_s$ is the weighting coefficient for minimizing the first and second terms in equation (4-8) and $R_T$ is the weighting coefficient for minimizing the second term.

The problem is subject to the following inequality constraints:

$$100 \leq T(t + j) \leq 500 \quad j = \{1, ..., N_c - 1\}$$
$$-20 \leq \Delta \beta(t + j) \leq 20 \quad j = \{1, ..., N_c - 1\}$$

4.4.2. Closed Loop simulation results

Based on the identified fuzzy model model, an NMPC structure is designed where the prediction horizon, $N_p$, is set to 20 steps and the control horizon, $N_c$, is set to 10 steps. The weighting coefficient for the difference
between states and the set points is set to 2 and the weighting coefficient for manipulated variable change is set to 1.

Figures 38-40 show the result of one run of this controller design for reducing the amount of porosity and roughness using the designed MPC in thin film deposition process.

![Figure 38. Open loop thin film deposition](image)

![Figure 39. Closed loop thin film deposition](image)
Figure 40. Variation in the substrate temperature as the manipulated variable

It is clear from the above figures that the evolution of porosity and roughness has been limited by applying the closed loop controller. The performance of the controller can be enhanced considerably by applying a robust optimization algorithm in the MPC controller design.
5. Conclusion

In this work, a model predictive control algorithm was developed to regulate the quantities of interest for two different processes. The first process which is the simpler one, was CO oxidation on Pt catalyst which has applications in pollution control. The second process is thin film deposition which is one of the most important microscopic processes with considerable and developing applications in different areas. Both processes were simulated using the KMC algorithm.

In KMC simulation of CO oxidation on Pt catalyst, the oxygen concentration over the surface which the reaction takes place was chosen as the manipulated variable. During the simulation, the evolution of CO and O\textsubscript{2} concentrations are observed. The manipulated variable is changed gradually during the simulation to catch the system approach in the case of increasing and decreasing of this variable. This simulation shows three different steady states for the system evolution depending on the initial condition which the simulation is assigned at start.

The thin film deposition process was modeled on a one-dimensional triangular lattice that involves two microscopic processes: an adsorption process and a migration process. The evolution of porosity and roughness as two important variables determining the quality of the thin film, are observed. Two manipulated variables for this simulation are material flux and substrate temperature. The roughness is introduced as the root mean square of the surface height profile and porosity is introduced as the ration of unoccupied sites over the lattice which have heights lower than the height of
surface at each site column to the total deposited particles at the specified time.

Because a closed-form model of the system is needed for the controller design, the fuzzy system identification is selected as the nonlinear modeling approach for finding an appropriate model to be used in model predictive controller design. The T-S fuzzy modeling has been selected for modeling these systems. For building such a fuzzy model, two main steps should be performed. The first step is a fuzzy model structure design in which the number of local linear models or rules and other parameters like those that define the centers and standard deviations of the membership functions should be determined. The Gaussian membership functions are selected for the fuzzy model.

The second step in the system identification is parameter optimization. The parameters which should be optimized are the local linear model matrices and the centers and standard deviations of the membership functions. With increasing the number of rules, the precision of the fuzzy model can be enhanced, but because increasing one rule adds at least 16 more parameters which should be optimized, the optimization problem makes a serious constraint on increasing the number of rules.

For taking into account the measurement noises, the idea of applying Kalman filter to the model has been used. The covariance type of Kalman filter is selected and for applying the Kalman filter to the fuzzy structure, at each instant, based on the contribution of each rule in the overall output of the system, the KMC simulation data at that time instant is divided between local linear models, then the Kalman filter is applied to each linear model and the output of the filters are accumulated to achieve the filtered output. The performance of this idea has been demonstrated to be very promising.
Finally, based on the identified model a model predictive controller is designed to regulate the states of the systems which have been modeled as the outputs of the fuzzy models. The important parameters affecting the performance of such controller design are the accuracy of the model, the prediction and control horizons of the MPC and the objective function defined for the MPC controller which should be minimized. Again in this step, an optimization problem should be solved at each step of controller act. Because an initial guess should be fed to the optimization procedure selected in this work, the performance of the controller is highly dependent on this initial guess at each step. For achieving a controller with more robust performance, using a robust and precise optimization algorithm for both the system identification step and especially in the controller design step is the objective of further work on this research.
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