Predictive Modeling of Key Process Variables in Granulation Processes based on Dynamic Partial Least Squares

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Abstract: Granulation is a multivariable process characterized by several physical attributes that are essential for product performance, such as granule size and size distribution. An optimally operated granulation process will yield, in a reproducible manner, product with tightly controlled performance attributes. In this paper predictive models of the dynamics of these key variables are developed using a dynamic partial least squares approach. The method, demonstrated here on process simulation as well as on an industrial mixer-granulator process, result in accurate predictions. These models motivate the development of model predictive controllers for these processes.

Keywords: Granulation, Process control, Dynamic modeling, Partial least squares

1. INTRODUCTION

Granulation is a complex process in which many input variables influence many product properties. As Iveson et al. describe in a review paper (2001), the understanding of the fundamental processes that control granulation behavior and product properties have increased in recent years. This knowledge can be used during process design, in choosing the right formulation and operating conditions, and it can also be used to improve process control. Although many variables are set constant during process design, variations during production in input variables occur due to the variable nature of the powder feed. Even if all granule properties, except for size, are ignored for process control, a one dimensional granule size distribution can be constructed by multiple discrete output variables, in order to represent the shape of the distribution (these can be mean sizes (with coefficients of variation), percentile sizes, moments or size bins). Model Predictive Control (MPC) is an effective method to control such multiple input, multiple output processes (García, et al., 1989). The majority of MPC applications in the chemical process industries utilize empirical models that are constructed from plant data. In this work, we explore the use of dynamic partial least squares to construct these empirical models.

2. METHODS

2.1 Partial Least Squares

Partial Least Squares (PLS) methods have been demonstrated as a useful tool for analysis of data and modeling of the systems from which the data are collected (Kaspar and Ray, 1993). Unlike related methods, such as Principal Component Analysis (PCA), which finds factors that capture the greatest amount of variance in the predictor (X) only, the PLS method attempts to find factors which both capture variance and achieve correlation. PLS handles this by projecting the information in high dimensional spaces (X,Y) down to low dimensional spaces defined by a small number of latent vectors ($t_1,t_2 \ldots t_a$). These new latent vectors summarize all the important information contained in the original data sets, by representing the scaled and mean-centered values of X and Y matrices as:

$$X = \sum_{i=1}^{a} t_i p_i^T + E$$
$$Y = \sum_{i=1}^{a} u_i q_i^T + F \qquad (1)$$

where the t_i are latent (score) vectors calculated sequentially for each dimension i=1,2,…a.

In the PLS method, the covariance between the linear combinations of X and the output measurement matrix Y is maximized at each iteration, using the vectors p_i and q_i which are the loading vectors whose elements express the contribution of each variable in X and Y toward defining the new latent vectors t_i and u_i. E and F are residual matrices for X and Y blocks, respectively. The optimal number of latent vectors retained in the model is often determined by cross-validation (Dayal et al. 1994).

In an industrial environment, it is more often the case that many of the predictor variables (X) are highly correlated with one another and their covariance matrix is nearly singular, which renders classical regression methods intractable. Reduced space methods such as PLS and PCA can overcome this problem (MacGregor and Kourti, 1995). PLS is also robust to measurement noise in the data and can be used in cases where there are random missing data and when the number of input variables is greater than the number of observations (Dayal et al. 1994). Various examples of the implementation of PLS analysis to industrial process modeling and control can be found in the literature (for example, Dayal et al., 1994, MacGregor and Kourti, 1995, and others).

