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A Nonlinear Predictive Control of Processes with Multiscale Objectives using a Fuzzy-System Identification Approach

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Abstract— **In this paper 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 control 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_2 on a Pt catalytic surface. The nonlinear fuzzy model gives a good 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.**

I. INTRODUCTION

For many chemical and biological processes of industrial interest, performance is measured both with respect to product yield and quality. The elusive latter term is usually dependent upon enforcing the product microstructure within strict limits. Multiscale models are traditionally used to quantify process evolution across all relevant length scales and characterize product behavior within the current computational limitations. Even such models however, pose significant challenges both from an analysis and control point of view [1]. Such difficulties are attributed in part to the unavailability of closed form models to describe the process evolution at molecular-level detail and their computationally intensive nature that prevents their real time implementation. An industrially relevant example is thin film deposition processes widely used by the microelectronics and solar energy industries (such as the production of photovoltaic systems). Due to the complex process dynamics and the strict quality requirements, a significant amount of research has focused on the design of feedback control structures. To circumvent the mentioned limitations, one of the proposed approaches identifies stochastic partial differential equation models to design the controller [2]. This approach however assumes specific structure to the nonlinear stochastic terms. Another approach relies on the off-line and subsequently the on-line identification of bilinear models for the process, which are then used for the controller synthesis [3]. To improve on the linear controllers an extension was proposed in [4], where the authors designed a nonlinear feedback controller to control the roughness of a one dimensional surface again employing stochastic KSE as the underlying process growth model. The proposed approach assumed a specific structure to the nonlinear stochastic terms.

In [5] linear models were identified directly based on the output from KMC simulators. The linear controller that was designed based on the identified model was used to control the lower order statistical moments of microscopic distributions. In a different approach [6] 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 finite set of ”coarse” observables. The identified state space model was used to design a receding horizon controller to regulate the roughness, during thin film growth, at a particular setpoint. 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 [7] a minimum set of coarse spatially invariant parameters that accurately describe the dominant behavior of the deposition surface during thin-film growth under adsorption and surface diffusion was identified and it was demonstrated 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 ([8]) a method was presented 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 [9] an approach was described in which targeted simulations are combined with systematic tools to elucidate the dynamics.

Another approach deals with the feedback linearization problem of nonlinear systems described by microscopic/ stochastic simulators, in which the lack of a closed form model was circumvented by directly calculating the

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quantities needed for design of nonlinear controllers from appropriately initialized microscopic simulations [10]. A shortcoming of this method however is that it is limited to stabilization and involves closed loop eigenvalue assignment constraints. In [11], [12] 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. Using the coarse variables nonlinear process models were identified offline 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 was developed in [22] 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 though exist that exhibit complex behavior 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.

This paper is organized as follows. In subsection II we present concepts from T-S Fuzzy Identification that has been used for nonlinear modeling of the system. In section III a nonlinear receding horizon controller is designed based on the identified nonlinear model. In section IV the information about the CO oxidation which is used as the example in this work is presented; in section V the results of system identification and controller design for the propose example are presented

I. TAKAGI-SUGENO FUZZY MODELING

Initially, Fuzzy modeling was based on considering expert knowledge using linguistic variables [13]. Subsequently, the concept of Fuzzy system identification using the available data from the system became the focus of interest [14]. Although the first fuzzy approaches were based on model-free designs [15], gradually interest increased in model-based fuzzy identification [16]. 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.

The T-S Fuzzy structure is considered for identification of nonlinear models of the form [17]

$$x(k+1) = f(x(k), u(k))$$
$$y(k) = g(x(k))$$

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 [18]:

$$If\ z(k)\ is\ F_i\ then\ x(k+1) = h_i(A_i x(k) + B_i u(k))$$
$$i = 1,2,...,r$$

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. 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.

The membership functions are chosen to have Gaussian distribution shapes [18] i.e.

$$h_i = \exp[-\frac{1}{2}(\frac{z_j - c_j^i}{\sigma^i_j})^2] \quad (1)$$

where $i=\{1,...,R\}$ defines the rule number i and $j=\{1,.. .,n\}$ 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:

$$f(x(k)|\varphi) = \frac{\sum_{i=1}^{R}(A_i x(k) + B_i u(k)) \prod_{j=1}^{n} \exp[-\frac{1}{2}(\frac{z_j - c_j^i}{\sigma^i_j})^2]}{\sum_{i=1}^{R}\prod_{j=1}^{n} \exp[-\frac{1}{2}(\frac{z_j - c_j^i}{\sigma^i_j})^2]} \quad (2)$$

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:

$$\varphi^* = \arg\min(\left| f(x(k)|\varphi) - x(k+1) \right|^2) \quad (3)$$

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.

