**A new look at the dynamic covariance structure of various approaches for batch process modelling**

When studying the Principal Component Analysis (PCA) modelling of batch process data, one realizes that there is a wide range of approaches. In many cases, new modelling approaches are presented just because they work properly for a particular application, e.g. on-line monitoring, and a given number of processes. A clear understanding of why these approaches perform successfully and which are the advantages and disadvantages in front of the others is seldom supplied. Many researchers agree that the PCA modelling of batch processes is in general bad understood and that some effort to show the differences among the approaches from a theoretical point of view is lacked.

Why does modelling after batch-wise unfolding capture changing dynamics? What are the consequences of variable-wise unfolding? Is there any best unfolding method? When should several PCA models for a single process be used? In this talk we show how these and other related questions can be answered by properly analyzing the covariances matrix used to calibrate the PCA models. Some of the conclusions have been pointed out elsewhere but some others are new, such as the theoretical evaluation of batch dynamic PCA (BDPCA) models (Chen and Liu, 2002), evolving and local PCA models (Ramaker et *al.,* 2005) and multi-phase PCA (MPPCA) models (Camacho and Picó, 2006). By looking at the dynamic covariance structure it will be shown that the latter approach is a general modelling framework where batch-wise and variable-wise models, BDPCA models and evolving and local models are included.

The discussion presented will be aimed to show when one modelling approach is preferable, taking into account the nature of the data to be modelled and also parsimony. This analysis help us to clearly determine how dynamics are built in the models, which parameters in the models are related with a single sampling time and which are averages of several/all sampling times, which information –if any- is discarded after unfolding or dividing in several submodels, and in which cases this is convenient.

This study assumes data have been properly aligned –if they were not yet- and preprocessed. Therefore, differences due to the use of different alignment or preprocessing methods are not treated.


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3. Camacho J., Picó J.. Online Monitoring of Batch Processes using Multi-Phase Principal Component Analysis *Journal of Process Control.* 2006;10:1021-1035.