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DRSM Model for the Optimization and Control of Batch Processes

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Abstract: Current Optimization and Model Predictive Control practices for batch processes are implemented using two models, one for determining the optimal trajectories and another identified around those trajectories for control purposes. Here we use the recently developed Dynamic Response Surface Modeling methodology from which the optimal trajectories and the local linear or nonlinear state-space models for control purposes are obtained. Because concentration measurements at each batch run are very infrequent, this might be the most attractive way to obtain a dynamic model for control purposes.

Keywords: Data-Driven Modeling, Optimization, Model-based Control, Batch Process, Dynamics, Nonlinear Models

1. INTRODUCTION

Data-Driven Modelling of batch processes for process control purposes has attracted substantial interest from both academic and industrial researchers in the past decades. Several model structures representing the nonlinear dynamics of the batch processes have been proposed, including the Hammerstein-Wiener (H-W) model and the Linear Parameter-Varying (LPV) model. The H-W models, consisting of two static nonlinear blocks in the inputs and outputs and a dynamic linear block in between (Bai 2002, van Wingerden, Verhaegen et al. 2009), have been applied for the modelling batch processes with linear kinetics and static nonlinear functions on the output, such as pH neutralization (Norquay, Palazoglu et al. 1999). The LPV model (Verdult and Verhaegen 2002) introduces scheduling parameters which vary with the evolution of the state variables in order to approximate bilinear dynamics. The aforementioned models are identified locally through Pseudo Random Binary Signal (PRBS) or Generalized Binary Noise (GBN) (Tulleken 1990) experiments in the vicinity of a pre-determined trajectory, possibly an optimal one. However, when the available measurements in a single batch are infrequent, the estimation of such a linear or nonlinear dynamic model of satisfactory accuracy is not feasible.

When the inner workings of the process are not known for a knowledge-driven model to be easily developed, the Design of Dynamic Experiments (DoDE) (Georgakis 2009) (Georgakis 2013) is a new and effective approach for data-driven process modelling and optimization with time-varying inputs. As a generalization of the traditional Design of Experiments (DoE) (Box and Draper 2007, Montgomery 2013), DoDE has been used to determine the optimal inputs for several batch processes (Troup and Georgakis 2013) (Fiordalis and Georgakis 2013) and has been experimentally verified (Makrydaki, Georgakis et al. 2010) on an industrial process. Usually the available data for estimating the corresponding Response Surface Methodology (RSM) model are collected at the end of the batch. If data are available also at fixed time intervals during the batch one can estimate a Dynamic RSM model (DRSM). This new type of model has been recently introduced in (Klebanov and Georgakis 2016) and will be briefly described and extensively used here. In contrast to the static RSM, the model parameters in DRSM are time-varying and do not require an excessive number of measurements during each batch. The DRSM model is used to calculate the optimal trajectory of a batch and will be also used here to estimate a dynamic model for control purposes in a receding horizon Model Predictive Controller (MPC). This saves the need for additional experimentation for the separate development of the model to be used by the MPC controller. Because the DRSM model captures both the linear and nonlinear dynamics of the process quite accurately, it can be used to develop either a linear or a nonlinear recursive dynamic model. Due to the limited length of this paper, we report here the control performances based on linear and nonlinear dynamic models and only the details on the estimation of the linear ones. The MPC controller here aims to achieve the desired concentration(s) at the end of the batch. An *in silico* illustration using an isothermal batch reactor with 3 reactions is presented.

Firstly, a DRSM model is estimated representing the dynamics of the process over the entire design domain in which the DoDE experiments are performed. This model is used to optimize the process. Part of the optimization task is to determine the optimal duration of the batch, easily achieved through the DRSM without the need to do experiments of different duration, lessening the experimental burden. From the DSRM, we identify local linear and Hammerstein-Wiener models, via subspace identification (Verhaegen and Verdult 2007) by sampling the DRSM in the

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vicinity of the optimal trajectory. To demonstrate that the proposed approach is more favourable when measurements are limited, we also identify local state-space models using PRBS experiments and compare the corresponding control performances. In all cases a Model Predictive Controller (MPC), utilizing a Kalman Filter (Kalman 1960), is used to control the desired concentration at the end of the batch.

2. DEVELOPMENT OF DRSM MODEL

The time-varying input profile in DoDE $u(\tau)$ is defined as

$$u(\tau) = u_0(\tau) + \Delta u(\tau) \times w(\tau) \tag{1}$$

Here $u_0(\tau)$ is a reference input profile of the dimensionless time $\tau = t/t_b$, where t_b is the batch time. The function $\Delta u(\tau)$ determines the size of the design domain within which the DoDE inputs are confined during experimentation. The function $w(\tau)$ is the dynamic factor, varying in the range [-1, +1]. We parameterize the time-varying dynamic factor $w(\tau)$ by a finite linear combination of Shifted Legendre polynomials. The input profile using only the first three of them is given by.

$$w(\tau) = z_1 P_0(\tau) + z_2 P_1(\tau) + z_3 P_2(\tau) \tag{2}$$

Here the coefficients, z_i, are called dynamic sub-factors and $P_i(\tau)$ is the $i-th$ Shifted Legendre polynomial. The first 3 such polynomials are:

$$P_0(\tau) = 1, P_1(\tau) = -1 + 2\tau, P_2(\tau) = 1 - 6\tau + 6\tau^2 \tag{3}$$

Other sets of orthogonal functions can be used as the functional basis, depending on the specific problem at hand.

