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Using Optimization to Detect Snowball Effects
T. J. McAvoy, *University of Maryland*

Frontiers in Industrial Process Automation – A Personal Perspective

P. Terwiesch, *ABB Process Industries GmbH*

The present contribution, from an industrial automation practitioner, looks at the operation of industrial processes as an integrated optimization problem that uses assets, labor, material, and energy to optimize profitability, subject to environmental, regulatory, health, and safety constraints. The extent to which available theories and tools have penetrated into industrial practice in each asset, material, energy, and labor optimization, is analyzed, as is the state of their respective combinations. Considering practical and economic barriers and opportunities, the author states his views on potentials for the application of control and optimization theories towards the optimized operation of industrial processes.

A Learning Theory Approach to System Identification

M. Vidyasagar, *Tata Consultancy Services*
R. L. Karandikar, *Indian Statistical Institute*

In this paper, we formulate the problem of system identification as a problem in statistical learning. By doing so, we are able to derive finite-time estimates of the proximity of the current model to the 'true system' if any, or to the 'optimal model' in case there is no true system. The main advantage of doing so is that traditionally system identification theory provides asymptotic results. In contrast, statistical learning theory is devoted to the derivation of finite time estimates. If system identification is to be combined with robust control theory to develop a sound theory of indirect adaptive control, it is essential to have finite time estimates of the sort provided by statistical learning theory. As an illustration of the approach, a result is derived showing that in the case of systems with fading memory, it is possible to combine standard results in statistical learning theory (suitably modified to the present situation) with some fading memory arguments to obtain finite time estimates of the desired kind. In contrast with earlier results in this area, the results presented here are applicable also to nonlinear systems. Moreover, no assumptions are made about the data to which a model is to be fitted, other than that it is a stationary stochastic process. This in contrast to earlier papers which assume that the data is generated by a model of known order. In fact, in the case of linear systems, the estimates presented here are not very conservative, but are more so in the case of nonlinear systems. As there is considerable scope for improving the specific bounds presented here, the results presented here should be viewed as just the beginning of a new theoretical approach.

A Systems Approach to Modeling and Analyzing Biological Regulation

F. J. Doyle III, *University of California, Santa Barbara*

Understanding regulation is a critical hurdle in unraveling complex biological systems. As gene-level architectures become known, the open challenge is to assign predictable behavior to a known gene structure, the so-called genotypeto- phenotype problem. In response to this challenge, the discipline of systems biology has emerged with an integrative perspective towards determining complex systems behavior. This research area lies at the intersection of classical fields such as microbiology and systems engineering, with strong influences from the more recent fields of informatics and genomics. In this paper, an overview of a number of quantitative tools from systems theory will be presented as enabling methodologies for unraveling biological regulatory systems, with an emphasis on (i) sensitivity analysis, (ii) identification methods, and (iii) optimization approaches.

New Developments in Industrial MPC Identification

Y.-C. Zhu, *Eindhoven University of Technology*

In industrial model predictive control (MPC), there is a demand for more efficient model identification methods. In this work we will review some recent developments in industrial MPC identification. The discussion will be around four fundamental issues of industrial identification: 1) test method, 2) parameter estimation, 3) order selection and 4) model validation/selection. Three industrial products will be discussed: 1) RMPCT identification package of Honeywell Hi-Spec Solutions, 2) DMCPlusä identification package DMCplus Model of Aspen Technology, and 3) Tai-Ji ID, the identification package of Tai-Ji Control. To show the benefits of modern approaches, two applications of Tai-Ji ID will be presented: an open loop identification of a crude unit and a closed-loop identification of a deethanizer.

Modelling and Control of Reactive Distillation Systems

M. O. Tadé, B. H. Bisowarno, Y.-C. Tian, *Curtin University of Technology*

Reactive distillation (RD) is an integrated functionality of reactor and distillation, which is gradually becoming an important unit operation in chemical process industry. Process modelling is crucial because the model should be basically accurate enough to represent the system complexity and feasible for real-time monitoring and control. Different applications also need different requirements for process modelling. In this work, the status of the current modelling techniques and their significance on process development are discussed. Strategies to tackle the challenging control problems associated with complex dynamics are also discussed. Some degree of intelligence in the control algorithms is required to compensate for the process uncertainties and unmodelled process dynamics. Therefore, model-based advanced controllers are promising tools for RD control. In this work, RD for ETBE production is used as a case study. Conventional PI controllers with proper control scheme can result in acceptable control performance. Set-point optimisation is presented to show the effects on chemical-physical interactions on profitability. Maximising product purity does not correspond to the maximum profitability. This optimisation framework can be used to develop a supervisory control system for RD column. Research gaps for future directions are identified.

