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Multivariate process control by transition scheme in soft-drink process using 3-Way PLS approach

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Abstract

Recently many attentions has been placed to process transitions, startups and restarts, since these abnormalities often arrives to the loss of production time, undesirable and not detectable variability increasing withproduction of off-grade materials. The present research deal with the modeling a continuous soft-drinks bottling process by a multivariate approach based on the 3-Way PLS. Process was modeled, filtering the high grade of autocorrelation and cross-correlation within the studied variables. The responsible variables for that behavior were detected by 3-Way PLS which could be useful to separate autocorrelated sources of variability enable to control this kind of industrial process.

Keywords: Multivariate Statistical Process Control; Transitions; 3-Way PLS; Soft-drink bottling process; PCA; MPLS.

1. Introduction

Statistical Process Control (SPC) has emerged as a tool for distinguishing between common causes and assignable causes, where the first are associated with inherent variability of the process, while assignable causes are occasional and generally unpredictable, due to abnormalities, which were not included in the process [1-3]. In this sense, the SPC provides a permanent and intelligent monitoring system, able to detect early the onset of changes in the process, identifying their origins.

Actually, industrial process are characterized by increased production speeds and highly automated plants, where large amounts of data are generated, being essential a simultaneous monitoring including all variables for the assessment of global process behavior, unlike the classical univariate approach [4]. An

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alternative to this conditions have been Multivariate Statistical Process Control (MSPC) methods based on Latent Projections [5]. These are able to deal simultaneously with large amounts of data and variables with high dimensionality and collinearity, extracting information about the direction of process variations [6]. These tools include the Principal Component Analysis (PCA) and Partial Least Squares Regression (PLS) and the so-called Multi-Way methods given the configuration in three dimensions with that process information [7]. In addition, in the last years, many attentions has been placed on process transitions, startups and restarts, since these abnormalities often arrives to loss in production time, increasing undesirable and not detectable variability, production of off-grade materials and inconsistent reproducibility of product grades [8, 9].

In this context, this research aims to analyze a continuous bottling process of carbonated beverages, configured as a sequential set of batches and variable length defined by a group of anomalies (detentions and unplanned restarts mainly) identified throughout the process. For this purpose, a 3-way PLS method was applied to assess the effect of these seeming transitions as a source of assignable causes (changes to the pattern of natural variability).

Nomenclature

CO_2: CO_2 content

°Brix: Sugar content

Cont.Net: Net Content

T1,T2,T3: Washer temperature

T4: Rinse Temperature

INC: Closing Torque

AP: Opening Torque

PCA: Principal Component Analysis

3-way-PLS: 3 way Partial Least Square Regression

MSPC: Multivariate Statistical Process Control

2. Materials and Methods

A systematic sampling every 15 minutes was applied in a continuous bottling process (13,500 bottles/min) for a carbonated soft-drink (PET 2 L). Totally 4608 cases were sampled and registered in a 4 months of production, reduced to 1938.

Measured variables: In each sample were assess a group of quality variables: CO_2 content, sugar content (ºBrix) and Net content. Likewise, a process variables: washer temperatures (T1, T2 and T3), rinse temperature (T4), closing torque (INC) and opening torque (AP).

The statistical methods used were: T^2 Hotelling Control Chart, Multivariable EWMA Chart, Principal Component Analysis (PCA) and 3-way Partial Least Squares Regression (3-Way-PLS).

All calculations and adjustments were made with SIMCA-P+ 12 (Umetrics, Umeå, 2009) and Statgraphics XVI (StatPoint Technologies Inc., 2009).

3. Results and Discussion

First, a missing data and abnormal situations identification stage was performed, thus a group of *transitions conditions* (in general changes from grade to grade, start-up of a continuous process, restart of a continuous process that went on hold due to a technical problem, and so on) was detected. Thus the dataset was "sliced" in a total of 23 batches chronologically sequential.

Then, the T^2-Hotelling and Multivariate EWMA charts (λ=0.25) were performed, since the two of ones are relatively knows in industry use (Fig. 1).

