Human Capital and Mobility Network in

CHEMICAL PROCESS CONTROL

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Second General Meeting

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Casa Diocesana – Seminário do Vilar
Porto, Portugal

edited by
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INDEX

Programme

Thursday, 26

17.00 - 19.00 - Early Registration

Friday, 27

08.30 - 09.00 - Registration and Coffee

09.00 - 09.15 - Welcome address

09.15 - 10.00 - ***Modelling Tools and Computer-Aided Design*** (W. Marquardt)

10.00 - 10.45 - ***Identification for Control*** (D. Bonvin)

10.45 - 11.15 - Coffee

11.15 - 12.00 - ***Non-linear Estimation and Control*** (P. Rouchon)

12.00 - 12.45 - ***Real-time Optimisation*** (S. Walsh)

12.45 - 14.30 - Lunch and posters

14.30 - 15.15 - ***Process Monitoring and Data Interpretation*** (J. Morris)

15.15 - 16.00 - ***Controllability Analysis and Plantwide Control*** (D. Rossiter)

16.00 - 16.30 - Coffee

16.30 - 18.30 - Posters

Saturday, 28

09.30 - 12.30 - General meeting of programme Coordinators

19.30 - Get Together Dinner

List of Participants

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Costas Kiparissides

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Fernando G. Martins
José Manuel Machado

Universitat Stuttgart, Stuttgart, Germany
Ansgar Rehm

Theme / Subgroup Reports

THEME 6: **Controllability Analysis and Plantwide Control**

Dr Diane Rossiter
Loughborough University, Department of Chemical Engineering, Loughborough, UK

Introduction

The main contacts and groups participating in this theme are Professor Waller, Abo Akademi (Finland), Professor Jorgensen, Danish Technical University (Denmark), Dr Walsh, Imperial College (UK), Dr Rossiter, Loughborough University (UK) and Professor Skogestad, Trondheim University (Norway). The main activities this year have been: a technical workshop hosted by Professor Jorgensen in Lyngby (May 1996) and participation in 3 invited sessions at the CONTROL'96 conference held in Exeter (September 1996) organised by Dr Rossiter.

The presentation at this meeting will focus on presenting an overview of the activities of the Theme in the last year and will discuss the plans for future collaboration under the TMR programme.

Lyngby Workshop 20 May 1996

The topic of the workshop was 'Plantwide Control and Controllability'. Each member of the theme was represented. However, attendance was not restricted to members of the Network so Elling Jacobsen (KTH, Sweden) and Morten Hovd (Fantoft Prosess, Norway) were invited. Eight presentations were given over the day on a variety of topics ranging from the effect of recycles on the plant zero dynamics (presented by Elling Jacobsen) to issues in control structure selection (presented by Professor Sigurd Skogestad). The attendants also had the opportunity to see the energy-integrated distillation column in the pilot plant at DTH. The day concluded with a discussion on the theme's contribution to the proposal for the Teaching and Mobility of Researchers chaired by Dr Walsh. This proposal incorporates new members namely, Dr Hovd, Fantoft Prosess (Norway), Professor Scali, Pisa University (Italy) and Dr Jacobsen, Royal Institute of Technology (Sweden).

CONTROL'96, 2-5 September 1996

This conference is to be held in Exeter. Three invited sessions incorporating 15 papers on the topic of Chemical Process Control have been organised by Dr Rossiter. These sessions include contributions from all the members of Theme 6 plus contributions from the other partners in the Network. A subset of the authors are to be invited to submit extended versions of their papers for consideration for a special issue in the Journal of Process Control.

List of Oral Presentations

SESSION: **Modelling Tools and Computer-Aided Design**

09.15 - 09.20 Bernd Lohmann: *Introduction*

09.20 - 09.25 C. Kiparissides: Short presentation of the poster *Computer Aided Design of LDPE Tubular Reactors*

09.25 - 09.30 T. Drengstig: Short presentation of the poster *A Formal Graphical Based Process Modeling Methodology*

09.30 - 09.50 B. Lohmann (on behalf of W. Marquardt*): Recent Progress In Computer-Aided Modeling at RWTH Aachen*

09.50 - 10.00 Discussion

SESSION: **Modelling and Identification for Control**

10.00 - 10.45 Individual contributions

SESSION: **Nonlinear Estimation and Control**

11.15 - 11.25 Olaf Abel: *Optimization of Batch Reactors: New Results*

11.25 - 11.35 Ansgar Rehm: *Recent Work On Nonlinear Control*

11.35 - 11.45 Bodil O. Recke: *title to be precised*

11.45 - 11.55 Pierre Rouchon: *One year within the network*

11.55 - 12.00 *Questions and conclusions*

SESSION: **Real-Time Optimization**

12.00 - 12.25 S. Walsh and C. Loeblein: *Real-time Optimisation of Batch Plants*

12.25- 12.45 The rest of the slot will be taken up with a discussion of the proposed continuation of work on real-time optimisation within the controllability/plant-wide control theme of the follow-on network.

