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File ID 76102
Filename SUMMARY

SOURCE (OR PART OF THE FOLLOWING SOURCE):

Type Dissertation
Title Statistical batch process monitoring
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Faculty Faculty of Science
Year 2004

FULL BIBLIOGRAPHIC DETAILS:

<http://dare.uva.nl/record/161629>

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◆ SUMMARY

This thesis describes the work of four years research carried out at the Process Analysis and Chemometrics group at the University of Amsterdam. The presented work contributes to the field of statistical batch process monitoring (SBPM) and provides the reader with a variety of topics such as an overview of existing methods and SBPM models, introduction of new models, improvements and applications.

First, an introduction is given about batch processes and their importance in industries such as the pharmaceutical or (bio)-chemical industry. The performance of a batch process can be expressed in terms of safety, end-product quality, process consistency, efficiency, and process disturbances. The fluctuations in these batch process parameters are a result of the variation present in a batch process. Multivariate statistical methods are well suited to supervise this variation. SBPM handles the concepts of SPC where statistical thinking holds a central place. The aim is to reduce and monitor the variation of the batch process.

SBPM can be seen as an integral part of a quality management program. In order to successfully implement SBPM in such a program, SBPM is put in a framework called the I.T.A.- trajectory: Initial phase, Training phase and Application phase. The I.T.A.- trajectory provides the user a stepwise approach to the most important parts of SBPM. The initial phase is an explorative analysis of the raw process data. In this phase, it is examined whether the process conditions can be recognized as 'normal operated' and if the process is statistically in-control. In the training phase, a model is built to capture the normal process variation and control charts are constructed. Then, in the application phase, new batches are monitored on-line using the control charts derived in the training phase. If abnormal behaviour is detected, the origin of this unknown variation is located. Finally, the source of variation that caused the process upset is removed and the process is improved.

The first step in the initial phase is to understand batch process data. That is, to study its origin, nature and behaviour. It is often required to preprocess the data before a model can be developed. Variable scaling is often necessary to account for differences in measurement units. Furthermore, synchronization of the batch data is necessary to align the "local time" of each batch. This forces specific events in the batches to occur at the same time in each batch. In this thesis a procedure based on dynamic time warping (DTW) for synchronization of batches is described. The DTW

algorithm is thoroughly explained and it is shown that certain 'inheritages' from speech recognition can be omitted.

In the training phase, an SBPM model is constructed. Two distinct classes of SBPM models can be distinguished: black models and grey models. Black models are purely data driven and commonly used in SBPM. There exist a wide variety of black models. The most well known models are explained and evaluated. This evaluation is expressed in terms of the false alarm rate and fault detection performance of the models. Two new black models are introduced: the time evolving and the local model. The results of a comparison study show that it is not always clear which model to use. Grey models are a combination of purely data driven models and prior information such as kinetics or mass/energy balances. The concept of grey models is explained and applied to an industrial polymerization process, which is monitored on-line by Near Infrared spectroscopy. Grey models are found not to give faster fault detection compared to black models but a significant improvement with respect to process understanding.

Based on a SBPM model, control charts are derived. The charts are examined by considering the statistics used for the chart and its mechanistics. The mechanistics are used to study the manifestation of process faults in the control charts. The initially proposed statistics for process monitoring are discussed. This discussion is partly based on the validity of the statistical assumptions made during the construction of the multivariate control charts. Some suggestions to improve the statistical properties of the charts are proposed. The most important improvements are the new formulation of the null hypothesis as well as the leave-one-out procedure.

The mechanistics of the control charts are discussed in two parts. First, the way of how process faults manifest themselves in the control charts. This behavior is examined for various models. By means of a simulation it is shown that in dynamic processes, faults are distributed in an unclear way in both control charts. This is due to the embedded error, but it depends highly on the choice of the model. Second, the ability of each model to capture the auto and cross-correlations present in batch process data is studied. It is shown that most models are well able to capture these correlations. In addition, for each model, the auto-and cross-correlations are distributed over the model parameters differently. Finally, general conclusions and future directions are given.