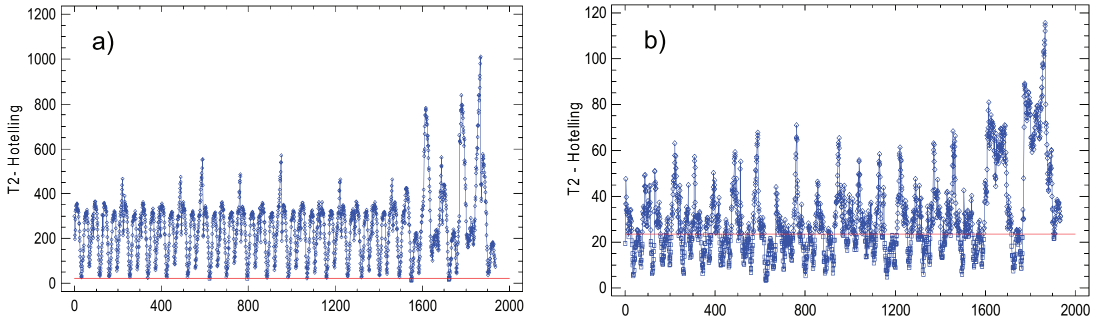

Fig.1(a) T^2 Hotelling Chart (b) Multivariate EWMA Chart

The T^2-Hotelling shown almost the 95 % the data was out of control, while Multivariate EWMA chart shown over 60 % of the dataset with a several shift. A later verification of the dataset, case by case for each variable, confirms that the ratio of real out of control signals considering the quality set points was very low.

Afterwards, a Principal Components Analysis (MSPC-PCA) was performed over the 23 batches trying to filter the autocorrelation detected (Fig. 2). The MSPC-PCA model retained 3 explaining the 78.2 % of total variance, while the predictive capability of the model was 31.8% (adequate value). The model was validated by a full cross-validation routine [10].

As seen in Fig.2, the MSPC-PCA shows the multivariate elliptic control limit at 95 % of confidence. The two main factors form a 2 dimensions orthogonal hyperplane. Factor 1 (37.8 % explained variance) arranges the samples according to high to low performance in quality variables (Net Content, CO_2 and ºBrix); whilst factor 2 (25.8% explained variance) clearly shows "pseudo stratums" associated to the autocorrelation of T1, T2 and T3. The behavior can be better explained by Contribution Plot (Figure 3).

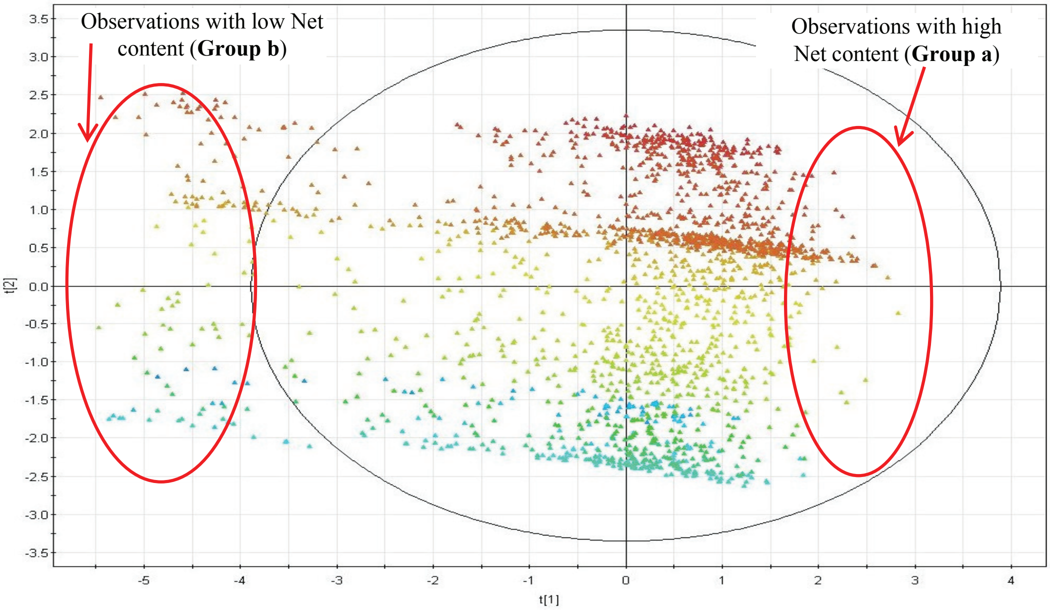

Fig.2 Principal Component Analysis (MSPC-PCA)

