Multivariate SPC for Startups and Grade Transitions

Carl Duchesne, Theodora Kourti, and John F. MacGregor
McMaster Advanced Control Consortium (MACC), Dept. of Chemical Engineering, McMaster University, Hamilton, Ontario L8S 4L7, Canada

Process transitions (grade changeovers, startups, and restarts) are very frequent in industry, and usually lead to the loss of production time, the production of off-grade materials, and to inconsistent reproducibility of product grades. Two aspects of using multivariate statistical methods based on PCA and PLS to improve process transition performance using historical records of transition data are discussed. First, multivariate SPC approaches are proposed to determine if the process conditions for the commencement of a transition ("startup readiness") are correct and to assess the successful completion of a transition ("production readiness for the new grade"). The latter is illustrated using a simulated fluidized-bed process for the production of different grades of linear low-density polyethylene. Second, analysis tools are suggested for diagnosing the reasons for past transition problems and for monitoring new transitions to ensure repeatable high quality transitions. The latter methods are aimed at reducing the amount of off-specification materials and reducing transition time, as illustrated on industrial data from restarts of a polymerization process.

Introduction

This article proposes several multivariate statistical approaches based on PCA and PLS for the analysis and monitoring of process transitions. By the term transition, we include continuous process transitions from grade to grade, the startup of a continuous process, or the restart of a continuous process that went on hold. In multiproduct continuous processes, transitions from grade to grade account for a significant portion of process time. As an example, it has been reported that gas-phase linear low-density polyethylene (LLDPE) reactors can cycle between as many as 50 different polymer grades (Xie et al., 1994) to satisfy customer demands. Other common types of transitions are process startups (from empty units after cleaning cycles) or process restarts after a process hold caused by disruption from steady-state production. Although necessary, all of these transitions lead to important loss of production time, off-grade materials, and inconsistent reproducibility of product grades.

Correspondence concerning this article should be addressed to T. Kourti.
Current address of C. Duchese: Laval University, Chemical Engineering Dept., Ste-Foy, Quebec G1K 7P4, Canada.

Grade transitions, startups, and restarts all share the same three common stages: the initial conditions, the transition, and the final steady state. This is shown in Figure 1 for a grade transition or a startup using three process variables. State 1 shows the steady-state process conditions of a grade (grade 1). At some point, the process conditions are modified (transition) aiming at another product (grade 2) corresponding to steady-state 2. When a large number of process variables are routinely collected, one could use a projection space to visualize the transition in a low dimensional space. This is shown in Figure 2, where the behavior of the process at each instant is summarized on a plane defined by two summary (latent) variables t_1 and t_2. Steady-state operating regions where the two grades can be successfully produced are shown as ellipses. Each dot in the ellipses of Figure 2 corresponds to the average steady-state conditions achieved during a past period when the corresponding grade was successfully being made. Just before a transition begins, the state of the process defines the initial conditions. These conditions may correspond to any of the points in "state 1" of Figure 2. Then, different transitions from one state to another are illustrated by the paths numbers I to IV in Figure 2. All paths shown in

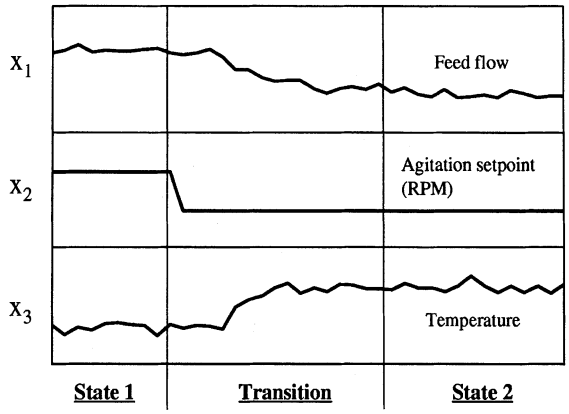

Figure 1. Three common stages of any process transition.

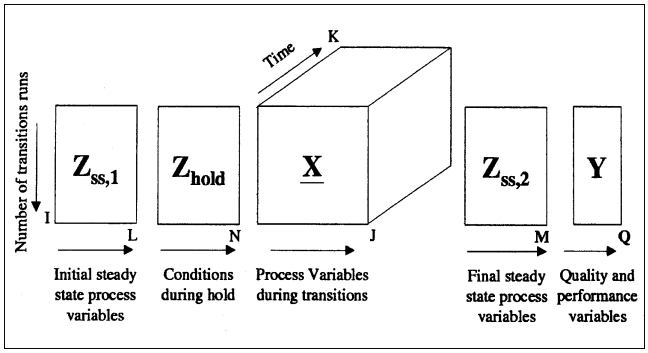

Figure 3. Nature of the data collected for the transition problem.

Figure 2 may achieve an acceptable quality of the *measurable* properties of the product at the final steady state. However, these paths take different times and produce different amounts of off-spec materials. Furthermore, not all the paths lead to process conditions within the ellipse of state 2. This implies that some aspects of the product for grade 2 may be questionable, even if the few measured product properties are within specifications.

This article addresses each of these problems. The general nature of transitional data is described, followed by the definition of "production readiness" regions within which the final steady-state process conditions must fall in order to ensure that the product will have high quality and be consistent with past periods of production for that grade. A similar problem of defining "startup readiness" regions is also addressed. Finally, we focus on historical transition data analysis including the diagnosis of reasons for poor transitions in the past and on the development of multivariate statistical process control schemes to test that new transitions are following an acceptable path.

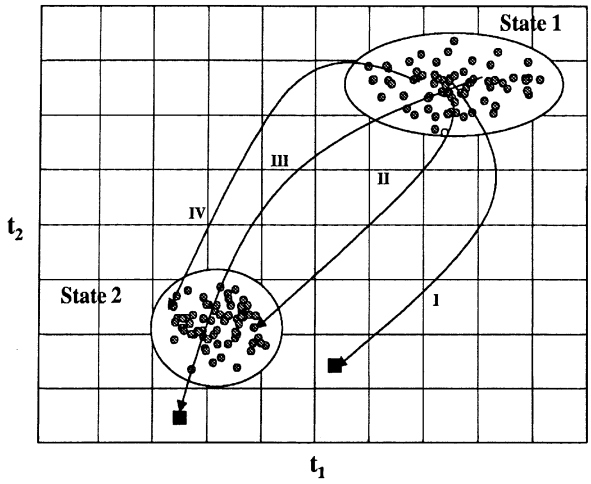

Figure 2. Three common stages followed by any transition.

Initial conditions: "state 1"; transition: paths I–IV; final steady state: "state 2".

Nature of Transitional Data

The type of database collected during the stages of different types of transitions is shown in Figure 3 for the general case. When $\boldsymbol{Z}_{\mathbf{hold}}$ does not exist, we then have a typical transition from one product (steady-state $\boldsymbol{Z}_{ss,1}$) to the other ($\boldsymbol{Z}_{ss,2}$). Initial conditions ($\boldsymbol{Z}_{ss,1}$) are characterized by a collection of L measurements obtained for I transition runs (and should fall within a certain range of conditions to guarantee successful transitions). If a process is put on hold for some reason and then restarted, a matrix $\boldsymbol{Z}_{\mathbf{hold}}$ gives a summary of N conditions that developed during the hold and describes the system just before restart ($\boldsymbol{Z}_{\mathbf{hold}}$ could also be a 3-way array, if the full transient behavior of the process for the duration of the hold needs to be considered). During each transition, process measurements are gathered on J process variables, sampled at K intervals, and are stored in a three-way array $\underline{\boldsymbol{X}}$. Then, at the end of each of the I transition runs, the final steady-state conditions are summarized by M process variables stored in a third block of data $\boldsymbol{Z}_{\mathbf{ss,2}}$. This latter data block may or may not be used in the analysis of transitions. However, it is used in the development of "production readiness" regions as is described in the next section. Finally, the last data block, $\boldsymbol{Y}$, contains Q measurements characterizing transition performance. It typically consists of transition time, amounts of off-grade materials, overall performance classification using "good"/"bad" categories and so forth. The data block $\boldsymbol{Y}$ should be viewed as the *objective function* used for improving transition policies and, therefore, any important measurements defining "desirable" transitions or any combination or function of them should be included in $\boldsymbol{Y}$.