Digital Imaging for Process Monitoring and Control with Industrial Applications

H.-L. Yu, J. F. MacGregor, *McMaster University*

The development of on-line digital imaging systems for process monitoring and control is illustrated through two industrial applications: i) the control of coating concentration and distribution on snack food products, and ii) the monitoring of boiler systems through imaging of the combustion processes. Feature information extracted from images using Multivariate Image Analysis (MIA) based on Principal Component Analysis (PCA), is used to develop models to predict product quality and process property variables. The imaging systems are used to monitor these product quality and process property variables, to detect and diagnose operational problems in the plants, and to directly implement closed-loop feedback control.

Monitoring Performance in Flexible Process Manufacturing

E. B. Martin, A. J. Morris, *University of Newcastle*

Partial Least Squares (PLS) is a popular method for the development of a framework for the detection and location of process deviations. A limitation of the approach is that it has generally been used to monitor one recipe, one product, for example, consequently applications may have been ignored because of the need for a large number of process models to monitor multi-product production. This paper introduces two extensions - multi-group and multi-group-multi-block PLS. These techniques enable a number of similar products, manufactured across different unit processes, to be monitored using a single model. The methodologies are demonstrated by application to a multi-recipe industrial manufacturing process.

Combined On-Line and Run-To-Run Optimization of Batch Processes with Terminal Constraints

C. Welz, B. Srinivasan, D. Bonvin, *École Polytechnique Fédérale de Lausanne*

This paper describes the optimization of batch processes in the presence of uncertainty and constraints. The optimal solution consists of keeping certain path and terminal constraints active and driving the sensitivities to zero. The case where the terminal constraints have a larger bearing on the cost than the sensitivities is considered, for which a two-time-scale methodology is proposed. The problem of meeting the active terminal constraints is addressed on-line using trajectory tracking, whilst pushing the sensitivities to zero is implemented on a run-to-run basis. The paper also discusses the run-to-run improvement of trajectory tracking via iterative learning control. The proposed methodology is illustrated in simulation on a batch distillation system.

Constrained Self-Optimizing Control via Differentiation

Y. Cao, *Cranfield University*

A new approach using differentiation to design ``self-optimization'' (Skogestad,2000} control system is proposed and applied to the evaporation process of Newell and Lee (1989). Using the chain rule of differentiation, an explicit expression of gradient in terms of system's Jacobian matrices has been derived for the first-order optimal condition of a constrained optimization problem. This gradient function can directly be used as a controlled variable to achieve self-optimization. To cope with conditionally active constraints, a cascade control structure has been proposed. With this structure, the optimal condition and conditionally active constraints can automatically switch each other to be active or inactive depending on disturbances so that both are satisfied. Both ideas have been demonstrated with the evaporator system. For the evaporation process, it is also shown that a traditional engineering judgement for level control structure selection may lead to a wrong decision. Simulation results show that the proposed control system does achieve self-optimization with various disturbances.

A Framework for Design of Scheduled Output Feedback Model Predictive Control

Z.-Y. Wan, M. V. Kothare, *Lehigh University*

We present a stabilizing scheduled output feedback Model Predictive Control (MPC) algorithm for constrained nonlinear systems with large operating regions. We design a set of local output feedback predictive controllers with their estimated regions of stability covering the desired operating region, and implement them as a single scheduled output feedback MPC which on-line switches between the set of local controllers and achieves nonlinear transitions with guaranteed stability. This algorithm provides a general framework for scheduled output feedback MPC design. The algorithm is illustrated with a highly nonlinear CSTR process.

Adaptive Backstepping Nonlinear Control of Bioprocesses

D. Dochain, *Université Catholique de Louvain*
M. Perrier, *Ecole Polytechnique de Montréal*

This paper deals with the design of adaptive and non adaptive nonlinear controllers based on backstepping techniques for bioprocesses. Backstepping techniques are known to be appropriate in particular to handle the control of systems with relative degree higher than one. In the present paper, we shall concentrate on one illustrative case study: the control of biomass concentration by acting on the influent susbtrate concentration. We propose the following sequence of controllers : we start with a non adaptive backstepping controller, then re-design the controller to include parameter estimation of uncertain model parameters. The design includes by construction the stability and convergence analysis of both controllers, whose performance are further illustrated in numerical simulations.