The 3-Way PLS model extracted 4 factors with a R2X = 77.1 % (Total X variance explained by the model) and a R2Y = 89.7 % (Total Y variance explained by the model), while the predictive capability of the model was 89.5 %. The model was validated by a full cross-validation routine to minimize the PRESS function (prediction residual sum of squares function) and avoid the overfit of the model. A detailed and separated in depth analysis by each factor was performed (Fig. 4 and 5).

Fig. 4 shows the evolution of the batches itemized by factor t1 with no signals of out of control, as well as is clear the weight of variables T1 and T2 respect all others. Since the temperatures variables are so autocorrelated and t1 is the main orthogonal factor (with bigger explained variance), is possible to affirm that this strong source of noise is hiding the variability of the quality variables, hampering the proper control of the process.

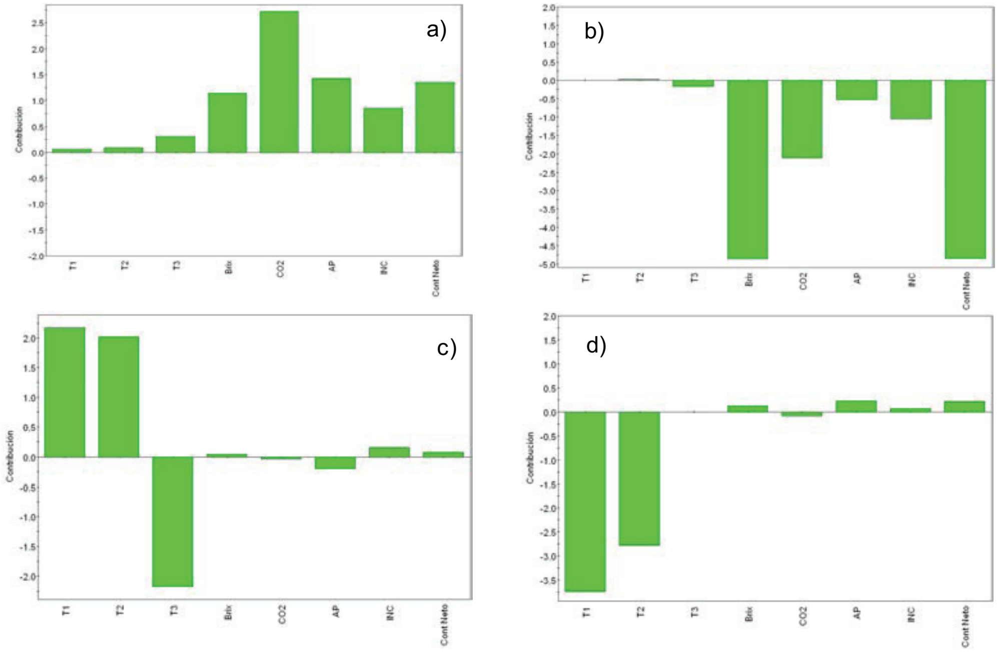

Fig. 3 (a) Contribution Plot for high level of Net Content (and CO_2) cases (b) Contribution Plot for low Net Content (and CO_2 and ºBrix) cases (c) Contribution Plot for high autocorrelation between T1 and T2 (d) Contribution Plot for low autocorrelation between T1 and T2 (and high T3)

*Note: All plots in standard deviation units.