SESSION: **Process Monitoring and Data Interpretation**

14.30 - 14.50 A.J. Morris and E.B. Martin: *A Brief Introduction to Multivariate Statistical Process Control and Demonstration*

14.50 - 15.02 J. Saltin: *Paper Machine Operation Monitored by Principal Components*

15.02 - 15.15 Lars Gregersen and S.B. Jorgenson: *Prediction and Monitoring Techniques for Fed-batch Fermentation Processes*

SESSION: **Controllability Analysis and Plantwide Control**

15.15 - 16.00 Individual contributions

Abstracts

On The Use of Observability Measures for Sensor Location in Fixed Bed Reactors

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In chemical industry and biotechnology a common problem of monitoring and control applications is the general lack of sensors. In order to overcome this difficulty, model-based state estimation techniques (e.g. Kalman filters, Luenberger observers) can be used to estimate state variables, that are not available from on-line measurements. However, it has to be verified, that the used sensors are sufficient, namely that the process is observable. In the case of distributed parameter systems, observability is affected not only by the choice of sensors, but also by the sensor location.

In the present contribution we will discuss the choice of optimal sensor positions for a fixed bed reactor example. Different observability measures, based on a process description by ODE's via spatial discretization (Damak *et al.*, 1992; Eising 1984; Kailath, 1980), as well as on the process description by PDE's (Curtain and Zwart, 1995), will be addressed for locating optimal sensor positions. Further, investigations will be shown for the influence of space discretization schemes on observability.

Results will be demonstrated in simulation studies, where state estimation is applied to a fixed bed reactor example.

Curtain, R.F., Zwart, H.J. “An Introduction to Infinite-Dimensional Linear Systems Theory", Springer-Verlag, 1995.

Damak, T.,Babary, J.P., Nihtila, M.T. “Observer design and sensor location in distributed parameter bioreactors”, 315-320, DYCORD'92, 1992.

Eising, R. “Between controllable and uncontrollable”, Systems and Control Letters, 4, 263-264, 1984.

Kailath, T. “Linear Systems”, Prentice-Hall Information and System Sciences Series, 1980.

Nonlinear Estimation and Control of Polymerisation Processes

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Thessaloniki Technology Park

The quality control of polymerisation processes is an extremely important but yet unsolved problem. The main purpose is the development of a dynamic structure interconnecting the measured and manipulated variables, so that the process would operate safely, in the most profitable fashion and certain desired processing objectives will be satisfied almost continuously. The fact that polymerisation processes are strongly nonlinear imposes the design and implementation of nonlinear controllers.

Accurate deterministic models, capable of predicting the propagation of all the fundamental state of the process with time have been developed. However, industrial polymerisation processes are subject to stochastic disturbances. Furthermore, it is not always technically feasible (mainly due to lack of robust and reliable sensors) and economically justifiable to measure the controlled variables. Measurement noises, often make the situation more complicated. Another obstacle, especially in batch processes, stem from the fact that most of the model parameters vary significantly with time during the process, due to changes in concentrations, temperature, viscosity, etc. These adverse effects, which sometimes cannot be acceptably overcome, even by the use of an advanced control algorithm, prevent the achievement of the desired control objectives and lead to unsatisfactory system performance and poor product quality.

For all the aforementioned reasons, if one simply solves the dynamic model, starting from some, not completely determined a priori, initial value, it will soon diverge from the real process. Thus, the first problem that must be addressed is the design of an effective non-linear state estimator that allows one to infer the important polymer properties during the reaction from a limited set of noisy measurements, so that necessary feedback control action can be applied. It is proven that the resulting dynamic-stochastic model with feedback information coming from reliable on-line sensors, can achieve excellent on-line tracking of the observable reactor states, providing the control system with its inference to adjust the control effort to erase the effect of the disturbances on product quality.