Advances in the Modeling and Control of Batch Crystallizers

Z. K. Nagy, J. W. Chew, M. Fujiwara, R. D. Braatz, *University of Illinois at Urbana-Champaign*

Despite the widespread application of crystallization, there are still a disproportionate number of problems associated with its control. These problems have become important in recent years as increased interest has been directed towards the crystallization of pharmaceuticals and proteins, which have additional complications compared to the inorganic crystallizations studied extensively in the past 50+ years. This paper covers recent advances in batch crystallization modeling and control. This includes a comparison in simulations and experiments between the classical temperature control approach developed in the 1970-90s with new concentration control approach developed in the last few years. The new approach, which uses ATR-FTIR spectroscopy and feedback control to follow a setpoint trajectory in the solution concentration as a function of temperature, results in reduced sensitivity of the product quality to disturbances. The resulting guidelines from the simulations are applied to the crystallization of paracetamol in water.

Joint Process and Control Designs of a Semibatch Emulsion Polymerization Reactor

F. Zaldo, M. Hernández, *Centro de Investigación en Polímeros*
J. Álvarez, *Universidad Nacional Autónoma de México*

The problem of jointly designing the equipment, the operation policy, and the calorimetric controller of a semibatch emulsion polymerization reactor is addressed within a nonlinear constructive control framework. A backstepping approach yields a passive cascade control structure, identifying the attainable closed-loop behavior, and the construction of a calorimetric controller. The designs of the equipment and of the operation are obtained from a recursive dynamic inversion in the light of safety, productivity, and quality considerations. The calorimetric controller tracks a prescribed temperature-free monomer profile by manipulating the heat exchange and monomer addition rates. The polymerization of vinyl acetate in an industrial size reactor is considered as application example with numerical simulations.

MPC in Statoil – Advantages with In-House Technology

S. Strand, J. R. Sagli, *Statiol R&D, Process Control*

Statoil has used an in-house developed model predictive controller (MPC) for the last six years. 26 applications are running closed loop today, with good performance and average service factors of approximately 99%. All application projects have used internal resources only, which means that the competence has been aggregated within the company and that the best practice has been integrated in the MPC software. As a result the basis for doing good projects improves continuously. The total cost of software development is moderate and the application project costs are definitely low. All applications are running with linear step response type of models, although the MPC also has the capability to use non-linear first principles based models. The paper presents the MPC algorithm, with specific focus on the practical issues which has to be considered for industrial process control. However, proper work in the application projects is even more essential than the software. How a typical MPC project is organized and executed have been outlined in this paper.

Modeling and Control of Thermal Microsystems

Y. J. Lee, S. Park, *Korea Advanced Institute of Science and Technology*
S. W. Sung, *LG Chem. Ltd. Research Park*
D. S. Yoon, G. Lim, *Samsung Advanced Institute of Technology*

A thermal microsystem is developed which consists of a microreactor integrated with a platinum sensor/heater, and automation equipment/software such as data acquisition system, control program and graphic user interface. From the control point of view, we analyze the dynamic characteristics of the fabricated microreactor and find some interesting dynamic features. On the basis of the analysis, we suggest an appropriate model structure and estimate the model parameters using the prediction error identification method. Requirements for a high-performance operation are discussed and a nonlinear control strategy is proposed to linearize the nonlinear dynamics of the thermal microsystem. We determine the parameters of the nonlinear controller using the optimal tuning method. The developed thermal microsystem shows much better control performances compared to commercial polymerase chain reaction (PCR) thermal cyclers. We successfully demonstrate the PCR of plasmid DNA using the thermal microsystem.

Modeling and Optimization on Energy Costs in Internal Thermally Coupled Distillation Columns of Non-Ideal Mixtures

X.-G. Liu, J.-X. Qian, *Zhejiang University*

Internal Thermally Coupled Distillation Column (ITCDIC) is the frontier of energy saving distillation research. In this paper, an evaluation method on the operating cost and its saving in the ITCDIC processes of non-ideal mixtures is presented. A mathematical model for optimization is first derived. The ethanol-water system is studied as an illustrative example. The optimization results show that the ITCDIC process of non-ideal mixture possesses an enormous potential of operating cost saving. The optimal operation conditions and the maximum percentage of operating cost saving are obtained simultaneously. The process analysis is then carried out and the results show the necessity and importance of optimal design on the rectifying pressure, the feed thermal condition, and the total heat transfer rate. These pave the way for the smooth operation and the further optimal design of ITCDIC processes for non-ideal mixtures.