Production Readiness Analysis

A problem which is not as straightforward as it may seem is to determine the successful completion of a transition from one grade of product to another. Only when the process has successfully achieved a new steady state in which all conditions are acceptable for the production of the new grade at an acceptable level of quality can one deem the transition

complete and the process in a state of "production readiness." Such a region should be based on the "complete" product quality (experienced by customers), and not just the few properties that are typically measured by the producer. This expanded set of properties should be used to determine if the final steady-state operation is consistent with producing a good quality product. Unfortunately, such an expanded (customer response) set of quality data is never available to process personnel at the end of transitions. Rather, only the few quality variables routinely checked by the quality control lab are available. A problem often encountered in practice is that these few routine quality measures may be within their new specification limits at the apparent end of a transition, even though the total quality as eventually seen by the customer is not. This situation often arises because the process operating conditions attained at the end of a transition are fairly different from what are normally used to produce an acceptable product for this grade. For example, some process variables may be left at the settings corresponding to a previous grade or another operating mode, because of preferences of different teams of operators or engineers, or because of economics, and so on. However, multiproduct processes are generally flexible enough to achieve specifications on the few measured quality properties, in spite of these differences. This situation is illustrated in Figure 2, where the final steady-state conditions for transitions I and III are different and fall outside the operating region that is normally used ("state 2" ellipse). These processing conditions may all still achieve the desired value of the measured properties, but the impact that a different combination of operating conditions may have on the "complete" product quality as seen by customers is unknown. For example, consider a linear low density polyethylene (LLDPE) fluidized-bed reactor transitioning between two grades of polymer. Grade quality of LLDPE copolymers is typically assessed using a measureable melt flow index (MI) and density (ρ) (McAuley and MacGregor, 1992). However, since MI and ρ only measure the location (mean) of the molecular weight distribution (MWD) and the copolymer composition distribution (CCD), respectively, they do not account for variations in the shape of these distributions, which is very important for customers. When buying two polymer products with the same MI and ρ, but produced under different conditions, a customer may find that they behave differently (that is, one is more difficult to process than the other).

Very few works related to this problem have been reported in the literature. McAuley and MacGregor (1992) briefly discussed that using only a few quality variables (such as Melt index and density) to define production readiness in a gas-phase LLDPE reactor does not ensure that the overall polymer quality (MWD and CCD) is on target.

Defining "production readiness" regions

A logical solution to the production readiness problem is to target processing conditions, as well as measured quality properties into a desirable region. This region should be based on steady-state conditions that have led, in the past, to good customer satisfaction. This can only be addressed based on a joint collaboration between suppliers and customers, as only customer feedback makes this problem observable. Once desirable steady-state periods are identified, multivariate projection methods, such as Principal Component Analysis (PCA) and Projection to Latent Structures (PLS), are used to develop production readiness regions. This is developed in a similar manner as for multivariate statistical process control charts for continuous processes (Kourti et al., 1996; Zullo, 1996).

The database available for defining a production readiness region consists of the final steady-state data block $\boldsymbol{Z}_{ss,2}$ shown in Figure 3. This data block contains M process measurements, collected for I steady-state periods. A second block of data $\boldsymbol{Y}$ may also be available for defining production readiness to help in identifying the successful steady-state production periods. It may consist of quality variables, including variables other than those used as product specifications, or of customer feedback on product quality obtained during all or some steady-state periods. Feedback could be simply in terms of a "good" or "poor" classification of quality. In the following a "production readiness" region will be defined using those process conditions which correspond to the "good" quality product defined in $\boldsymbol{Y}$.

To define a production readiness region as discussed above, one needs to build a PCA model of the $\boldsymbol{Z}^{cc}_{ss,2}$ database, which is a subset of $\boldsymbol{Z}_{ss,2}$ containing only successful steady-state production periods (that is, common cause sources of variations around a nominal operating point). The result of PCA is a reduced dimensional space defined by a set of score variables, $t_1, t_2, \ldots, t_A$. Usually, the first few scores (t_1 and t_2) are enough to summarize the major sources of variations in the data ($\boldsymbol{Z}^{cc}_{ss,2}$). The production readiness region will be defined by the value of these scores, as well as by the model residuals expressed as a squared prediction error (SPE), or perpendicular distance to the reduced dimensional space. An elliptical region of the form of $T^2 = \sum_{i=1}^{A} t_i^2/s_{t_i}^2$ is used to define the boundary of the production readiness region on the plane spanned by the scores of the PCA model. Here, $t_1, t_2, \ldots, t_A$ are the first A principal components and $s_{t_i}^2$'s are their sample variances. The critical value of T^2 at the α-level of significance is obtained from the Hotelling's T^2 distribution where $T^2 \sim [[(I-1)(I+1)A]/I(I-A)]\ F_\alpha(A, I-A)$ (Anderson, 1984). I is the number of observations in $\boldsymbol{Z}^{cc}_{ss,2}$ and A is the number of components used in the PCA or PLS analysis. The perpendicular distance of the ith observation from the plane is defined as $SPE_i = (z_{ss,2,i} - \hat{z}_{ss,2,i})^\top (z_{ss,2,i} - \hat{z}_{ss,2,i})$, where $\hat{z}_{ss,2,i}$ is the estimate of $z_{ss,2,i}$ obtained by PCA or PLS: $z_{ss,2,i} = \boldsymbol{t}_i \boldsymbol{P}^\top + \boldsymbol{E} = \hat{z}_{ss,2,i} + \boldsymbol{E}$. Approaches for computing upper limits on SPE are discussed in Nomikos and MacGregor (1994b). In some literature the statistic $DMODZ_i = \sqrt{SPE_i/(N-A)}$ is used as a measure of the distance to the model of the $\boldsymbol{Z}$ space (residuals). When this distance is higher than a given limit, this suggests that a combination of operating conditions reflects a different correlation structure than seen before in the historical database. A valid production readiness, therefore, consists of two monitoring charts, one for the projection space (score space) and one for the distance from this projection space or residuals (either SPE or $DMODZ$). Final steady-state operation has reached this region when projected conditions fall within the limits of the projection space and when the residuals are below an upper limit. Only when both processing conditions and measured

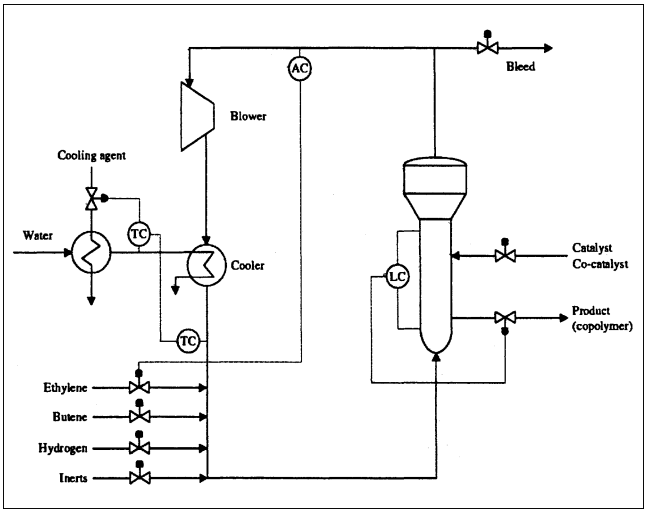

Figure 4. Gas-phase LLDPE reactor.

quality have reached their successful regions should the transition be considered terminated and the process deemed to be in a state to satisfactorily produce the new grade.