Several important considerations must be addressed in any state estimation procedure. Firstly, process nonlinearities and continually changing reactor conditions cannot be ignored. Secondly, the state estimator must be formulated in such a way that bias free state estimates can be obtained under all types of unknown model mismatch and process disturbances that might be encountered during implementation. Finally, for the case of a short duration reaction the speed of convergence of the state estimator from initialisation errors is critical.

A well established estimation technique, Extended Kalman Filtering, (EKF) can then be employed to calculate and correct the states. The application of EKF to batch and continuous processes has been studied, especially in the case of process-model mismatch. A modification able to handle multirate sampled data has also been successfully applied. The significance of introducing meaningful stochastic states for the development of a simultaneous state and parameter estimator has been emphasised. Finally, the application of reiterative EKF to batch processes with uncertain initial values has been examined. In all cases, experimental results have been presented, displaying significant improvement.

The basic assumption behind EKF is that the process can be described adequately by a deterministic model. If this is not the case, Neural Network (NN) techniques can be used to model the process and to implement a controller design. The application of NN on estimation has been presented briefly, along with a comparison between the EKF estimation techniques and a Neural Network based estimator.

Implementation of an Artificial Neural Controller in a Batch Chemical Reactor

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This work deals with the problem of temperature control of batch reactor processes. Generally the control schemes used in chemical reactors are complex due to the time dependent variables, presence of different kind of uncertainties in batch cycles, utility restrictions and to accomplish safety rules. The most common control mechanisms adopted in industrial processes, are single or cascade control systems based in standard proportional-integral-derivative (PID) algorithms.

Although this type of control is satisfactory in most situations, new control schemes are being developed to enhance performance and reliability. The objective of this study is to explore a new strategy to control the reaction temperature in highly exothermic reactions.

An artificial neural network (ANN) was developed to control the batch chemical reactor. The database used to generate the structure of the controller is obtained from the dynamic simulations of the process model.

The results obtained from the simulations concerning conventional control system and the artificial neural networks control model show a better performance for the artificial neural network based control system. However, our approach should be proved in a pilot scale process and field results will be the final test of our theoretical previsions.

A FORMAL GRAPHICAL BASED PROCESS MODELING METHODOLOGY

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1. INTRODUCTION

The development of mathematical models for complex chemical processes is a demanding task involving personnel from several different scientific disciplines. A means for making this task more efficient, is to employ a representation of the process that the participants in the model development phase has a joint understanding of. Our main goal is to develop such a representation scheme and to utilize it in the development of a modeling methodology. However, developing a general representation scheme is a demanding task due to the great variety of chemical processes. We therefore need to identify some common features or characteristics of the class of chemical processes we are focusing on.

2. MODELING METHODOLOGY

The modeling methodology presented here consists of two main parts, a topological and a phenomenological part. To the topological part belongs the decomposition of the process into modules representing volumes and boundaries. This approach follows the principles described by Marquardt (1994). However, in this paper we focus on the phenomenological part. The material presented in this paper is based on the work done in Drengstig *et al.* (1996).

We have chosen three process characteristics as a basis for the representation scheme, i.e. TRANSPORT, REACTION and ACCUMULATION. These characteristics are related to the following extensive quantities, *mass* and *energy*. *Momentum* is not considered. The quantity *mass* is the mass of each chemical species. For these characteristics and quantities we have defined the symbols given in Table 1. We have also introduced **relations** in Table 1. These relations are used as connecting elements between the other symbols when creating a network representing the process. The direction of the arrows is not an indication of the direction of the flow, but rather it defines the *positive* direction for the flow. The arrows with two directions are used in equilibrium modeling.

Table 1: Symbols and relations defined in the modeling methodology

	ACCUMULATION	TRANSPORT	REACTION	**relations**
chemical species	□	diffusion ◹ convection ▭	Surface R^s Volume R^v	material flow ↘ material eq. ↘
energy	△	conduction △ convection ▲ radiation ✳		energy flow ⇢ thermal eq. ⇢

We further introduce a view where the network of symbols is constructed. This view is termed TRAV[1]. Having defined this formal representation scheme, we now propose to use it as a basis for a modeling methodology. This implies that the representation of the process is a visualization of the phenomenological model of the process. However, a chemical process may have different models and also model representations, depending on the purpose of the model and the assumptions made during the modeling. In order to make a mathematical model, i.e. as a collection of differential and algebraic equations, the symbols in the TRAV must be related to equations. For instance, in Table 1 we find the symbol for ACCUMULATION of *chemical species*. This symbol would typically

[1] Transport, reaction and accumulation view.

be related to a balance equation in the modeling methodology. Similarly, the TRANSPORT symbols would typically be related to algebraic equations.