Multi-objective Robust Control of an Evaporation Process

W.-J. Yan, *Zhejiang University*
Y. Cao, *Cranfield Univeristy*

In this paper, a new multi-objective robust control design approach is applied to an evaporation process. The new approach extends the standard generalized-l2(Gl2) control problem with the G-shaping paradigm resulting a set of new linear matrix inequality (LMI) conditions. Using this approach, a multi-objective robust control problem consisting of robust stability and robust performance objectives with various frequency and transient performance requirements, can be less conservatively solved using computationally tractable algorithms. A comparison of simulation results with controllers designed with different techniques demonstrates the superiority of the new method.

Nonlinear Control of a Fluid Catalytic Cracking Unit

Q. Yang, S.-R. Li, X.-M. Tian, *University of Petroleum (East China)*

The dynamics of a fluid catalytic cracking unit (FCCU) is a typical nonlinear system. A nonlinear control of a FCC unit via feedback linearization is developed based on the mechanistic model of a FCC unit. The servo and robustness properties of the closed loop system are verified by simulation for a sample FCC unit. The simulation shows that the controller is valid and can be implemented to practical FCC units.

Estimator Design with PLS Model for Consistent Control of Refinery Main Fractionators

P. Dante, B. Alessandro, G. Pannocchia, *University of Pisa*

In this paper the problem of designing product quality inferentials for refinery main fractionations is addressed by using the PLS regression. A simulated crude distillation unit is chosen as case study, and several linear steady-state estimators are designed and compared in terms of accuracy and consistency, i.e. the estimator ability of guaranteeing low closed-loop offset. The paper shows the importance of the auxiliary measurement choice in order to build an effective inferential control scheme. Moreover, it shows that the use of only temperature measurements is not sufficient to guarantee an acceptable estimator performance. Additional measurements as the operating pressure and internal flows have been used to improve the estimator accuracy and consistency.

Actuator Selection based upon Model Insights for an Energy Integrated Distillation Column

H. W. Li, R. Gani, S. B. Jørgensen, *Technical University of Denmark*

A method for development of actuator structures based upon model insight is presented. The method contains three steps. First dynamic degrees of freedom are handled using suitable level actuators and control loops. Second the feasible operating region is developed and third static control structures are proposed and screened. The advantage of the three-layered strategy is that the second and third layers can be dealt with early during process development while the first layer may assure perfect control initially. Later during process design where dynamic process information is available the dynamic loops of the first layer may be designed and subsequently high level control can be designed to fit appropriate control objective for plant.

Study on the Soft-Sensor and Control Scheme for an Industrial Azeotropic Distillation Column

S. Zhang, C.-M. Bo, J. Li, C.-Y. Sun, Y.-R. Wang, *Nanjing University of Technology*

In this paper, control problems of an industrial Azeotropic distillation column were discussed and improved. At first, the soft-sensor of water content in the bottom of the column was built based on on-the-spot data collected by distributed control system (for short, DCS), through applying soft-sensor technology of regression, and a self-correcting module was also designed. The functions of estimation, display and correction about water content were realized on the DCS. At the same time, according to the actual quality control targets, an inferential control scheme based on soft-sensor was designed, in which the on-line estimating values of soft-instrument were used. The close-loop control of the product quality was realized in the scheme. As a result of increasing of Boolean calculation with constrained condition in the inferential control arithmetic, the reliability and practicability of the control system is strengthened. Application of the control system to the column showed that the control system can resolve effectively the problems that the product quality cannot be measured on-line and be close-loop controlled directly, and has realized the bounder control of water content in the bottom of the column.