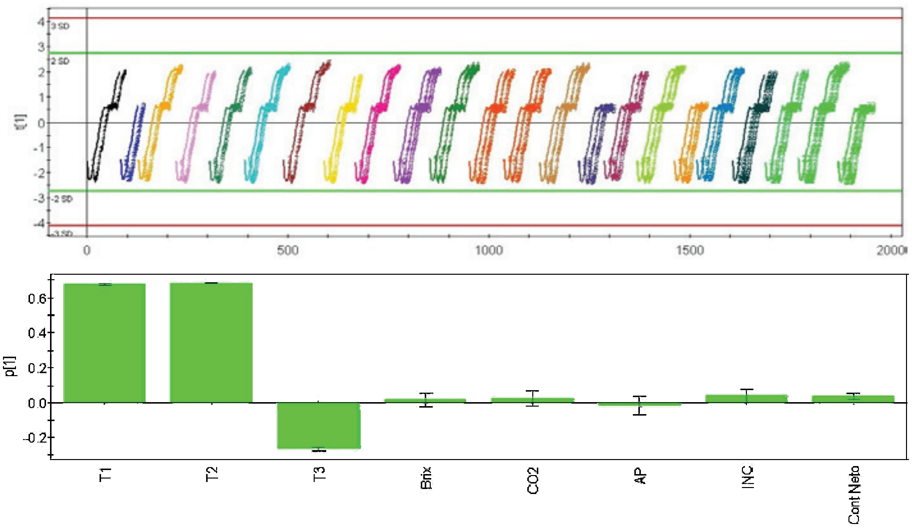

Fig. 4 Evolution of the 23 batches itemized by factor t1

Fig.5 shows the evolution of the batches itemized by factor t2 (considering that all the variability associated to factor t1 was filtered). Clearly the behavior pattern is not constant and shows some several shifts, even now with moderate signals of out of control of batches 5, 11, 13 and 14, and strong signals of out of control of batches 19, 20, 21, 22 and 23. Thus the source of variability of this situation is associated mainly to Net Content, CO_2 and ºBrix, scilicet the quality variables of the final product.

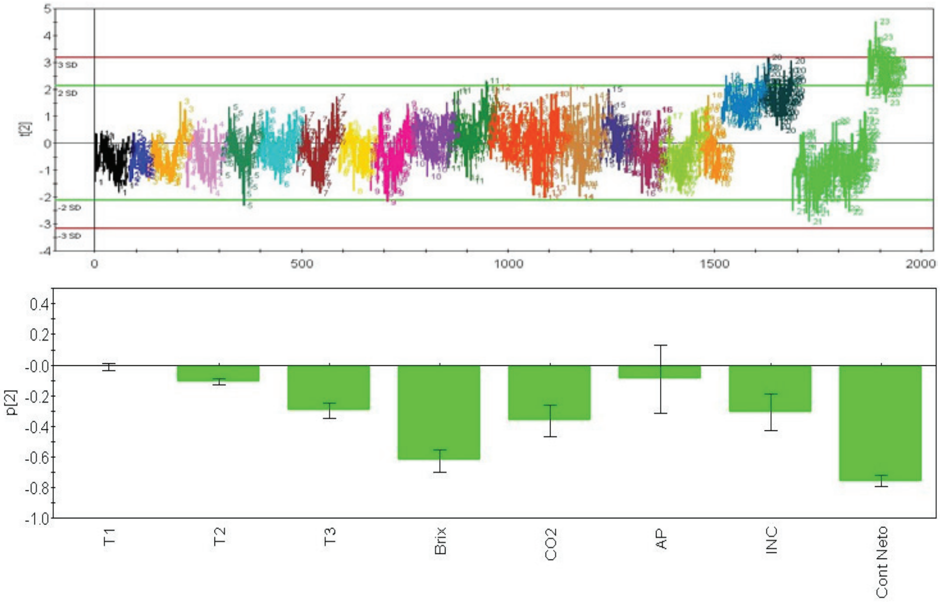

Fig. 5. Evolution of the 23 batches itemized by factor t2

4. Conclusion

MSPC-PCA and 3-Way PLS methods appear like useful tools to separate autocorrelated sources of variability, it enable to apply a proper routine to control industrial process.

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