3. CASE STUDY

We will here exemplify the use of the methodology on an aluminum electrolysis cell, see Fig. 1. The modeling of this process is done in cooperation with Hydro Aluminium A.S.

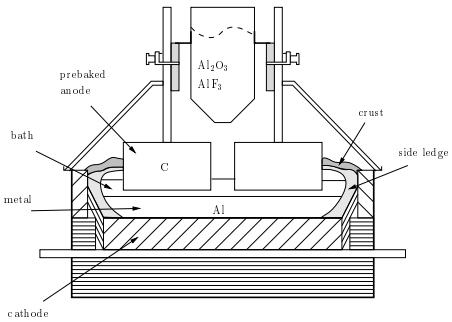

Figure 1: Sketch of an aluminum electrolysis cell.

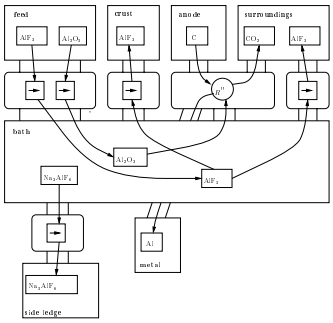

Figure 2: TRAV for the aluminum electrolysis cell (only mass aspect).

The main feed, Al_2O_3, is dissolved in the bath and electrically reduced to aluminum according to $2Al_2O_3 + 3C \rightarrow 4Al + 3CO_2$. This reaction is in Fig. 2 modeled as a surface reaction. AlF_3 is added to reduce the melting point of the bath. However, the observed cell behavior after adding AlF_3 is not fully understood. Hence, the aim of our work is primarily to develop a model of the AlF_3 dynamic, and secondly, to use it for model based control. Note that the crust is modeled as consisting of AlF_3 and the side ledge as consisting of Na_3AlF_6.

One of Elkem's high carbon ferro manganese furnaces has also been modeled using the modeling methodology (Wasbø and Foss 1995).

4. DISCUSSION

An advantage of the modeling methodology is that it facilitates easy model development and enlargement. However, a disadvantage is that the representation scheme becomes crowded if the number of chemical species and/or reactions are high. However, techniques for representing only parts of the TRAV could be an alternative. The main application of the methodology is to model lumped parameter systems using extensive quantities, e.g. number of moles, rather then intensive, e.g. concentration. However, to generalize the method, Drengstig *et al.* (1996) proposed a representation for distributed parameter systems. Equilibrium modeling and index problems are also addressed. Based on the phenomenological representation it is possible to develop modeling rules and thereby achieve consistent modeling.

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Marquardt, W. (1994). Trends in computer-aided process modeling. In: *Proceedings of PSE'94*. pp. 1–24.

Wasbø, S. O. and B. A. Foss (1995). Object-Oriented Model of a Ferromanganese Furnace. In: *INFACON7 TRONDHEIM June 1995* (J. Kr. Tuset, H. Tveit and I. G. Page, Eds.). "The Norwegian Ferroalloy Research Organization (FFF)". pp. 545–554.

Computer-Aided Process Modeling with the Modeling Environment Modkit

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Due to environmental and safety regulations, growing demands on product quality as well as increasingly competitive markets, the continuous improvement of chemical processes and the development of new ones is an important prerequisite for the success of chemical process industries. Tight time and cost constraints force these industries to continuously reduce their experimental effort during process development and to facilitate, even routinize, the application of model-based process technology. Nevertheless, the effort of setting up a detailed mathematical model for a chemical process remains still high because of the large variety of chemical process units and physical phenomena as well as increasing requirements on the sophistication of models. In order to overcome these limitations as systematization of modeling as well as the development of computer-aided modeling environments is required. Established tools and most of the recent explorative prototypical environments developed by other university groups are confined to the specification and representation of model building blocks and lack support for the process of model development. The modeling environment ModKit that is currently being developed provides high-level knowledge on modeling concepts and offers guidance in order to facilitate the development of detailed mathematical models.