Grey-Box Modelling as a Tool for Improving the Quality of First Engineering Principles Models

N. R. Kristensen, H. Madsen, S. B. Jørgensen, *Technical University of Denmark*

A systematic framework for improving the quality of first engineering principles models using experimental data is presented. The framework is based on stochastic grey-box modelling and incorporates statistical tests and nonparametric regression in a manner that permits systematic iterative model improvement. More specifically, the proposed framework provides features that allow model deficiencies to be pinpointed and their structural origin to be uncovered through estimation of unknown functional relations. The performance of the proposed framework is illustrated through a case study involving a model of a fed-batch bioreactor, where it is shown how an incorrectly modelled biomass growth rate can be uncovered and a more appropriate functional relation inferred.

Identification of Multirate Sampled-Data Systems

J.-D. Wang, T.-W. Chen, B. Huang, *University of Alberta*

This paper studies identification of a general single-input and single-output (SISO) multirate sampled-data system. Using the lifting technique, we associate the multirate system with an equivalent linear time-invariant lifted system, from which a fast-rate discrete-time system is extracted. Uniqueness of the fast-rate system, controllability and observability of the lifted system, and other related issues are discussed. The effectiveness is demonstrated through simulation and a real-time implementation.

System Identification from Multi-rate Data

R. B. Gopaluni, H. Raghavan, S. L. Shah, *University of Alberta*

In this paper, we provide a novel iterative identification algorithm for multi-rate sampled data systems. The procedure involves, as a first step, identifying a simple initial model from the multi-rate data. Based on this model, the ``missing" data points in the slow sampled measurements are estimated following the expectation maximization approach. In the second step, using the estimated missing data points and the original data set, a final elaborate model is obtained. An application of the proposed method to an industrial data set is also included.

Robust PID Tuning using Closed-Loop Identification

Y.-C. Zhu, *Eindhoven University of Technology*

Identification based PID tuning is studied. The proposed approach consists of the identification of linear or nonlinear process model and model based control design. The identification test can be performed in both open loop and closed-loop. The so-called ASYM method is used to solve the identification problem. The method can identify a low order process model with a quantification of model errors (uncertainty). The PID tuning is based on the internal model control (IMC) tuning rules. Two case studies will be performed to demonstrate the proposed methodology. The first one is the adaptive control of the dissolved oxygen of a bioreactor; the second one is the nonlinear PID control of a PH process.

Estimation of Reaction Rates by Nonlinear System Inversion

W. Marquardt, A. Mhamdi, *RWTH Aachen*

The estimation of reaction rates is an important problem in mechanistic modeling, monitoring and control of chemical reactors. In contrast to standard estimation techniques where a model must be chosen for the reaction rates, we consider them in this work as unknown time-varying functions, which also may be interpreted as inputs. The resulting estimation task is an ill-posed inverse problem. The paper addresses this estimation problem based on systematic methods for nonlinear system inversion and filtering resulting in efficient estimators. A theoretical analysis reveals the conditions for reaction rate reconstruction are those for system invertibility. Our estimation scheme is a regularization method which eliminates the difficulties arising with ill-posed problems. Guidelines for the design of the estimator structure and the selection of the regularization parameters are presented.

An Incremental Approach for the Identification of Reaction Kinetics

W. Marquardt, M. Brendel, A. Mhamdi, *RWTH Aachen*
D. Bonvin, *EPFL*

This paper proposes an incremental approach for the identification of complex reaction kinetics in chemical reactors. The reaction fluxes for the various species are first estimated on the basis of concentration measurements and balance equations. This task represents an ill-posed inverse problem requiring appropriate regularization. In a further step, the reaction rates are estimated without postulating a kinetic structure. Finally, the dependency of the reaction rates on concentrations, i.e. the kinetic laws, are constructed by means of feed-forward neural networks. This incremental approach is shown to be both efficient and flexible for utilizing the available process knowledge. The methodology is illustrated on the industrially-relevant acetoacetylation of pyrrole with diketene.

Development of a Technique for Performance Evaluation of Industrial Controllers

C. Scali, M. Rossi, *University of Pisa*
M. Amadei, *Polimeri Europa*

The paper describes a method to account for different issues of performance monitoring of industrial control systems, under SISO control: detection of poorly tuned loops, process identification, controllers retuning and evaluation of performance improvements. The procedure can be completely automated and applied on-line or off-line; it starts from the analysis of plants data and ends up with a suggestion to the operator about the new controller settings. Characteristics and effectiveness of the technique are illustrated by simulations results and application to industrial plant data.