Simulation example

The concepts related to definition of production readiness are now illustrated with data obtained using a detailed mechanistic model of a gas-phase LLDPE reactor (McAuley et al., 1990; McAuley, 1992). The LLDPE reactor is shown in Figure 4. This fluidized-bed reactor is used to carry out copolymerization of ethylene and butene (copolymer) by the means of a Ziegler-Natta catalyst. The fresh feeds of the system consist of ethylene (F_{Et}), butene (F_{But}), hydrogen as a chain transfer agent (F_H), and inerts (nitrogen). These gases maintain the fluidization of the bed, within which polymer particles are growing. Feed rates of ethylene and inerts are also used to control reactor pressure (P). The catalyst (F_{cat}) is fed directly into the reaction zone. The bed level or weight (B_w) is controlled by manipulating the polymer outflow rate ($F_{\text{poly,out}}$). Since the conversion per pass is low, unreacted monomers coming out of the reactor are recycled.

A bleed stream is necessary to prevent buildup of impurities. Bleed rate (F_{bleed}) is adjusted using the bleed valve position (ν_p). Since the reaction is exothermic, heat is removed from the recycled gas stream before returning into the reactor, using a water-cooled heat exchanger. Reactor temperature (T_r) is controlled using a cascade control system, adjusting the cooling water temperature feeding the exchanger ($T_{w,\text{in}}$). To stabilize the polymerization reaction, ethylene concentration in the recycle stream is also controlled at a specific level using the rate of fresh ethylene feed. A nonlinear property control scheme is implemented on the process to maintain the two measured polymer quality variables, instantaneous MI and ρ close to their set points (McAuley and MacGregor, 1993). "Complete" polymer quality can be assessed by the overall compositional and molecular weight distributions (CCD and MWD), computed using Stockmayer's bivariate distribution for a two monomer system (McAuley et al., 1990).

Table 1. Process Nominal Conditions

	T_{sp} (K)	$B_{w,sp}$ (tonne)	F_{cat} (kg/h)	ν_p (%)
Nominal value	360.00	65.0	5.00	0.30
Std	1.19	0.9	0.11	0.02

To simulate a common cause variation region for acceptable process operation ($\mathbf{Z}^{cc}_{ss,2}$), 20 steady-state periods for the production of a specific polymer grade ($MI = 12$ g/min, $\rho = 920$ g/L) were generated, by introducing small random variations, in the reactor temperature set point (T_{sp}), the bed level set point ($B_{w,sp}$), the feed of catalyst (F_{cat}), and the bleed valve position (ν_p), around nominal conditions. The values of these variables were maintained constant during the entire steady-state periods, but were varied between them. Nearly nonstationary autoregressive disturbances on the amount of impurities and on the relative amounts of each type of catalyst active sites, as well as random measurement error on MI and ρ, were also added to the simulations. For each production period, the nonlinear controller maintained MI and ρ near their specifications in spite of disturbances and variations in operating conditions. Table 1 shows the nominal values and sample standard deviation for each of the four process variables. To introduce some collinearity within the four manipulated process variables, $B_{w,sp}$ and F_{cat} were varied in a correlated manner with a sample correlation coefficient of 0.84.

Three additional operating conditions were also simulated, but including systematic differences not seen in the common cause data. However, even for these conditions, similar MI and ρ were obtained due to compensation from the nonlinear controller. Steady-state periods number 21 and 22 were generated in a similar manner to those for the common cause variation data, but the reactor temperature set point was left at other settings in both cases. Values of 350.1 K and 369.5 K were implemented on T_{sp} for runs number 21 and 22, respectively. Steady-state period number 23 was also generated as common cause data, but $B_{w,sp}$ and F_{cat} were varied in a negatively correlated fashion. Figure 5 shows the measurements on MI and ρ averaged over each of the 23 steady-state periods. Clearly, the apparent polymer quality as measured by MI and ρ still appears to be good for operating periods 21 to

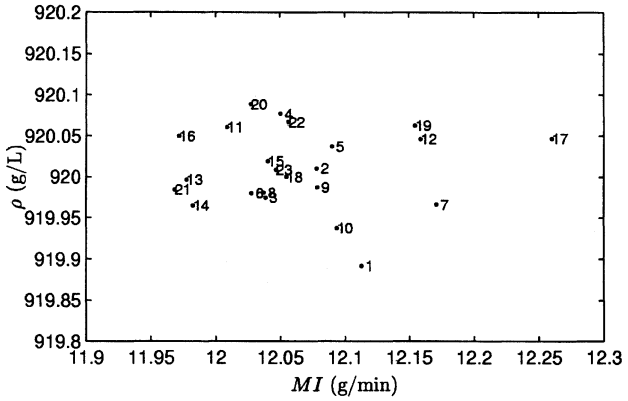

Figure 5. Averaged measurements on melt index and density over each of the 23 steady-state periods.

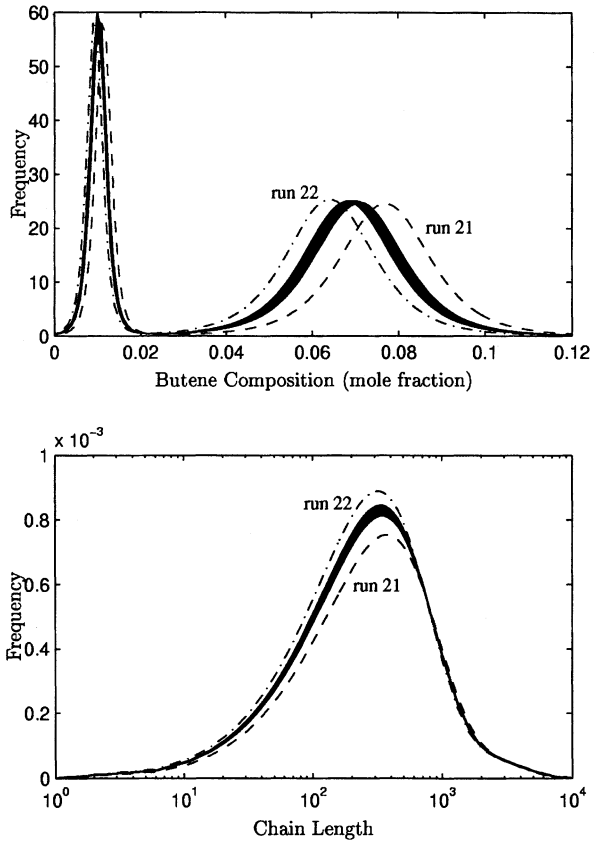

Figure 6. Overall polymer quality for the 23 runs, as described by the overall composition and chain length distributions.

Solid lines: runs 1–20 and 23, dashed line: run 21, dashed-dotted line: run 22.

23. This demonstrates that the process has enough flexibility to achieve the same measured polymer properties in spite of all sources of variations.

If polymer quality could have been completely characterized by measuring the overall CCD and MWD for all 23 production periods, the results shown in Figure 6 would have been obtained. Average steady-state process conditions were used for computing the CCDs and MWDs. Distributions associated with periods 1–20 and 23 are very similar and only vary due to the common cause sources of variations. However, operation in periods 21 and 22 clearly lead to a very different product, even though MI and ρ were within specifications. It is expected that a supplier would have received complaints for these products, without having evidence for such poorer quality. For this reason, we assume that a supplier would use steady-state periods 1–20 and 23 as an initial basis for developing the production readiness region.

A total of 11 process variables ($\boldsymbol{Z}_{ss,2}$) are currently measured on the fluidized-bed reactor: F_{Et}, F_{But}, F_H, F_{cat}, F_{bleed}, $F_{\text{poly,out}}$, T_r, $T_{w,\text{in}}$, P, B_w, and ν_p. These measurements were averaged over their corresponding steady-state periods. Mean centering and scaling to unit variance was applied to $\boldsymbol{Z}_{ss,2}$ and a PCA was performed. However, period 23 had a large residual or perpendicular distance to the projection space ($DMODZ = \sqrt{SPE/(N-A-1)}$), since $B_{w,sp}$ and F_{cat} had an unusual negative correlation during this period. These results are not shown here for sake of conciseness. Although no major customer complaints would be expected for materials produced under period 23, it would be safer to remove such outlier observations before developing production readiness regions. We, therefore, proceed with the development of the production readiness region with periods 1–20.