The development of any software tool to support an engineering activity requires the conceptualization of the problem domain which finally results in a sound methodology of process modeling. Such a methodology comprises two principal issues: the definition of model building blocks which can be aggregated to form a consistent model and the development of modeling procedures which support both, the derivation of models from scratch, and the reuse and evolutionary modification of an existing model. The formal representation of model building blocks and modeling procedures requires a data model that supports a declarative description of modeling knowledge. At the same time this data model forms the basis for the design of the knowledge-based modeling environment ModKit. This environment is based on Gensym's knowledge-based software environment G2 which provides procedural, object-oriented, and rule-based programming facilities as well as a sophisticated graphical user interface and an interface for inter-process communication.

Canonical modeling objects for the structural and behavioral description of chemical processes have been developed and implemented in ModKit. A graphical model editor is used to build a chemical process model just by selection, modification and aggregation of modeling objects. Experts as well as less experienced users are supported by a predefined but extensible set of modeling steps, guiding the user through the process of modeling. These modeling steps are defined using a Grafcet approach which is similar to Petri nets. The structural description can be decomposed into arbitrary hierarchical levels. Elementary modeling objects contain the behavioral description in an equation-oriented manner. Moreover, alternative models together with comprehensive hypertext documentation can be represented in order to support the multifacetted nature of modeling.

ModKit is an open environment intended to utilize different well-known and state-of-the-art software tools. First of all, Aspen Technology's simulation software SpeedUp as well as gPROMS from Imperial College have been integrated. A code generator automatically maps ModKit's internal model representation into the representation required by a specific simulator. During a simulation run inter-process communication through G2's Standard Interface GSI is used in order to visualize the simulation results within ModKit.

Computer Aided Design of LDPE Tubular Reactors

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The development and application of computer-aided design tools has become increasily important in the past fourty years and the perspectives for the near future are even more promising. The present work describes the development of an integrated software package for the simulation and control of high pressure polyethylene tubular reactors. The overall goal of this software package is to build powefull, flexible, adaptive simulation tools for the prediction of the operating conditions and the molecular properties of various polyethylene products.

Low Density PolyEthylene (LDPE) and its copolymers are widely used for a large variety of applications and commonly produced in either autoclave-type vessels or tubular reactors. A fairly general reaction mechanism is employed to describe the complex free-radical kinetics of ethylene polymerization. The mechanism includes, initiator decomposition, chain initiation and propagation reactions, chain transfer to monomer, solvent and polymer, intramolecular transfer, and b-scission of sec and tert radicals and termination and disproportionation reactions.

The main functions of the package are built around a comprehensive mathematical model which describes the important chemical and physical phenomena that occur in this type of polyethylene reactor. The mathematical model includes the material, energy and momentum balances of the tubular reactor supported by the thermodynamics and transport properties of the reacting mixture evaluation equations. The method of moments is employed for the solution of the infinite polymer species balances, while for the case of multi-component polymerization the pseudo-kinetic rate constants approach is adopted.

The incorporation of an on-line parameter estimator provides the capabillity of real time prediction of the molecular properties of produced polymer, the estimation of control moves of key process variables as well as the prediction of the operational and product characteristics of alternative design options. Using the appropriate reactor measurements, the on-line parameter estimator adjusts certain key process variables in order to match the actual reactor performance.

A very powerful and user friendly interface is developed under Windows environment, which operates as a front-end for running the various support programs (reactor model and a number of on-line estimators) that do the actual design. A number of databases is available to the user to load automatically whole sets of input data and several state and output variables can be graphically represented. The whole design process is carried out under the Windows environment, offering maximum flexibility, extensive error checking during data input, using plethora of dialog boxes, buttons and controls that aid the engineers to spend their time in the design process.

Some Properties of the Orthogonal Collocation Method used for Approximating Distributed Parameter Process Models

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The dynamics of fixed bed reactors are described by partial differential equations (PDE's) derived from mass and energy balances. Either for (dynamic) simulation or for control design, the PDE's model is commonly reduced to a set of ordinary differential equations (ODE's) by using approximation methods (e.g. finite differences, orthogonal collocation,...) (Georgakis *et al.*, 1977). The approximation procedure may result in extensive computation studies before obtaining a satisfactory model approximation. For orthogonal collocation (which presents the advantage of substantially reducing the number of required ODE's), in spite of interesting attempts, e.g. Cho and Joseph (1983), there exists no systematic procedures for choosing the reduction parameters (like the number of collocation points, or the value of the parameters α and β of the Jacobi polynomial, which influence the location of the discretization points). The systematic use of orthogonal collocation requires a better understanding of its properties and of its influence on the discrtetized process model dynamics. The objective of this paper is to present some properties of orthogonal collocation concerning the choice of the Jacobi polynomials for locating the collocation points and its interpretation as a possible optimal choice, and the properties of the matrices which represents the approximation of the space derivatives with respect to the number of collocation points and the parameters α and β of the Jacobi polynomial.