Performance Assessment of Constrained Controllers

C. Georgakis, *Polytechnic University*
L.-L. Huang, *Lehigh University*

The paper presents a new deterministic framework for assessing constrained control loop performance. The proposed dynamic performance index is based on the dynamic operating work of Uzturk and Georgakis (2002). It focuses on the time related characteristics of controllers' response to set-point changes or step-type disturbances. It explicitly takes into account the existence of constraints on manipulated variables. These constraints include minimum and maximum values as well as an upper limit on the rate of change of the input variables.

Performance Envelopes of Process Intensified Systems

S. R. Abd Shukor, M. T. Tham, *University of Newcastle upon Tyne*

Intensified processes may have response times orders of magnitudes faster than conventional units. Thus, the dynamics of control loop elements such as valves and measurement devices may no longer be negligible. This paper presents the results of an investigation into how the dynamics of control loop components influence the performances of controlled intensified processes. By adopting a particular controller design methodology, it was found that only the process delay and the time-constant of the feedback transmitter affect closed-loop performances. Further analysis showed that there are threshold values for these two parameters, beyond which closed-loop behaviour can be severely degraded, even in the nominal case. In terms of operability, the degree to which a process is intensified may therefore be limited. The results also reveal that advanced control techniques may be necessary if acceptable control of intensified systems is to be achieved.

Fault Diagnosis Based on Limit Measurements of Process Variables

H. A. Preisig, *Norwegian University of Science and Technology (NTNU)*
Y. X. Xi, K. W. Lim, *National University Singapore*

Industry uses mostly information on measurements passing limits as inputs to diagnostic systems. Asking the question on what can be achieved by such systems, we aim at an optimal design of diagnostic systems. The approach is, in contrast to the currently available techniques, based on continuous models that are mapped into discrete-event dynamic systems in the form of nondeterministic automata, with faults being constraint to have event-dynamic, that is, they occur and persist. We compute domains in which faults can be isolated or detected and discuss guidelines on how to design an application-optimal fault detection and isolation mechanisms.

Optimal Experimental Design for Training of a Fault Detection Algorithm

T. Duever, S. J. Lou, H. Budman, *University of Waterloo*

This paper focuses on Optimal Experimental Design to train a Projection Pursuit Regression (PPR) model used for fault detection. A novel experimental design method, referred to as Gaussian Probability Design, is proposed and compared with the conventional Factorial Design. The Gaussian Probability Design automatically searches for the sparseness of the data, and adds pairs of training data on both sides of a class boundary in areas where the data density is the lowest. This design method outperforms the Factorial Design in reducing the fault misclassification more effectively with the same amount of new training data.

Fault Diagnosis and Fault Identification for Fault-Tolerant Control of Chemical Processes

K.-K. Noh, E. S. Yoon, *Seoul National University*

Fault-tolerant control (FTC) of nonlinear systems is presented within an adaptive control framework. FTC can be accomplished by three subtasks; fault-diagnosis, fault identification and adaptive nonlinear control. In order to diagnose a fault at a time, a set of residual generators for fault diagnosis is designed by means of unknown input observers. When disturbances exist, disturbance-decoupled model could be derived for reliable diagnosis. Fault identification following fault diagnosis is an analogue to control task; the diagnosed fault is regarded as a control input and found out such that the residual from residual generator incorporating identification task is driven to reference zero. And, feedback linearizing control is liked with fault diagnosis and fault identification to compensate for a fault to the process. A three-tank system is taken as an example for demonstration of the presented FTC.

Constraint Handling in Reduced Order MPC: Application to Paper Machines

Y. Arkun, *Koç University*
A. Rigopoulos, *Weyerhaeuser Corp.*

This paper presents a method to handle input constraints when a large scale system is to be controlled by a model predictive control algorithm which uses a reduced order model of the process under consideration. A paper machine is used throughout to motivate and illustrate the method.