Process dynamics can be incorporated into the PLS model by including columns of lagged outputs and/or inputs into the predictor block (*X*) (Dayal et al., 1994, Kaspar and Ray, 1993, Juricek et al. 2001). The resulting PLS model is actually an ARX type input-output model of the form:

$$A(q^{-1})y_i(k) = \sum_{j=1}^{nu} B_j(q^{-1})u_j(k - nk_j) \tag{2}$$

$$A(q) = 1 + a_1 q^{-1} + a_2 q^{-2} + \ldots + a_m q^{-m} \tag{3}$$

$$B_j(q) = b_{j,1} q^{-1} + b_{j,2} q^{-2} + \ldots + b_{j,m} q^{-m} \tag{4}$$

where *y* denotes the output variable (e.g., median particle size, d_{50}), and *u* denotes the manipulated variable (e.g., binder flow). The terms *A* and *B* contain the autoregressive and exogenous terms of the model, respectively. The autoregressive term captures dynamics through lagged terms of the output, and the exogenous term captures dynamics through lagged terms in the input.

Once the models have been calculated from the plant data, it is useful to evaluate their properties using several key statistical measures. Some of the useful statistics that are associated with reduced space models (Wise et al. 2006) are outlined below:

Q residual – is simply the sum of squares of each row of *E* (from eq. 1), i.e. for the ith sample in *X*, x_i:

$$Q_i = e_i e_i^T \tag{5}$$

where e_i is the ith row of *E*. The Q statistics is a measure of the difference between a sample and its projection into the *a* principal components retained in the model.

Hotelling T^2 is a measure of the variation in each sample within the model. Its value is the sum of normalized squared scores, defined by:

$$T_i^2 = t_i \lambda^{-1} t_i^T \tag{6}$$

where t_i are the score vectors (eq. 1) and λ is a diagonal matrix containing the eigenvalues corresponding to *a* eigenvectors (principal components) retained in the model.

Together, the T^2 and Q residual statistics are useful in evaluating the fitness of a PLS model to specific data. It is possible to calculate statistically meaningful confidence limits for both cases.

2.2 Simulation studies

In our previous work, a nonlinear one dimensional population balance model (1D-PBM) was successfully used to model a laboratory continuous drum granulation process with fine particle recycle (Glaser et al., 2008). The same model is used here as a base for a process simulation (Figure 1) for a preliminary evaluation and sensitivity test of the applicability of the dynamic PLS modeling technique for granulation.

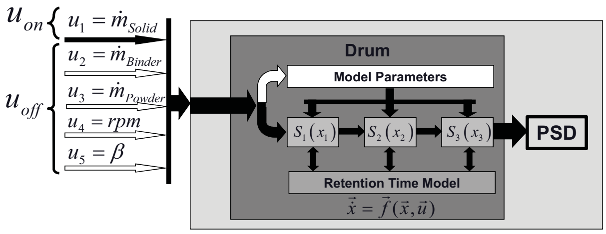

Fig. 1. Simulator structure: five inputs are included in the simulator: binder spray rate, fine powder feed-rate, drum rotation-rate and the drum inclination angle. The model is divided into three well mixed drum compartments, each described by an individual set of ODEs, a retention time model and a set of global parameters that influence the model behavior (taken from Glaser 2008).

Both particle median size (d_{50}) and, separately, particle size distribution width (d_{84}/d_{16}) were used as output variables for this study. The predictor (*X*) was constructed from 4 manipulated variables (solid feed flow rate, binder feed flow rate, drum rotation speed, recycle rate) and the computed recycle flow as an additional input variable. Process dynamics were incorporated into the *X* block by including columns of lagged output variables. The lag time was estimated using an autocorrelation function. Delay times of each of the input variables were estimated using cross correlation function, and the predictor matrix was adjusted according to the obtained delay vector. During the simulation, the 4 manipulated variables were randomly perturbed around their nominal values at steady state sequentially, i.e. input variables were perturbed one after the other in fixed time gaps. The resulting PLS-based ARX model's short horizon predictive ability was tested by cross validation with a set of separately calculated simulation sequences with different excitation regimes. For each of these cross validation sequences, the root mean square error of the model based prediction (RMSEP), relative to the simulated plant measurements was calculated for a given short horizon period. In order to make a more representative quantification of the predicting ability of the model, the short horizon start point was moved along the time axis of the data one time step after another thus creating a set of RMSEP measures out of which an average and maximum RMSEP could be calculated. All variables were mean centered and scaled to unit variance prior to processing.