Multi-Phase Analysis Framework for Handling Batch Process Data

Principal Component Analysis (PCA) and Partial Least Squares (PLS) have been successfully applied to batch process data for monitoring and quality prediction. Since batch data is three-way, the data matrix has to be conveniently rearranged in a two-way matrix for applying bilinear models as PCA and PLS.

The multi-phase modelling approach is based on calibrating independent models for different intervals of a batch process to improve the modelling. To design a multi-phase model, the phases of the process have to be determined by expert knowledge (Ündey and Çinar, 2002), process analysis (Kosanovich et *al.*, 1996) or automatic recognition (Lu et al., 2004). In some cases, the phases may not have a clear physical interpretation and so they cannot be determined by fundamental knowledge. On the other hand, the identification of the phases by process analysis can be a challenging task. The automatic identification of the phases overcomes these problems and seems to be a good alternative, as long as the recognition algorithm performs adequately.

The goal of the Multi-Phase (MP) algorithm (Camacho and Picó, 2006a and 2006b) is to find the phases of the batch process, i.e. the segments of the batch well approximated by a linear (for instance PCA) model. In this talk we present several enhancements of the previous versions of this algorithm for its general use with any unfolding procedure (batch-wise, variable-wise and batch dynamic) using either PCA or PLS. Also, a set of postprocessing algorithms have been defined to reduce the complexity of the model and to mixture several multi-phase models into one. The convenient use of the postprocessing methods, as it will be shown, helps to improve the process understanding. The combination of the MP algorithm, the postprocessing methods and the application of Analysis of Variance (ANOVA) conform the MP Analysis Framework presented here, with application to off-line and on-line monitoring, final quality prediction and estimation of trajectories of variables. The MP framework has many advantages: First, the sampling time ordering is used implicitly for the identification of the phases. Second, the parameters defined for the algorithms allow the designer to handle the data in a flexible and well-defined way. Third, the MP Framework can be used in a straightforward manner to efficiently investigate the process under study.

Data from several batch processes of very different nature (a polymerization process, a fermentation process and a waste-water treatment process) will be used to show the capabilities of the modelling framework proposed.

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