Simulation-Based Dual Mode Controller for Nonlinear Processes

J. M. Lee, J. H. Lee, *Georgia Institute of Technology*

This paper presents a simulation-based strategy for designing a nonlinear override control scheme to improve the performance of a local linear controller. The higher-level nonlinear controller monitors the dynamic state of the system under the local controller and sends an override control action whenever the system is predicted to move outside an acceptable operating regime under the local controller. For this purpose, a cost-to-go function is defined, an approximation of which is constructed by using simulation or historic operation data. The cost-to-go function delineates the ``admissible" region of state space within which the local controller is effective, thereby yielding a switching rule. The same cost-to-go function can also be used to calculate override control actions designed to bring the system state back into the admissible region as quickly as possible. One potential problem of this approach is the lack of robustness when the simulation data sparsely cover the state space and the data-based approximation of the cost-to-go function is extrapolated to a region previously unseen. Hence, successful application of the proposed method requires safeguarding against undue extrapolations. For this reason, a kernel-based local approximation, instead of a global approximator like a neural network, is used to interpolate the cost-to-go values. It is shown that the kernel-based local regression provides convenient means to implement a risk-sensitive control scheme which avoids excessive extrapolation. The proposed scheme is demonstrated and discussed with nonlinear examples.

Nonlinear Model Predictive Control of Multicomponent Distillation Columns using Wave Models

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A. Kienle, E. D. Gilles, *Max-Planck-Institut für Dynamik Komplexer technischer Systeme Magdeburg*

A novel control concept for multicomponent distillation columns is presented. The concept is based on nonlinear wave-propagation phenomena that occur in counter-current separation processes. On this basis a reduced order model has been developed in previous work that not only considers profile positions but also the profile shape itself. The reduced model gives direct access to key parameters of the plant, such as the separation front positions. Furthermore, it allows real-time computations for multicomponent distillation columns. Such a model is used for both, the nonlinear model predictive control (NMPC) and the observer design. The observer uses temperature measurements and gives estimated temperature and concentration profile positions as well as compositions in the product streams. The robustness of the observer is shown intuitively and in simulation studies. The control of multicomponent distillation is formulated within the NMPC framework by penalising the deviation of the front positions from their reference points and ensuring the product specifications by means of constraints. By directly taking account of product specifications the presented control concept differs from inferential control schemes known from literature. Due to the fact that the concept is based on simple temperature measurements an industrial application seems easily possible.

Nonlinear Model Predictive Control of Cement Grinding Circuits

R. Lepore, A. Vande Wouwer, M. Remy, *Faculté Polytechnique de Mons*

Based on a reduced-order model of a cement grinding circuit, a nonlinear model predictive control strategy is developed. The first step of this NMPC study is the definition of control objectives which consider product fineness, product flow rate and/or grinding efficiency. At this stage, one of the main concerns is to relate these objectives to easily measurable particle weight fractions. Second, NMPC is implemented so as to take the various constraints on the manipulated variables and operating conditions of the mill into account. Third, robustness with respect to model uncertainties is analyzed, and the most critical parameters are highlighted. Finally, an NMPC scheme, combining a stable inner loop for controlling the mill flow rate and a DMC-like compensation of the model mismatch, is proposed.

Optimal Operation and Control of a Reactive Simulated Moving Bed Process

A. Toumi, S. Engell, *University of Dortmund*

In this paper, we investigate the continuous production of High Fructose Corn Syrup (HFCS) in a Reactive Simulated Moving Bed process (RSMB). The RSMB process combines a quasi-continuous chromatographic separation with an enzymatic biochemical conversion of glucose to fructose. For the equilibrium limited glucose isomerization such an integration is suitable. The optimal operation of the RSMB process is determined using a sequential approach based on a rigorous mathematical model of the plant. In addition, we propose a new strategy to determine the distribution of the columns over the zones in the RSMB plant circumventing the solution of a Mixed Integer Nonlinear Problem (MINLP). During the operation of the RSMB process, disturbances occur (e.g. continuous decrease of the enzyme activity) which lead to an off-spec product. The control objective is to maintain the product purity while injecting a minimal additional amount of eluent. We propose a nonlinear model predictive controller which can deal with the complex hybrid dynamic of the RSMB plant as well as with hard constraints. The parameters of the non-linear process model are periodically estimated by least-squares fitting to online measurements. The efficiency of the whole control concept is shown in simulation studies for a 6-column RSMB plant.

Combinations of Measurements as Controlled Variables: Application to a Petlyuk Distillation Column

V. Alstad, S. Skogestad, *Norwegian University of Science and Technology (NTNU)*

This paper consider how to best implement the optimal operation policy in the presence of uncertainty (disturbances and implementation errors) by selecting the right set of controlled variables c to be kept at constant setpoints c_s. More specific, we focus on how to select controlled variables that are linear combinations of a subset of the available measurements with good self-optimizing properties.

