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♦ FUTURE DIRECTIONS*

In the second chapter of this thesis a framework (the I.T.A.-trajectory) is presented for statistical batch process monitoring. Although this framework is far from complete, the authors of this thesis believe that it is necessary to present the ideas of statistical batch process monitoring in such a manner. The implementation of similar statistical tools in total quality programs, own their success because the techniques are encapsulated in such management programs. It is often the plant manager that needs to be convinced of the advantages that statistical batch process monitoring has to offer. It is not the mathematics that are interesting for the plant manager, but the advantages that can be reached by using the philosophy of statistical batch process monitoring. Presenting statistical batch process monitoring in a framework such as the I.T.A-trajectory makes it easier to communicate with non-technicians.

Another important issue is the lack of proven examples in industry. If rough numbers would be available for the savings that statistical batch process monitoring can accomplish for every kilogram of produced product, another argument can be brought into the discussion with the plant manager.

In the initial phase of the I.T.A-trajectory, batch data is collected. In the past, collecting batch process data was a serious stumbling block. Many potential applications failed because of the time consumption that data collection took. However, it is our experience that through the years of this research, this barrier seems easier to take. The platforms used in production plants are increasingly improved for proper data warehousing. Nowadays, it is quite easy to log in from a remote location to the main database system, and retrieve the batch data in well-organized data sheets. This trend definitely increases the potential of statistical batch process monitoring and is in accordance with the expectation that the availability of data will exponentially increase in the next decade.

The third chapter deals with synchronizing batch data prior to modelling. The problem of batches having unequal run length is evident for almost all datasets. There are hardly any industrial applications where the operation of batches guaranties equal run length. The results for dynamic time warping showed that, dynamic time warping,

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as a synchronizing tool seems to work well over a broad range of applications. However, the issue of on-line synchronization is not crystallized and is still in a research-stage. Also, the proposed method for synchronizing a set of batches has the disadvantage that intensities of the signals are changed. It is unclear how this affects the performance of SBPM models. Ideas exist to extent the dynamic time warping-algorithm from warping two pairs of signals to warping *n*-pair of signals at the same time. It can be concluded that the issue of synchronization is not only hot in the area of statistical batch process monitoring, but also in other fields of chemistry where the same problems can be recognized. Further research in this area is therefore worthwhile to undertake.

Black models for statistical batch process monitoring have been discussed and existing approaches are compared to new approaches. Using component models for statistical batch process monitoring gives rise to many new ideas for other black models. Besides the suggested approaches in this thesis, many more black models were used along the research period. Still, there is more research required to investigate the applicability of such models and moreover, their properties.

It became very clear that many complex questions came up from using relatively 'simple' black models. Therefore, it is important to understand 'simple' models first before more complex models are used.

The ideas about grey models and their application are discussed in chapter five. It is very appealing to combine the advantages of black and white models into grey models. Although the application of real first principle models for batch process monitoring is not considered in this thesis, some aspects of such approaches are captured in the application of grey models. Statistical batch process monitoring is typically a data-driven approach that originates from the field of chemometrics and data analysis. This might clarify the fact that engineers, at first sight, are hesitant to apply these techniques. The concept of grey models definitely brings the views of engineers and chemometricians together. It is shown that grey models can be very advantageous especially for diagnosing purposes. It is expected that the application of grey models will gain much interest in fields such as bio-technology where interpretation of the model parameters are highly desired.

Chapter six of this thesis discusses the mechanistics and statistical properties of the control charts derived from various SBPM models. Much effort is put into assessing the performance for the various models by introducing performance indices and studying the statistical characteristics. Studying the performance of the control charts is mainly induced because of the poor detection performance of the *D*-chart. It is common to quantify the performance of SBPM models by the detection power of faulty batches. In this research, the performance is based also on another important chart characteristic: the type I error. The results for the type I error show that the performance can be problematic. More research is required to set the control limits according to the type I error to overcome this problem. It seems that the statistics and mechanistics for this control chart are not without problems. It is our feeling that another statistic for the scores is required. Therefore, testing the performance of control charts needs to be based on either more robust statistics or non-parametric tests.

Testing the underlying statistical assumptions highly depends on the validity of the used statistics, which can be quite conservative. The fact that drawing such conclusions about statistical properties are related to the number of samples in the dataset is not hopeful considering the fact that statistical batch process monitoring models suffer from this. Therefore, it would be interesting to investigate batch-monitoring tools that require only few samples. Ideally, models are developed on a laboratory scale, scaled up to industrial reactors and then applied to various plants worldwide.

An important issue in quality improvement programs is the relation of the process operation with the end product quality. Hence, the relation between process performance and the end product specifications, expressed, as capability indices should be studied. The focus should be on the product observability of the system and the use of multivariate methods in combination with capability indices.

Another important issue in process monitoring is fault diagnosis. Although contribution plots are very successful in diagnosing process upsets, the way of diagnosing process upsets can be improved by fault reconstruction. That is, understanding how historical, known faults can be used to diagnose future batch runs.

Batch processes are complex with respect to the correlation that exists between batches and process variables over time. It is very interesting to study these correlations and how these correlations are being captured by statistical batch process monitoring models. However, because of the complexity of real process data and lack of samples, detailed and extensive simulations of batch processes with prior information about these correlation structures are required.

Batch processes are commonly monitored using typically engineering variables. In this thesis, various spectroscopically monitored batch processes are studied. Spectroscopic measurements have the ability to gain insight information about te chmeistry of the process. An very interesting question is how this spectroscopic data can be used together with physical or/and biological data. Combing different sources of process measurements gives a total view of the process. Such data fusion is believed to be necessesary in order to relate process variation to end-product quality.

Despite all the questions, it is clear that statistical batch process monitoring is very useful for monitoring batch processes and is therefore well suited to be a part of a quality improvement program. Various applications from literature clearly show the excellent performance of statistical batch process monitoring in detecting process upsets.

However, it is now important to evaluate practical applications of those models that are well understood and continue to develop models that are better capable of dealing with the disadvantages that are inherent to batch processing such as changing recipes and a relative low number of historical samples.