Georgakis, C. Aris, R.; Amundson, R. “Studies in the control of tubular reactors - I. General considerations”, Chem. Eng. Sci., 32, 1359-1369, 1977.

Cho, Y.S. and Joseph, B**. “**Reduced-order steady state and dynamic models. Part I and II”, AIChE J., 29(2), 261-276, 1983.

An Introduction to Multivariate Statistical Process Control and Demonstration

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Statistical Process Control (SPC) is a tool for achieving and maintaining product quality. Classical univariate statistical techniques have focused on the monitoring of one quality variable at a time and are not appropriate for analysing process data where variables exhibit collinear behaviour. Minimal information is derived on the interactions between variables which are so important in complex manufacturing processes. These limitations are addressed through the application of multivariate statistical process control (MSPC) to the process. The basis of MSPC are the projection techniques of principal components analysis and projection to latent structures. The philosophy behind these approaches is to reduce the dimensionality of the problem by forming a new set of latent variables to obtain an enhanced understanding of the process behaviour. If the variables are highly correlated, then the process can be defined in terms of a reduced set of latent variables, which are a linear combination of the original variables. This talk presents an overview of multivariate statistical process control. The power of the methodology is demonstrated by application to an industrial process.

Paper Machine Operation Monitored by Principal Components

J. SALTIN
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Principal components analysis was applied to paper quality data and paper machine process data. Four to seven principal components were required to explain the majority of the underlying variability. A specialised procrustes rotation technique was then used to interpret these principal components as underlying physical phenomena that determine the interrelationships among the paper quality variables. To do this, process experience is used to manipulate the principal components into a recognisable phenomena. For example an experienced paper maker knows that when the sheet becomes highly oriented, the CD tear will increase while the MD tear will decrease. In addition, MD tensile and elongation will increase while the CD properties decrease.

After the principal components have been identified, the components can then be predicted using the process variables through principal components regression.

These techniques are used to trace changes in paper quality due to the underlying causes. This can be used to improve the control and/or the operation of the paper machine.

Prediction and Monitoring Techniques for Fed-batch Fermentation Processes

LARS GREGERSEN AND STEN BAY JØRGENSEN

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Fed-batch fermentation processes are characterized by their nonlinear dynamics, which is in general poorly understood.

Due to the large number of types of microorganisms that the industry uses in fermentation processes the effort that is needed to develop deductive dynamic models for simulation, fault detection and control design seems too large to be overcome in the near future.

Existing databases of already running processes containing process operations and conditions can be used for inductive modelling instead.

This paper describes the use of such databases mainly for statistical process control (SPC) and fault diagnosis. Statistical methods such as principal component analysis (PCA) and projection to latent structures (PLS) provides new latent variables based on the original data sets. The latent variables form a basis for on-line monitoring of the process in a reduced variable space. This dimensionality reduction simplifies the task of detecting faults and isolating the variables that contain information about the origin of the fault.

The methods described can also be used for prediction purposes. The product concentration is one of the key variables of the process when the performance is to be evaluated, but it is not measured on-line due to the expenses of on-line chemical analysis.

One of the ways to evaluate the process performance it to predict the final product concentration. This is done using PLS and is thus not more expensive in terms of computer time than the fault detection. The accuracy of the prediction has been found to be approximately equal to the accuracy of the chemical analysis, but is faster and cheaper.

Estimation of Reactive Impurities and Reactor Fouling in Batch Polymerisation Reactors Using Multivariate Statistical Methods

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Advanced process control of polymerisation processes is of great importance. Polymer manufacturers face increasing pressures for production cost reductions and more stringent "polymer quality" requirements. Significant economic advantages can be obtained by operating polymerisation reactors in an optimal way such that product uniformity is maintained. The main goals in operating a polymer reactor include high yield, consistent product quality and safe operation. To achieve these goals one needs well-structure control strategies, efficient process monitoring and reliable polymer characterisation techniques. A number of limitations have inhibited the polymer reactor monitoring and control schemes: the lack of on-line sensors for measuring quality variables, the poor understanding of the process dynamics, the highly sensitive and non-linear behaviour of polymer reactors and the difficulty of developing accurate mechanistic models.