II. Receding Horizon Controller Synthesis

A receding horizon 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 receding horizon controller, the objective is to dynamically force the system from an initial stationary state to a desired stationary state.

Receding horizon 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 receding horizon control objective is to minimize a cost function *J*:

$$J = \sum_{i=1}^{N_p} R_s (S_i - x_i)^2 + \sum_{i=1}^{N_c} R_\beta \Delta\beta_i^2 \quad (4)$$

where S_i is the i-th set point, x_i is i-th controlled state variable, $\Delta\beta_i$ is the i-th change in the manipulated variable β, N_p is the prediction horizon, N_c is the control horizon, R_s is the weighting coefficient for minimizing the first term in (4) and R_β is the weighting coefficient for minimizing the second term in (4). Note that in the specific formulation there is no final time penalty, employing large enough prediction horizons to ensure stability of the controller [19], while also $N_p >> N_c$.

The problem is subject to the following inequality constraints:

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

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 receding horizon controller design is a nonlinear model predictive control (NMPC) [19].

In the receding horizon 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). After this optimization, the first value for the change in the manipulated variable $\Delta\beta_1$ is applied to the system 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) by changing the values of R_s and R_β. For example if the value of R_β is increased, there is more weight for changing the manipulated variable on the cost function *J*, so we can achieve more smooth change in the manipulated variable β by increasing R_β.

III. Illustrative Example: CO Oxidation

We illustrate the system identification and control methodology presented in the section II on a KMC realization [20], [21] (using 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. The process involves adsorption of A, dissociative adsorption of B_2, and a second-order surface reaction the products of which desorbs immediately [22]. The mean-field Langmuir-Hinshelwood approximation equations for this process in the absence of adsorbate interaction would consist of a set of two ODES [23],

$$\frac{d\theta_A}{dt} = \alpha(1 - \theta_A - \theta_B) - \gamma\theta_A - 4K_r\theta_A\theta_B$$
$$\frac{d\theta_B}{dt} = 2\beta(1 - \theta_A - \theta_B)^2 - 4K_r\theta_A\theta_B \quad (5)$$

where θ_A, θ_B represent the surface coverage of CO, and O_2, respectively, α, β are the rate constants for adsorption of CO and O_2, respectively, γ is the rate constant for CO desorption and K_r is the reaction rate constant. We employed β as the manipulated input. The values of these parameters are taken to be $\alpha = 1.6$, $\gamma = 0.04$ and $K_r = 1$ [23]. 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 β, the system exhibits multiple steady states, where the first steady state (Table I) and the third steady state are locally stable while the second steady state is unstable [23]. These values are shown in Table I for value of $\beta = 3.5$.

The probability of the lattice being in a specific configuration is given by the following master equation [25]:

$$\frac{\partial P(\sigma,t)}{\partial t} = \sum_{\sigma'} W(\sigma',\sigma)P(\sigma',t) - W(\sigma,\sigma')P(\sigma,t) \qquad (6)$$

Where $P(\sigma,t)$ is the probability that the system is in state σ at time t and $W(\sigma,\sigma')$ is the probability per unit time of transition from configuration σ to σ'. KMC provides a numerical solution of the above master equation through Monte Carlo sampling [24]. 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.

Table I
CO oxidation steady state values

SS1	$\theta_{A,ss,1}$	0.13944	$\theta_{B,ss,1}$	0.63553
SS2	$\theta_{A,ss,2}$	0.67526	$\theta_{B,ss,2}$	0.11452
SS3	$\theta_{A,ss,3}$	0.97101	$\theta_{B,ss,3}$	0.00137

IV. FUZZY SYSTEM IDENTIFICATION AND CONTROLLER DESIGN RESULTS

In order to perform the fuzzy system identification using the approach presented in section II, 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 $\sigma^i{}_j$. In this work 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 $\sigma^i{}_j$). The values of these parameters are part of parameter vector φ in (3). The remainder of φ includes the elements of the matrices A_i and B_i that are identified by solving the optimization problem.

After fuzzy system identification phase, which is done based on the data from KMC simulation, a new set of data are created using KMC with different initial conditions and different manipulated variable. In this example initial conditions include the concentrations of CO and O_2 and the manipulated variable is β, the rate constant for adsorption of O_2. The values of β is changed smoothly between 3 and 5, as shown in figure 1. 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 variable.