Three components were found significant by leave-one-out cross-validation and a summary of modeling results is given in Table 2. The R^2_{cum} value gives the cumulative percentage of the total sum of squares of $\boldsymbol{Z}_{ss,2}$ that is explained by the fitted PCA model with A components, $A = 1, 2, 3$. The Q^2_{cum} value gives the cumulative percentage of the total sum of squares of $\boldsymbol{Z}_{ss,2}$ that can be predicted with this model using a leave-one-out cross-validation procedure. With more than two components (3 in this case), the production readiness region is presented using the Hotelling's T^2 statistic (see the previous sub-section), as shown in Figure 7.

The averaged steady-state conditions for periods 21 and 22 were projected onto the reduced space of the PCA model, as if they would be monitored on-line, and their projection results are also shown in Figure 7. Clearly, these sets of operating conditions are different, both in the projection space (T^2) and in the distance from this space (DMODZ), due to unusual temperature set points. Had a production readiness region been implemented on-line, the operators or engineers would have been warned that a state of "production readiness" had not been reached. Contribution plots to T^2 and DMODZ (Kourti and MacGregor, 1996) would then have shown that the reactor temperature was the major contributor to these deviations and corrective actions could be taken. The production of large amounts of poor quality materials could have, therefore, been avoided.

In this example, the two abnormal situations arose from fairly large temperature biases which, one might argue, could have been noticed by the process engineer. However, in general, such abnormal situations can arise from combinations of small biases in many variables, none of which may draw the attention of the engineer, but together result in an abnormal condition leading to poor quality products. The multivariate "production readiness" charts would be equally effective at detecting these more subtle situations.

"Startup readiness" regions

Definition of "startup readiness" is another practical problem that could be solved in a similar fashion to that of the "production readiness" problem. An example of startup readiness issues encountered in the film coating industry is described here; it involves synchronizing two sections of the process before the startup of coating operation begins. One section is aimed at bringing the materials and solutions involved in the coating operation to specified temperatures, viscosities, and so on. The second section of the process involves equipment for conveying the material to coating devices and requires some time to be ready for coating. Furthermore, coating solutions generally age and need to be within a certain time window. Clearly, if the decision to initiate the startup happens too early and the temperatures and viscosities of the materials have still not attained the correct combination of conditions, or too late, and the solutions have aged, then this may cause poorer transient performance or

Table 2. PCA Model: Cumulative Percent Explained and Percent Predicted Variance of $Z_{ss,2}$, $R^2_{Z_{ss,2},\text{cum}}$ and $Q^2_{Z_{ss,2},\text{cum}}$

A	$R^2_{Z_{ss,2},\text{cum}}$ (%)	$Q^2_{Z_{ss,2},\text{cum}}$ (%)
1	46.0	28.3
2	78.8	62.8
3	97.1	92.6

failure of the startup procedure. Therefore, a startup readiness region could be developed to help with sychronizing the processing conditions in both sections of the process and, hence, ensure desirable startup performance. This region will be developed for the process conditions $\boldsymbol{Z}_{ss,1}$ (see Figure 3), prevailing over some time window just prior to initiating the startup procedures that led in the past to desirable performance (stored in $\boldsymbol{Y}$). Again, this would involve building PCA or PLS models on the time histories of the variables over this period to define a startup readiness region. A similar problem was presented by Wurl et al. (2001), who proposed the use of multivariate process monitoring to reduce the startup time of a batch filament extrusion process. Their approach consists building a Projection to Latent Structure (PLS) model on good production data and use this model to monitor processing conditions during the startup. The model allows one to detect operational conditions that are inconsistent with good production.

It is important to note that both the production readiness and startup readiness regions are based on data from past transitions. They are defined to include past conditions that successfully led to good transition startups and endings, and exclude those that did not. However, as with all data-driven methods, they cannot predict what might happen when a combination of conditions arises that has never occurred before. This implies that there will almost certainly be conditions outside of these regions that might be perfectly acceptable. All one can do when such a transition is encountered is to add those conditions to the database and update the model and the regions. Eventually, once most conditions have been encountered the regions will stabilize.

Analysis of Transition Policies

Transition policies are traditionally developed using detailed mechanistic process models, in conjunction with optimization algorithms (Sargent and Sullivan, 1979; Farber and Laurence, 1986; McAuley and MacGregor, 1992; Xie et al., 1994; Ohshima et al., 1994; Flender et al., 1996; Wang et al., 2000; Cervantes et al., 2002). The evaluation of sub-optimal policies based on first principles models is a topic also encountered in the literature. A discussion of the relative merits of a few, sub-optimal grade transition policies for olefin polymerization is provided by Debling et al. (1994), while Verwijs et al. (1995) proposes qualitative rules for achieving successful startups of continuously operated chemical reactors. Mechanistic models are, however, often not readily available or difficult and time consuming to develop. In these situations, a database approach to improve transition policies would be very useful.

In this section, we propose an empirical approach to help improve transition performance through the analysis of historical data from past process transitions. Past data from

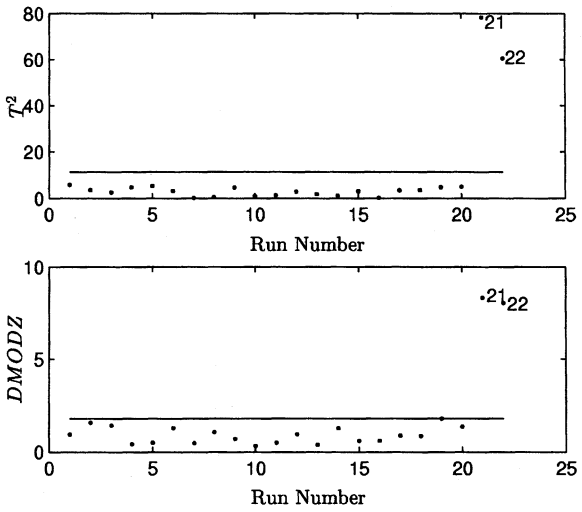

Figure 7. PCA model built on the 20 steady-state production periods within common cause variations.

Hotelling's T^2 and distance to the model (residuals) after 3 components (DMODZ).

transitions that produced different amounts of off-grade material and had different durations are analyzed. A scheme is then suggested to monitor the process to ensure consistent performance during transitions. The idea of this approach comes from the fact that databases collected during transitions (Figure 3) are similar to those obtained from batch processes, for which the analysis and monitoring of trajectories (Nomikos and MacGregor, 1994a,b, 1995; Kourti et al., 1995), and the optimization of trajectories (Duchesne and MacGregor, 2000) have already been addressed.

Depending upon the range of variations available in the historical transition databases, two scenarios could be used for improving transition policies, in the sense of reducing transition time and amounts of off-grade products. The first scenario represents situations where a wide range of variations exist in past transition policies (that is, several distinct policies were implemented in the past). In such cases one could extract the features of these policies that are associated with shorter transitions and smaller amounts of off-grade and subsequently use these to optimize the transitions. The upper plot of Figure 8 illustrates how distinct transition policies would appear in a score plot of a latent variable model. A wide range of variations could also be obtained when designed experiments are added to current transition policies. From a number of transition policies, one could choose the one closest to the pursued objectives (such as minimize wastes and transition time). An approach to the identification of trajectory features for transient optimization has been presented in Duchesne and MacGregor (2000).