Although important batch process issues have been extensively studied, such as design, scheduling, simulation, operation planning, optimisation and control, practically very important aspects, which have not been considered, are the problems of estimation of reactive impurities and reactor fouling, which commonly exist in practice. When there are reactive impurities and reactor fouling, the calculated optimal control policies and batch ending times are not appropriate and corrective actions should be taken to prevent off-specification production.

This paper addresses the issues of reactive impurities and reactor fouling estimation and present a multivariate statistical approach, based on the statistical projection methods of Multiway Principal Components Analysis (MPCA) and Multiway Projection to Latent Structures (MPLS), for on-line estimation of reactive impurities and reactor fouling at an early stage of the polymerisation process. These techniques have been successfully applied to a pilot-scale methyl-methacrylate (MMA) polymerisation reactor.

Batch Process Monitoring for Consistent Production

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A number of limitations have inhibited the success of batch process monitoring: the finite and variable duration of a batch, the presence of significant non-linearities, the lack of on-line sensors for measuring quality variables, the absence of steady-state operation, the difficulty of developing accurate mechanistic models, and process measurements that are autocorrelated in time as well as being correlated with one another. Recent approaches to the monitoring of batch behaviour have been based on extensions of the statistical projection methods of Principal Components Analysis (PCA) and Projection to Latent Structures (PLS) - multi-way PCA and multi-way PLS. These techniques form the bases of the multivariate statistical process control charts for batch process monitoring. The control limits for detecting when a process is moving out of control for multivariate SPC charts are based upon Hotelling's T^2 statistic. A new approach which allows the nominal data to dictate the form and shape of the bound, the M^2 statistic, is reviewed. Finally, an application of multivariate SPC and the impact the different confidence bounds have on process operation is highlighted by application to a batch methyl methacrylate polymerisation reactor.

Process Monitoring Using Non-Linear Principal Component Analysis

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Multivariate process monitoring is founded on the technique of principal components analysis (PCA). For non-linear systems, linear PCA may give misleading or uninformative distinctions between different operating conditions and mask the occurrence of process malfunctions. The application of non-linear PCA, in particular, accumulated non-linear PCA scores has provided a significant improvement in the separation of different operating conditions/faults. The methodologies are applied to a polymerisation reactor and a large industrial metals manufacturing process.

The concept of extracting features from highly non-linear data has been discussed by a number of researchers, with most techniques being based upon artificial neural networks. Of particular interest is the ability of the autoassociative neural network topology to provide a transformation which has been referred to as non-linear principal component analysis, NLPCA. The architecture of this network comprises five layers: input layer, mapping layer, bottleneck layer, demapping layer and output layer. Kramer proposed that the outputs of the bottleneck layer were non-linear principal components. This has been questioned by a number of researchers, since substituting the sigmoids by linear functions does not result in the extraction of linear principal components. A more appropriate terminology is that of non-linear feature analysis. The use of non-linear features has been shown to successfully describe the underlying structure of non-linear data. The generation of non-linear principal components requires the use of the statistical technique, principal curves. Non-linear Principal Components Analysis can be used in a similar way to PCA; the identification and removal of correlations amongst process variables as an aid to dimesionality reduction, data visualisation and data exploration in non-linearly correlated data.

The application of non-linear PCA, in particular, accumulated non-linear PCA scores has provided a significant improvement in the separation of different operating conditions/faults. The methodologies are applied to a polymerisation reactor.

Robustness Issues in Spectral Data Calibration

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It is known that many of the traditional regression techniques display potential instability so that the regression results are often sensitive to the selection of the calibration samples. Some techniques are under investigation in Newcastle to counteract such problems. These include stabilising these procedures through bagging regression, stacked regression and other data augmentation techniques.

The techniques of Principal Components Regression (PCR) and Projection to Latent Structures (PLS) have been shown to be able to handle collinear and high dimensional data for a range of problems. However, of interest to industry is whether by applying these techniques, acceptable calibration models can be developed from a minimal number of samples. This paper investigates the problem of sample sparsity through noise augmentation and bootstrapping techniques.