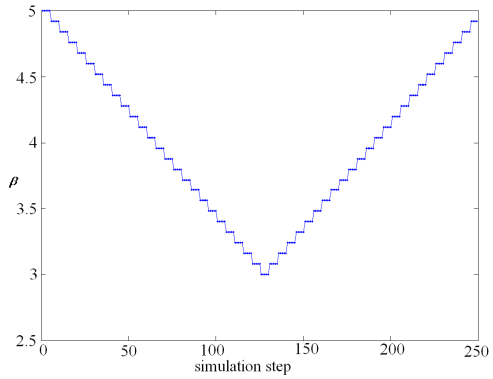

Fig.1. The changes of manipulated variable β in the KMC simulation

The evolution of the identified fuzzy model with the new initial condition and β and the results of the KMC simulation are displayed in figures 2, 3, 4 for different initial values. The sampling step is every 4 seconds of the evolution of the process.

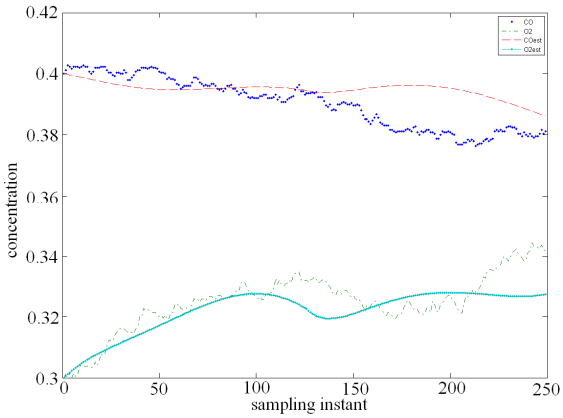

Fig.2. evolution of θ_A and θ_B, $\theta_{A0} = 0.4$ $\theta_{B0} = 0.3$

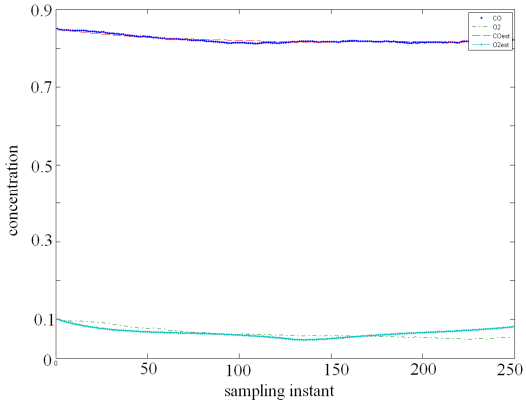

Fig.3. evolution of θ_A and θ_B, $\theta_{A0} = 0.85$ $\theta_{B0} = 0.1$

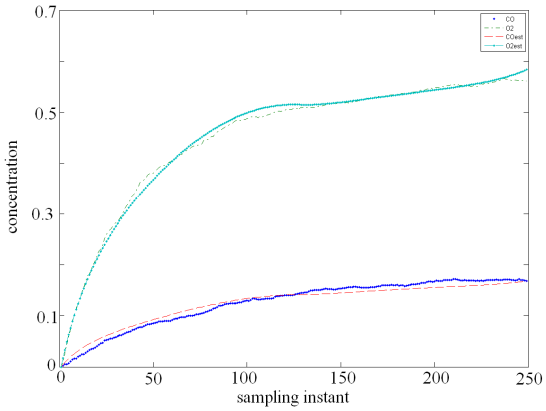

Fig.4. evolution of θ_A and θ_B, $\theta_{A0} = 0$ $\theta_{B0} = 0$

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 2, 3 and 4. 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 θ_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 5, 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.

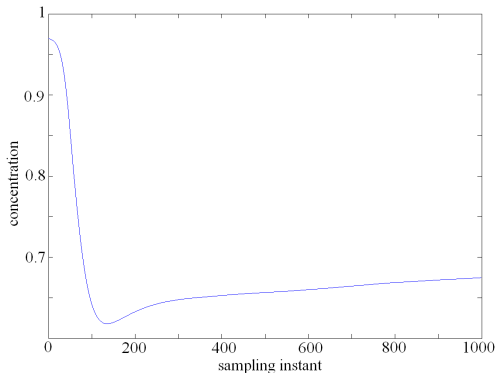

Fig.5. The evolution of θ_A from initial steady state θ_A =0.97 to the set point θ_A =0.67

The temporal profile of the manipulated variable β that was employed for achieving this goal is displayed in the figure 6. We observe that the manipulated variable β attains values close to zero to drive the system to reducing the coverage and then β increases again. It is important to note that no chattering in β 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.