The second scenario is a more frequent situation where only one nominal transition policy has been used in the past, but with some variations in its implementation, due to decisions from operators and engineers and various process disturbances. This situation is illustrated by the lower plot of Figure 8, where the dots and the crosses represent transitions that resulted in good and poor performance, respectively. The

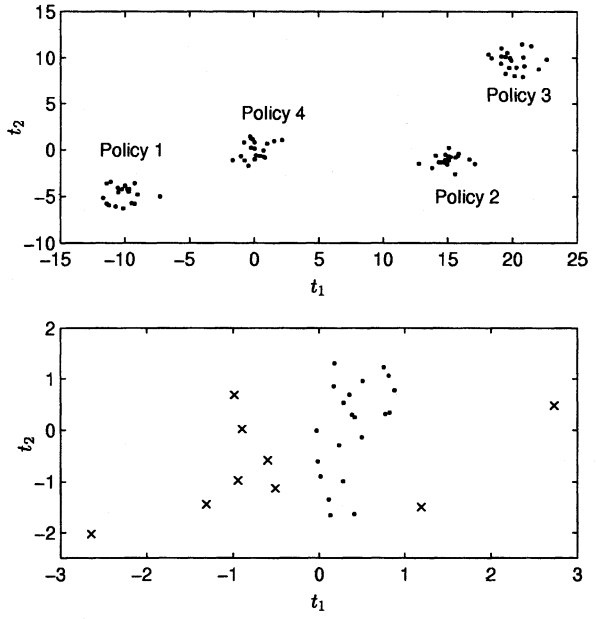

Figure 8. Transitions history using a latent variable model.

The upper plot illustrates the situation where several policies were used and the lower plot, the situation where only one policy was used, but with variations in its implementation (dots: good transition performance; crosses: bad transition performance).

range of variations in such a situation would be too small to allow transition policy optimization as in the first scenario, but one could still improve transition performance through the development of a monitoring scheme for these transitions, based on those that have led to the best performance in the past. By removing systematic variations around the current policy, one should expect a reduction in transition time and amounts of off-grade products. This section of the article addresses this latter approach.

Developing a multivariate monitoring scheme for transition policies involves the following four steps:

(1) Alignment of the transition trajectories for transitions which had different durations;

(2) Analysis of historical transition data to verify if problems leading to poorer transition performance are observable from the available data, and to eliminate any identified causes of poorer transitions;

(3) Development of statistical control charts to monitor transitions; and

(4) Implementation of the control charts to monitor new transitions.

Each of the steps mentioned above are discussed in turn in the remainder of this section and are illustrated with data collected from a continuous industrial polymerization process. The problem with this process is one of recovering from disruption of steady-state production. When operating in steady state, interruption of the process operation may occur for many different reasons. When this happens, the process remains on hold (flows to and from the process unit are stopped) until the problem is fixed, and then the process is restarted. During the hold period, the content of the different process units remains within the units and so, reactions continue to evolve. The restart operation, therefore, consists of recovering steady-state production regardless of the state that the process reached during the hold.

Alignment of trajectories

The first issue that needs to be addressed is the alignment of trajectories collected during transitions ($\boldsymbol{X}$). Since the way transitions are implemented is often left to the discretion of operators and engineers, large variations in the duration of these transitions can occur. The issue of alignment is to remove the time duration factors leaving only the trajectory shape factors to be analyzed by the multivariate statistical methods (multiway PCA and PLS). The different time durations of various sections of the transition or the total time can be included into the $\boldsymbol{Z}$ or $\boldsymbol{Y}$ data blocks, or a cumulative time indicator can be included in the $\underline{\boldsymbol{X}}$ block (Westerhuis et al., 1999a). Several approaches already exist for aligning trajectories: the indicator variable approach (Nomikos and MacGregor, 1994b; Kourti et al., 1996) and the dynamic time warping approach (Kassidas et al., 1998). A more complete review of methods for aligning trajectory data is also provided by Westerhuis et al. (1999b).

For the industrial example, it was decided to align the trajectory data ($\underline{\boldsymbol{X}}$) using the indicator variable approach. The indicator variable used was the cumulative mass-flow rate of a key reactant divided by the estimated weight of the reactor content (which is full at all times). This indicates the number of residence times that have passed since the beginning of the restart procedure. It always starts at zero, but needs to be truncated at a point where final steady state is reached. In this example, truncating after six residence times was found appropriate as most of the material that remained within the units during the hold is discharged and a stable steady-state behavior is obtained after this number of residence times. As an example of alignment, consider Figure 9 showing the trajectories of one process variable from the industrial process before and after being aligned. Note, in particular, the alignment of the early part of the trajectories for that variable.

Analysis of historical transitions

The second step of the procedure for improving transition policies involves a post-analysis of all the available data, as shown in Figure 3 (except for $\boldsymbol{Z}_{ss,2}$), to detect whether one

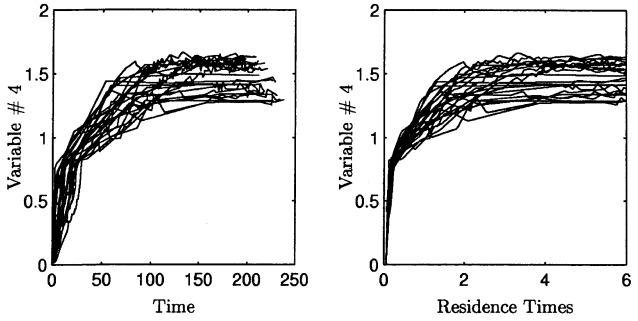

Figure 9. Alignment of trajectories collected on variable No. 4 for a total of 24 restarts.

Lefthand side: raw trajectories; righthand side: aligned trajectories.

Table 3. Multiblock, Multiway Discriminant PLS Analysis*

	R^2_{cum} (%)				Wt. %		
Component	Z_{ss}	Z_{hold}	X	Y	Z_{ss}	Z_{hold}	X
1	13.02	43.95	12.36	40.27	17.88	51.52	30.60
2	21.21	45.67	21.01	27.00	27.94	14.60	57.46

*R^2_{cum} is the accumulated percentage of variance explained by the model, and wt. % gives the relative importance of each block to that component.

can distinguish between good and bad transition performance, and to identify and rectify any apparent causes of poor transitions. This is essential to verify if known problems are observable from the collected process data and, furthermore, once observability is established, to determine if the problems can be diagnosed. Multiway, multiblock PLS or discriminant PLS (Wold et al., 1984) can be used to provide such evidence, depending on what type of Y data is available.

For the industrial example used to illustrate the concepts of this article, a total of 24 restarts were available for the production of a specific polymer. The data is organized into four blocks: the steady-state operation just prior to hold $Z_{ss,1}$ (24×26); the conditions during the process hold just prior to restart Z_{hold} (24×6); the restart trajectories $\underline{X}$ ($24\times13\times100$), and the restart performance criteria Y (24×4). The restart performance criteria included the amounts of two types of off-specification materials produced during the restart, and the restart duration. An "overall" classification of transition performance into "good" and "acceptable" and "poor" categories was made by process engineers based on these three measures of restart performance. This overall classification was then used in the post-analysis. Furthermore, since it was found impossible to discriminate between restarts falling into the "good" and "acceptable" categories using the available data, these two groups were merged. The performance criterion (Y) is, therefore, a simple dummy variable, taking a value of $+1$ for "good" or "acceptable" restarts and a value of -1 for "poor" restarts.