One approach for the generation of robust models is based upon the standard bootstrap. A series of new data sets are created through the statistical technique of the standard bootstrapping, i.e. sampling with replacement. A calibration model is then developed for each data set and the corresponding outputs are averaged to give the final model.

The data augmentation technique is similar in concept but it is built upon the addition of noise to the data. The methodology originated in the field of computerised vision. More recently, it has also received attention as a method for improving neural network training. In this report the data set is augmented with Gaussian noise and twenty new data sets, each the same size as the original are created. The level of noise added ranged from 0 to 20% of the variability for each individual wavelength. A PLS model, in the form of a regression vector is then calculated for each new data set and the resulting twenty PLS models are then averaged to produce the final calibration model. Two alternative approaches were examined, the augmentation of both the spectra (process) and reference (quality) variables and the augmentation of the spectra alone.

The ability of the data augmentation techniques and bootstrap regression to produce robust calibration models for specific properties of an industrial data set are investigated on an industrial data-set.

Control Structure Selection Techniques

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Control structure selection is an important step in the design of control schemes for chemical processes. How to efficiently select manipulable inputs and measureable outputs for multi-input multi-output processes is what is of interest.

This work presents systematic approaches for considering how using a theoretical basis the process (and/or control) engineer can make informed choices for which of the available inputs should be selected to have the most effect on the outputs. A measure, the Single Input Effectiveness SIE [1,2], for each candidate input has been derived and used to rank the inputs. Other work on the selection of inputs that achieve the best disturbance rejection structure is also covered [3]. A new indicator the Input-Disturbance Alignment measure (IDA) is presented. Case studies will be used to validate the design tools.

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Control Structure Selection for Energy Integrated Distillation Column

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This contribution concerns a case study on control structure selection for an almost binary destillation column. The column is energy integrated with a heat pump to transfer heat from the condenser to the reboiler.

This integrated configuration renders the possible control structure somewhat different from what is usually seen. Further the heat pump enables disturbances to propagate faster through the system. The plant has six possible actuators of which three must be used to stabilize the system. Hereby three actuators are left for product purity control and/or pressure control. A MILP sceening method based on a linear state space model is used to determine an economically optimal set of controlled and manipulated variables. The algorithm searches all possible structures rejects the ones with forces any output beyond a specified maximum deviation, when the system is subjected to worst case disturbances. The generated set of inputs and outputs are analysed with freqency dependent RGA and singular values to determine the best pairring of the variables in terms disturbance rejection. The paring and controller design are implemented and evaluated through nonlinear simulation.

The suggested control structure is also compared to a control structure applied experimentally.

Analysis of Control Systems for Processes for Processes with Recycle

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Recycle streams are very common in chemical plants, where integration of units is favoured for economic and enviromental reasons. The design of the control system for process with recycle presents some specific difficulties, because all the units linked by recycle streams must be accounted for simultaneously. Neglecting the effect of the recycle leads to unsatisfactory performance and in some cases instabilities may appear in the closed loop response.

Studies about the effect of the recycle parameters on the overall dynamics have been the object of intense research in the last years [1, 2, 3,]. In [4] alternative process designs are compared, for a typical reactor/stripper configuration, in order to optimize economics and controllability of the plant. As a rule to avoid amplification of disturbances (snow-ball effect) is proposed to fix the flow rate of the recycle loop. In [5] a plant including three distillation columns and two recycle streams is proposed as benchmark.

Detrimental effect of recycle can be eliminated by acting at the stage of design of process equipments, or at the stage of design of the control system by a careful selection of the control configuration and by a proper design of the controller.

In our reserch activity [6,7] the possibility of eliminating the problem at the stage of design of the control system has been faced by analysing the performance of different control systems with and without recycle compensators [8] for SISO and MIMO processes. It is shown that for SISO systems the recycle compensators becomes necessary for a fast soppression of disturbances. For MIMO processes the adoption of a compensator in many cases largely simplifies the design of the control system; in fact the elimination of the effect of the recycle, which is the main cause of interaction, allows satisfactory results even with simple diagonal PI controllers. The robustness of control structures based on the compensator has been investigated for different dynamics of the forward and of the recycle process in the presence of uncertainty and variation of parameters caused by changes of operating conditions.

In the case of complex plants there is not a general methodology to assist the choice of alternative control schemes; therefore a technique to analize all the possible combinations of controlled and manipulated variables (on the basis of a defined objective function) has been developed and applied on the proposed benchmark.

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