The set of experiments is designed by systematically varying the values of the dynamic sub-factors, z_i in the normalized range of [-1,+1] and within the following constraining equations $-1 \le z_1 \pm z_2 \pm z_3 \le +1$. In Figure 1, we plot the DoDE inputs designed for the batch process discussed later in section 4. The dotted lines are the reference input profile (middle) and the upper limit of the design domain. The solid lines are the designed set of input profiles to develop the DRSM. In these experiments, the functions $u_0(\tau)$ and $\Delta u(\tau)$ have a linear dependency on time. With the output data collected from the designed experiments, a quadratic DRSM with 3 factors in the following form is fitted:

$$y(\tau) = \beta_0(\tau) + \sum_{i=1}^{3} \beta_i(\tau) z_i + \sum_{j=1}^{3} \sum_{i<j}^{3} \beta_{ij}(\tau) z_i z_j + \sum_{i=1}^{3} \beta_{ii}(\tau) z_i^2 \tag{4}$$

where y is the output. Here again we select the shifted Legendre polynomial as the basis for the parameterization of each function $\beta(\tau)$. If the first R Shifted Legendre polynomials are used, the $\beta_q(\tau)$ is given by

$$\beta_q(\tau) = \gamma_{q,1} P_0(\tau) + \gamma_{q,2} P_1(\tau) + \ldots + \gamma_{q,R} P_{R-1}(\tau) \tag{5}$$

With $q = 0, i, ij$ or ii; for $i = 1, 2, \ldots, n$ and $j > i$. Function $\beta_q(\tau)$ can be expressed as an inner product of two vectors, $\beta_q(\tau) = \boldsymbol{\gamma}_q^T \mathbf{p}(\tau)$ where $\mathbf{p}(\tau) = [P_0(\tau), P_1(\tau), \ldots, P_{R-1}(\tau)]^T$ is the column vector of the first R Shifted Legendre polynomials and $\boldsymbol{\gamma}_q = (\gamma_{q,0}, \gamma_{q,1}, \ldots, \gamma_{q,R-1})^T$ is the column vector consisting of the $\gamma's$ parameterizing $\beta_q(\tau)$. The estimation of the $\gamma's$ will be obtained by solving the following linear regression problem, eq (6), formulated in matrix form.

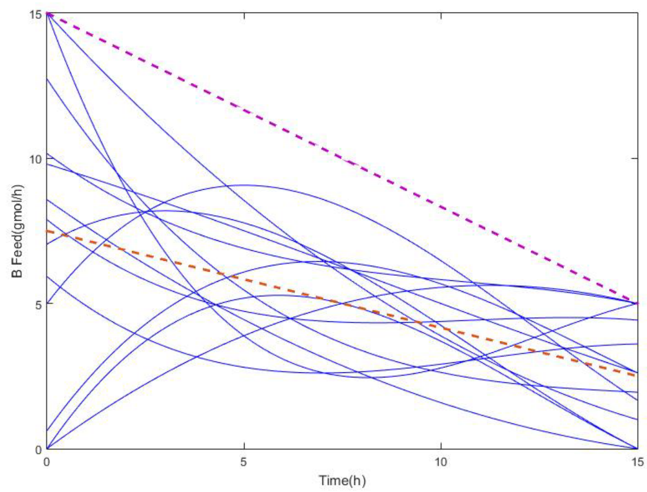

Figure 1: Input Profiles of Reactant B parameterized by 3 Dynamic Sub-Factors

We here list the variables, which define the dimensions of the vectors and matrices involved in eq (6). They include the

- n : Number of dynamic Sub-factors
- p : Number of parametric functions $\beta_q(\tau)$
- R : Number of polynomial parameterizing each $\beta_q(\tau)$
- M : Number of experiments
- K : Number of measurements during each experiment

There are two constraints on the above variables: $M > p$ and $K > R$. Here we arrange the measurements from the M experiments in the $M*K$ matrix $\mathbf{Y} = (\mathbf{y}(\tau_1), \mathbf{y}(\tau_2), \ldots, \mathbf{y}(\tau_K))$ where column vector $\mathbf{y}(\tau_k) = (y_{1,k}, y_{2,k}, \ldots, y_{M,k})^T$ has the measurements made at time instances τ_k, (k=1, 2,…, K) across all M experiments. We now express the dependence of output, $\mathbf{Y}$ on the inputs and the parameters as

$$\mathbf{Y} = \mathbf{Z \Gamma P} \tag{6}$$

Matrix $\mathbf{\Gamma}$ consists of the constants γ parameterizing the $\beta_q(\tau)$ functions. Matrices $\mathbf{Z}$ and $\mathbf{P}$ defined below are of full rank. For the illustrative example of two dynamic sub-factors, the matrices are given by:

$$\Gamma = \begin{pmatrix} \gamma_{0,0} & \gamma_{1,0} & \gamma_{2,0} & \gamma_{12,R-1} & \gamma_{11,0} & \gamma_{22,0} \\ \gamma_{0,1} & \gamma_{1,1} & \gamma_{2,1} & \gamma_{12,R-1} & \gamma_{11,1} & \gamma_{22,1} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \gamma_{0,R-1} & \gamma_{1,R-1} & \gamma_{2,R-1} & \gamma_{12,R-1} & \gamma_{11,R-1} & \gamma_{22,R-1} \end{pmatrix}^T$$