Multiblock, multiway discriminant PLS (MBPLS) was used to perform a post analysis of the 24 restart data sets. In this analysis, ones tries to extract features from the process transition data ($Z_{ss,1}$, Z_{hold} and $\underline{X}$) that allow one to discriminate "poorer" restarts from "good" and "acceptable" ones, as assessed *a priori* by process experts (Y). The features extracted by MBPLS should contain information on the process vari-

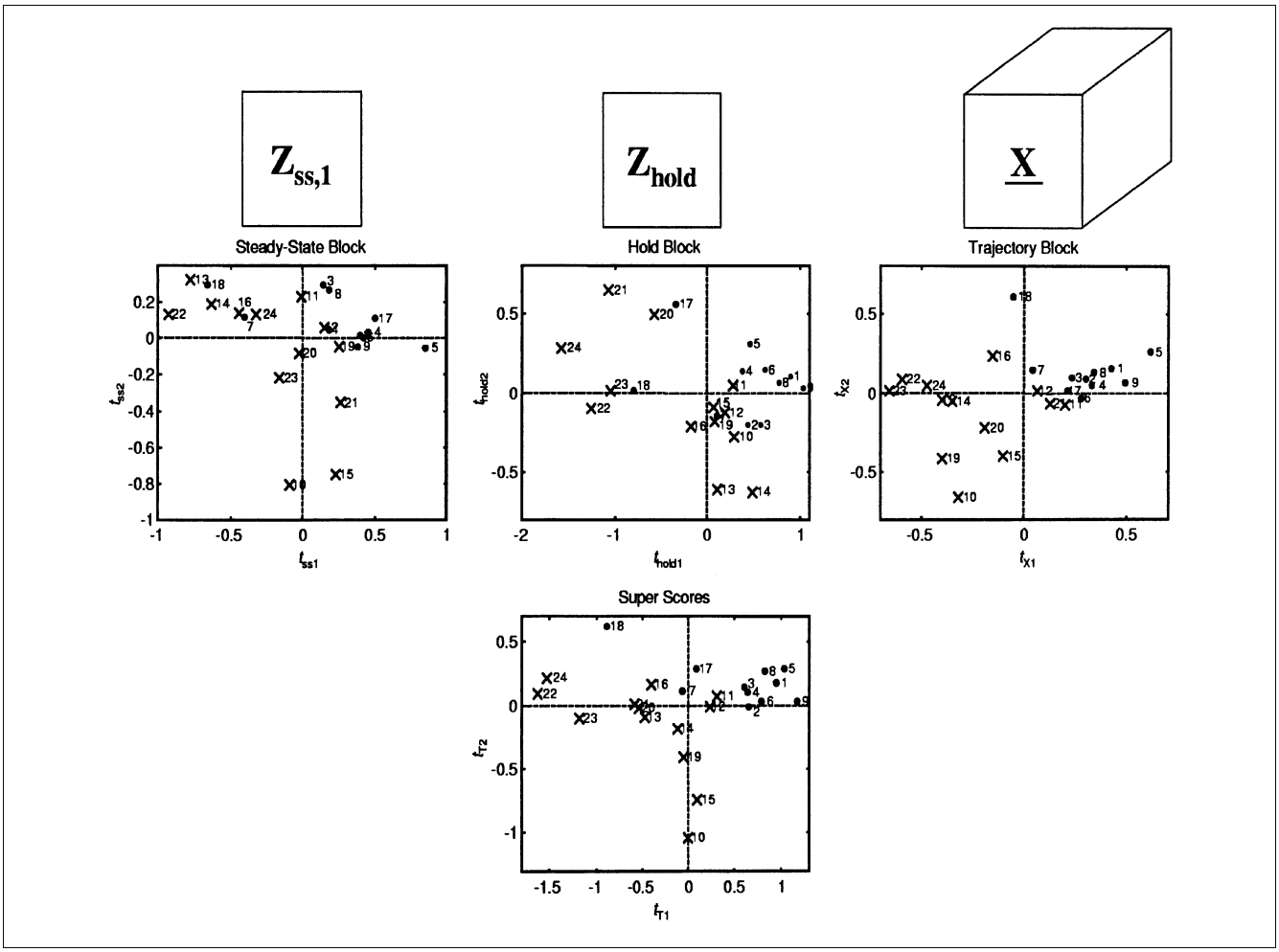

Figure 10. Multiblock discriminant PLS analysis of the 24 available restart data sets.

Dots: "good" startups; crosses: "poor" startups.

able changes that are the most correlated with the "good" and "poor" transition performance classification. Process knowledge is then used to interpret the extracted features in order to diagnose the reason for "poorer" restart performance and, subsequently, to decide on a procedure to improve performance. The multiblock PLS algorithm used is the one published by Westerhuis and Coenegracht (1997). This modeling approach and related algorithms are described in details in the Appendix section. Although MBPLS has a similar predictive ability as PLS (with all predictor blocks as one matrix), it has a twofold advantage for data interpretation due to its hierarchical structure. Its "super level" of modeling (see Figure 14 in Appendix) produces super scores ($\boldsymbol{t}_T$) that are useful for monitoring the whole system, and super loadings ($\boldsymbol{w}_T$) to compare the relative importance of each predictor block in modeling $\boldsymbol{Y}$. On the other hand, at the "sublevel," scores and loadings are computed for each predictor block which makes it possible to monitor each predictor block separately and to evaluate the relative importance of each process variable to the variation in that block.

Satisfactory discrimination between "good" or "acceptable" and "poor" restart data sets was obtained using two MBPLS components (cross-validation results revealed that only two components were statistically significant). A summary of the MBPLS results is given in Table 3. The first two components explain a total of 67% of the variance in $\boldsymbol{Y}$ (40% by the first component and 27% by the second component). The percentage of explained variance for each predictor block ($\boldsymbol{Z}_{ss}$, $\boldsymbol{Z}_{\mathbf{hold}}$ and $\underline{\boldsymbol{X}}$) indicates how much variation in that block is used in modeling $\boldsymbol{Y}$ for each component in the model. The importance of each predictor block (wt. %) is also shown in Table 3. It is computed as the percentage that each super weight accounts for in the norm of the super weight vector ($w_{T,b}^2/\|\boldsymbol{w}_T\|$ for predictor block b, see Appendix for algorithm and notation). Super weights $w_{T,b}$ give the relative importance of each predictor block in explaining variations in $\boldsymbol{Y}$ in a given MBPLS component. In the example, the first component focuses more on the hold data block and the second, on the steady state and restart trajectories. All three predictor blocks appear important in explaining $\boldsymbol{Y}$ (dicrimination), although $\boldsymbol{Z}_{\mathbf{hold}}$ and $\underline{\boldsymbol{X}}$ are clearly more important.

Figure 10 shows the score plot for each predictor block separately, as well as the plot of the super scores of the MBPLS model. The super score plot can be viewed as a monitoring space for the whole system, while the monitoring of each predictor block is performed via the score plots corresponding to each block. In each of these score plots, dots are used to identify "good" or "acceptable" restarts and crosses are used for "poor" restarts. The plot of the super scores show a very clear distinction between the "good" or "acceptable" and the "poor" restarts. Furthermore, there appears to be two kinds of "poor" restarts, one in the negative direction of t_{T1} and the other in the negative direction of t_{T2}.

The first dimension of the model mainly explains variations in the hold block ($\boldsymbol{Z}_{\mathbf{hold}}$) and in the trajectory $\underline{\boldsymbol{X}}$ block (as apparent from wt. % in Table 3). Therefore, one can diagnose the cause for poor performance of restarts in t_{T1} direction using the data included in these two blocks. The data collected during the hold ($\boldsymbol{Z}_{\mathbf{hold}}$) reveal a very important aspect of the restart problem. Two clusters appear in the $t_{hold1} - t_{hold2}$ plot, one including observations 17–18 plus 20–24,

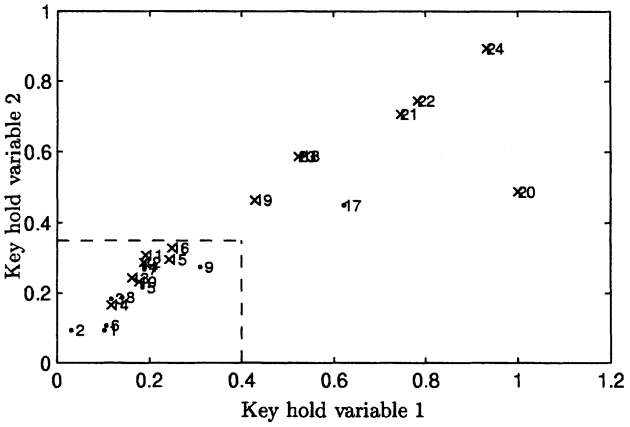

Figure 11. Values reached by two key process variables during the 24 hold periods.