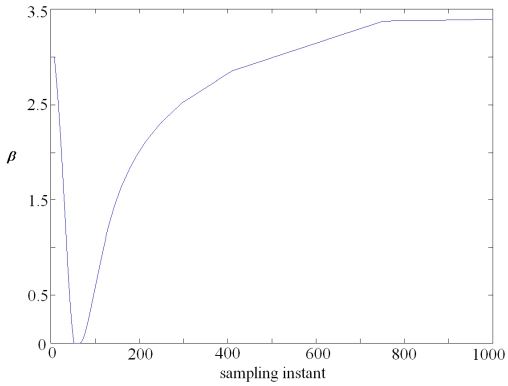

Fig.6. manipulated variable β for driving the CO coverage from initial steady state θ_A =0.97 to the set point θ_A =0.67

The value of the cost J of equation 4 is displayed in figure 7. As shown in this figure, the value of cost J is reduced fast in the first steps of evolution of the system under controller effect and it reached values close to zero as the process is steered to the desired steady state.

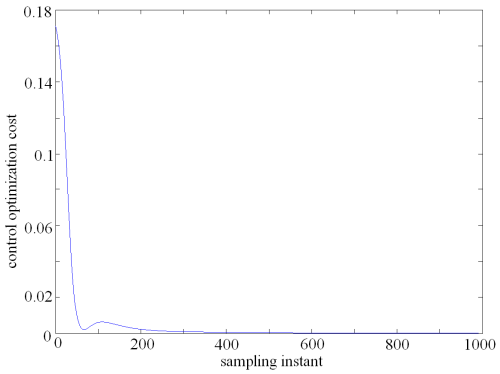

Fig.7. evolution of cost J after each optimization step in receding controller design procedure

To evaluate the capability of the controller 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 8 we present the temporal profiles of the system states, while the manipulated variable temporal profile is shown in the figure 9. It is observed in figure 8 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.

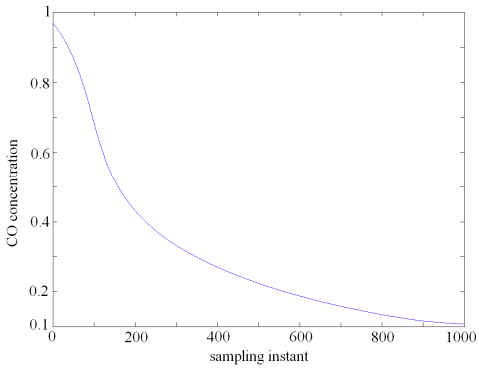

Fig.8. The evolution of θ_A from initial steady state θ_A =0.97 to the set point θ_A =0.13

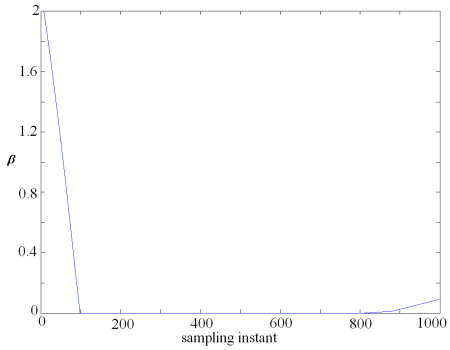

Fig.9. manipulated variable β for driving the CO coverage from initial steady state θ_A =0.97 to the set point θ_A =0.13

V. CONCLUSION

In this contribution, the problem of model-based controller design for microscopic system was investigated. The problem was addressed via the identification of nonlinear models that were subsequently used for NMPC design. The model was constructed in this two step procedure using fuzzy system identification algorithms. The data required for this system identification were produced using KMC simulations. The proposed approach was illustrated on a KMC realization of the catalytic oxidation of carbon monoxide. The resulting models of the fuzzy system identification step captured the process evolution well, while the stochastic noise didn't severely affect the model performance. Subsequently, a receding horizon controller was designed that successfully forced the system from an open-loop stable steady-state to a desired open-loop unstable steady state. Furthermore, the designed controller was successfully employed to force the system to traverse a separatrix and stabilize the system at a different open-loop stable steady-state.

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