Dots: "good" restarts; crosses: "poor" restarts.

and the second including the remaining observations. Since restarts numbered 17–24 had much longer hold periods than usual, this leads one to suspect that hold duration has a significant impact on restart performance. While the process is on hold, it acts as a batch process, such that the concentration of one reactant (the only one continuously fed during the hold) and heat accumulate. When holds have extended durations, this accumulation is such, that reactions bring some of the key process conditions to a very different region, and this explains the two clusters in the scores of the hold block. The scaled values taken by two such key variables are shown in Figure 11, where the long holds fall outside the dashed box. The fact that most data sets in the range of 17–24 fall in the "poor" category suggests that once the longer hold region is reached (region outside the dashed box in Figure 11), it becomes difficult or even impossible to recover from these holds with "good" restart performance. Polymer reaction engineering knowledge on the particular polymer system also supports this empirical evidence. Therefore, when this region is reached, one could empty part or all content of the process and then start up with fresh materials. This would avoid the costs associated with processing even more materials that are bound to produce large amounts of off-grade materials.

"Poor" restarts are also associated with negative t_{X1} values in the trajectory block ($\underline{\boldsymbol{X}}$). These negative values of t_{X1} are associated with heat balance problems introduced by longer hold periods and by the feed policy of some key reactants.

The second component of the model mainly explains variations in the trajectory block ($\underline{\boldsymbol{X}}$) and the steady-state block ($Z_{ss,1}$) (see wt. % in Table 3). Restarts number 10, 15, and 19 have large negative values of the second super score (t_{T2}). This negative t_{T2} was found to be associated with an operational problem; a delay in turning on one process unit after the restart was initiated while no corrective actions were taken. Restarts number 10 and 15 also cluster on negative t_{ss2} in the steady-state block due to some extreme variations in a few process variables (these might have been the reason for putting the process on hold).

The proposed solution to this restart problem involves first eliminating the sources of the problems identified in the above

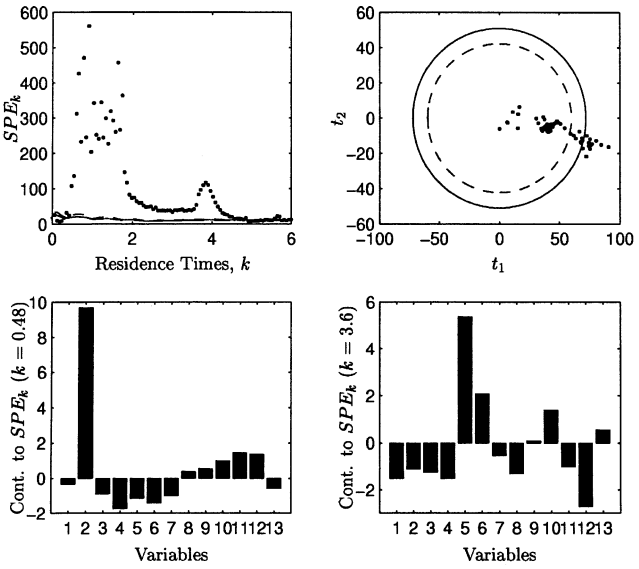

Figure 12. Multivariate statistical process monitoring of restart number 10.

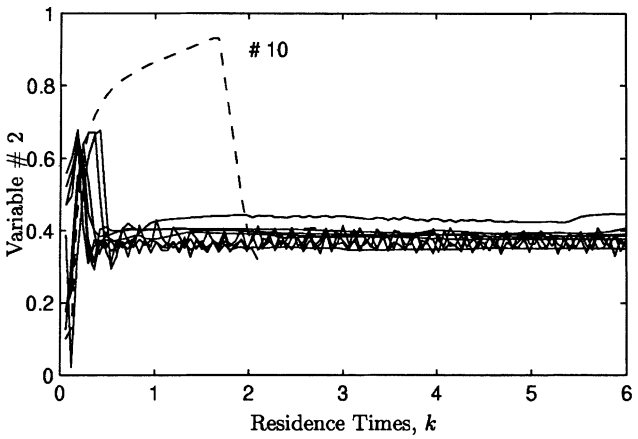

Figure 13. Behavior of variable No. 2 during startups.

Plain line: "good"-"acceptable" data sets No. 1–9; dashed line: "poor" startup No. 10.

analysis and then developing a monitoring procedure for the hold periods ($\mathbf{Z}_{\mathbf{hold}}$), and restart trajectories ($\underline{\boldsymbol{X}}$). The latter scheme is presented in the next section.

An MSPC scheme for monitoring transition trajectories ($\underline{\boldsymbol{X}}$)

To develop a monitoring scheme for the restarts ($\underline{\boldsymbol{X}}$), a multiway principal component (MPCA) model is built using only the data corresponding to the restarts with "good" and "acceptable" performance. Data sets numbered 17–24 are not used in this analysis, since they appear to correspond to a different class of operating conditions (longer holds), and only 2 "good" or "acceptable" restarts are available in this region. The model is, therefore, built using only 9 restarts. Establishing a monitoring scheme with such a small number of data sets can be misleading, as the range of variation corresponding to desired transient behavior may not be entirely spanned. However, the analysis shown next is a good illustration for the methodology proposed in this article. The procedure for building a monitoring scheme for data arranged in a three-way array is described in Nomikos and MacGregor (1994b). The restarts are aligned again here with the procedure described earlier. A two-component MPCA model was found to be sufficient to characterize the good restart histories and to detect abnormalities associated with the "poor" restarts. Figure 12 shows the results that one would have obtained if restart number 10 would have been monitored. This figure shows multivariate monitoring charts for the instantaneous square prediction error at time k(SPE_k) and for the scores (t_1 and t_2) of the MPCA model. This makes it possible to monitor model residuals as the transition evolves. The dashed and plain lines on the plots of Figure 12 correspond respectively to 95% and 99% limits. Contributions to deviation in SPE_k (MacGregor et al., 1994; Kourti and MacGregor, 1996) are also shown in Figure 12 for two different residence times (k).

The alarm on SPE_k early in the transition ($k = 0.48$) is associated with variable number 2. The behavior of variable 2 during these restarts is shown in Figure 13 and is compared to its normal or desired behavior, defined by the "good" and "acceptable" sets (1–9). Clearly, variable 2 reached a much higher value and remained at this high level for a much longer period of time than what is normally observed. This explains the alarm on the scores as well. Variable number 2 has a strong influence on the heat balance of the process and, hence, on the reactions. When this variable reaches higher values for a longer period of time (caused by a delay in turning on some specific units), especially early in the restart, and when no corrective actions are implemented, then variable 5 and 6 generally take a longer time to settle to desired steady-state values. This is shown in the contribution plots for $k = 3.6$, where variables 5 and 6 have higher values than usual. Polymerization knowledge again supports this empirical evidence and suggests that this behavior on variable 5 and 6 is strongly associated with production of more off-grade material.

The faults for the other "poor" restart data sets were also identified, but not shown here. The procedure described in this article has demonstrated that if an on-line monitoring scheme had been in place, these problems in the process operation would have been detected early enough to alert operators and probably prevent off-specification material from forming.

Control charts can also be set up for the hold data ($\mathbf{Z}_{\mathbf{hold}}$), or the $\mathbf{Z}_{\mathbf{hold}}$ data can be combined with trajectory data ($\underline{\boldsymbol{X}}$) in a multiblock monitoring scheme (MacGregor et al., 1994).

Conclusion

Empirical methodologies for improving transition policies (grade changeovers, startups and restarts) and for defining production readiness have been presented in this article. These can be used for improving process and product quality when mechanistic models are not readily available. Improvement and optimization of trajectories during transitions would result in reduced amounts of off-specification materials and transition time, and this could also lead to faster response to market demand. Furthermore, a better definition of produc-

tion readiness should ensure that at the end of a transition the process conditions are such that the product grade produced at the new steady state will be of high quality and will be consistent with past production.

In flexible multiproduct plants, many combinations of steady-state operating conditions may allow one to meet specifications on a small number of measured product quality variables. However, product quality is never completely characterized by only these few measured quality variables. The impact of using different operating conditions on the unmeasured aspects of product quality is unknown. A customer buying such a product may find that it behaves differently or is more difficult to process, even though the quality specifications on a few variables are met. To alleviate this problem, we propose defining target regions for process conditions, as well as for the few measured quality variables. Principal component analysis (PCA) is used for defining the desirable steady-state operation regions at the end of a transition ("production readiness region") or at the commencement of a transition ("startup readiness region"). It was shown, by simulation studies of a linear low density polyethylene (LLDPE) reactor, that targeting the steady-state process operation to such a desirable region improves product quality and consistency, regardless of which operation region one is transitioning from.

Improving startup or grade transition from an empirical point of view is based on the fact that in the past, some transitions were better than others, in terms of amounts of off-grade materials, transition duration, and safety conditions. Developing a monitoring procedure for transient periods, based on the best transitions achieved in the past, seems to be a logical solution. This involves the use of multivariate statistical techniques such as multiway principal component analysis (MPCA) and multiblock multiway projection to latent structures (MBPLS). The concepts were illustrated using restart data from an industrial polymerization process. Insightful empirical evidence was obtained by analyzing such data on how to achieve a reduction in amounts of off-specification materials.

Acknowledgments

This work was supported by the Natural Sciences and Engineering Research Council (NSERC) of Canada and by the McMaster Advanced Control Consortium (MACC).

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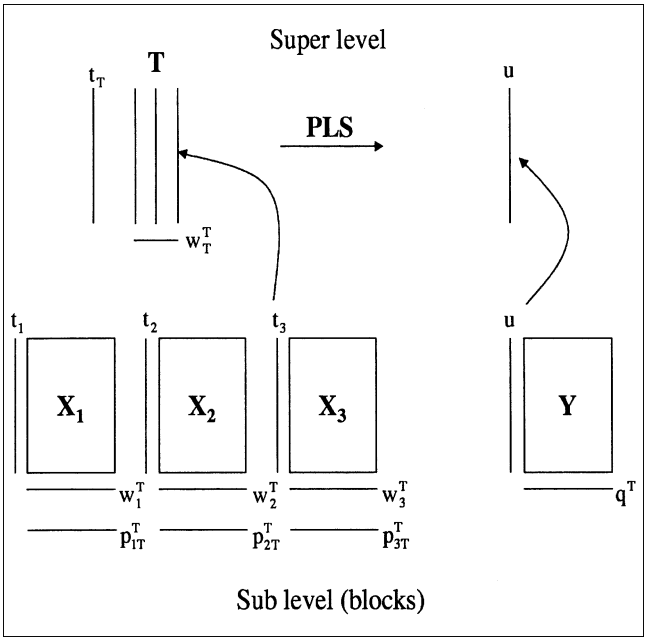

Figure A1. Multiblock PLS algorithm with 3 *X* blocks.

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Appendix

Multiblock PLS (MBPLS) models are used in this work to analyze historical transitional data. The general structure of the MBPLS model is illustrated in Figure A1, for the situation where three process variable blocks ($\boldsymbol{X_1}$ to $\boldsymbol{X_3}$) and one quality variable block ($\boldsymbol{Y}$) are available. This structure is equally valid for a larger number of $\boldsymbol{X}$ and $\boldsymbol{Y}$ data blocks.

The MBPLS model is based on a two-levels modeling hierarchy: the block level (or sublevel) and super-block level. At the block level, the variance within each $\boldsymbol{X}$ block and the $\boldsymbol{Y}$ block is decomposed into a number of latent vectors ($\boldsymbol{t_1}$ to $\boldsymbol{t_3}$ and $\boldsymbol{u}$), similarly as PLS does. The corresponding set of loadings for each block are the vectors $\boldsymbol{w_1}$ to $\boldsymbol{w_3}$ for the $\boldsymbol{X}$ blocks and $\boldsymbol{q}$ for the $\boldsymbol{Y}$ block. The scores of each $\boldsymbol{X}$ block are then used at the super-block level to form a score matrix $\boldsymbol{T}$. A PLS model is then built at the super-block level between $\boldsymbol{T}$ and $\boldsymbol{u}$ to yield the super-block model, with the super-block loadings $\boldsymbol{w_T}$ and super-block score $\boldsymbol{t_T}$. The iterative algorithm used to estimate the scores and the loadings at both the sub and the super levels is provided below. The hierarchy of the MBPLS model allows to build a monitoring space for the whole system using the super score space ($\boldsymbol{t_T}$), as well as a monitoring space for each predictor block $\boldsymbol{X}$ using the sublevel scores ($\boldsymbol{t_1}$ to $\boldsymbol{t_3}$). Another useful feature of the MBPLS model is that one could assess what predictor blocks are the most important in explaining the variance of $\boldsymbol{Y}$ using the super block loadings $\boldsymbol{w_T}$, while the loadings of the sub level ($\boldsymbol{w_1}$ to $\boldsymbol{w_3}$) can be used to assess what process variables are the most important in explaining the variations in each block. The MBPLS model leads to the same predictive ability as for a PLS model with all predictor blocks included in the same matrix. However, the MBPLS model improves data interpretability over the conventional PLS model.

The iterative algorithm used in this article to estimate the various MBPLS parameters is the one published by Westerhuis and Coenegracht (1997), which makes use of the super score deflation. In this algorithm, the $\boldsymbol{X}_b$ blocks, $b = 1, 2, \ldots, B$ represent the various predictor blocks used in the model, with m_{Xb} being the number of variables in block b. Appropriate centering and scaling of the data ($\boldsymbol{X}_b$ and $\boldsymbol{Y}$ blocks) should be performed before the analysis. The MBPLS algorithm is described below.

1. Start with $\boldsymbol{u}$ equal to some column of $\boldsymbol{Y}$
2. $\boldsymbol{w}_b = \boldsymbol{X}_b\boldsymbol{u}/\boldsymbol{u}^T\boldsymbol{u}$
3. normalize $\boldsymbol{w}_b$ to unit length
4. Compute block scores: $t_b = \boldsymbol{X}_b\boldsymbol{w}_b/m_{Xb}^{1/2}$
5. $\boldsymbol{T} = [\boldsymbol{t}_1 \ \cdots \ \boldsymbol{t}_B]$
6. Compute super block loadings: $\boldsymbol{w}_T = \boldsymbol{T}^T\boldsymbol{u}/\boldsymbol{u}^T\boldsymbol{u}$
7. Normalize $\boldsymbol{w_T}$ to unit length
8. Compute super block scores: $\boldsymbol{t}_T = \boldsymbol{T}\boldsymbol{w}_T/\boldsymbol{w}_T^T\boldsymbol{w_T}$
9. $\boldsymbol{q} = \boldsymbol{Y}^T\boldsymbol{t_T}/\boldsymbol{t}_T^T\boldsymbol{t}_T$
10. $\boldsymbol{u} = \boldsymbol{Y}\boldsymbol{q}/\boldsymbol{q}^T\boldsymbol{q}$
11. Check convergence of $\boldsymbol{u}$. If no convergence, go to 2.
12. $\boldsymbol{p}_{bT} = \boldsymbol{X}_b^T\boldsymbol{t}_T/\boldsymbol{t}_T^T\boldsymbol{t}_T$
13. $\boldsymbol{E}_b = \boldsymbol{X}_b - \boldsymbol{t}_T\boldsymbol{p}_{bT}^T$
14. $\boldsymbol{F} = \boldsymbol{Y} - \boldsymbol{t}_T\boldsymbol{q}^T$
15. Compute next dimension by returning to 1, using $\boldsymbol{E}_b$ and $\boldsymbol{F}$ as the new $\boldsymbol{X}_b$ and $\boldsymbol{Y}$.

Manuscript received Feb. 12, 2001, and revision received June 27, 2002.