Self-optimizing control is when an acceptable loss can be acheived using constant setpoints for the controlled variables (without the need to reoptimize when disturbances occur).

A new method is proposed, that from a local point of view give controlled variables with perfect self-optimizing properties. This is acheived by selecting controlled variables c=Hy, where H is selected in the left null space of F, where F is the optimal constrained mapping delta y_opt=F delta d. The proposed method is illustrated on a Petlyuk distillation colum.

A Complete Dynamic Model for Twin Screw Extruders

Y. Le Gorrec, S. Choulak, F. Couenne, C. Jallut, *LAGEP*
P. Cassagnau, A. Michel, *LMPB*

A one-dimensional physically motivated dynamic model of a twin-screw extruder for reactive extrusion has been developed. This model can predict extruder behaviour such as pressure, filling ratio, temperature and molar conversion as well profiles as residence time distribution under various operating conditions such as feed rate, screw speed, monomer/initiator ratio and heat flux supplied to the barrel. The model consists of a cascade of perfectly stirred reactors which can be either fully or partially filled with backflow. We consider the mass balance coupled with the momentum balance for the calculation of the pressure profile and the flows between the different reactors. At each reactor is associated the concentration in monomer, the temperature of the matter, the temperatures of the associated piece of screw and barrel. The final model consists of a set of differential algebraic equations. The experimental validation is only made on flow aspects of the model by using experimental RTD's.

A Data-Driven Model for Valve Stiction

S. L. Shah, M. A. A. S. Choudhury, *University of Alberta*
N. F. Thornhill, *University College London*

The presence of nonlinearities, e.g., stiction, hysteresis and backlash in a control valve limits control loop performance. Stiction is the most common problem in spring-diaphragm type valves, which are widely used in the process industry. Though there have been many attempts to understand the stiction phenomena and model it, there is lack of a proper model which can be understood and related directly to the practical situation as observed in real valves in the process industry. This study focuses on the understanding, from industrial data, of the mechanism that causes stiction and proposes a new data-driven model of stiction, which can be directly related to real valves. It compares simulation results generated using the proposed model with industrial data.

A Software Sensor for a Wastewater Treatment Plant

T. Lopez, *Instituto Mexicano del Petróleo*
A. Pulis, M. Mulas, R. Baratti, *Universita' di Cagliari*

In this work, a software sensor is presented in order to monitor the pollutant concentrations in an activated sludge process for industrial and municipal wastewater treatment. The software sensor consists of a model-based state estimator to infer the (unmeasured) biodegradable substrate and ammonia concentrations, based on a reduced process model with approximated model parameters and considering only on-line measurements of dissolved oxygen and nitrate concentrations. The software sensor performance is showed with experimental data from a real process and it is compared versus a complex process model, obtaining good estimated concentrations.

Experimental Verification of Gap Metric as a Tool for Model Selection in Multi-Linear Model-Based Control

A. Palazoğlu, *University of California, Davis*
O. Galán, *ABB Australia Limited Paper*
J. A. Romagnoli, *University of Sydney*
Y. Arkun, *Koç University*

A nonlinear system can be modeled using a set of linear models that cover the range of operation. A model-based control strategy then can be employed that uses the local models in a cooperative manner to control the nonlinear system. The decision of how many models are sufficient for effective control can be tackled by the use of the gap metric that quantifies the distance between two linear operators. A pH control experiment is used to demonstrate the effectiveness of gap metric as a tool for model selection.

Bayesian Estimation of Unconstrained Nonlinear Dynamic Systems

W.-S. Chen, B. R. Bakshi, P. K. Goel, *Ohio State University*
S. Ungarala, *Cleveland State University*

Accurate estimation of state variables and model parameters is essential for efficient process operation. The Bayesian formulation of the estimation problem suggests a general solution for nonlinear systems. However, a practically feasible implementation of the solution has not been available until recently. Most existing methods have had to rely on simplifying assumptions to obtain an approximate solution. For example, extended Kalman filtering estimates the system state by linearizing the nonlinear model and assuming Gaussian distributions for all random variables. Moving horizon estimation assumes Gaussian or other fixed-shape distributions to formulate a constrained least-squares optimization problem. In this paper, Bayesian estimation is implemented by sequential Monte Carlo sampling. This approach can represent non-Gaussian distributions accurately and efficiently with minimum assumptions and computes moments by Monte Carlo integration. The features of the Monte Carlo approach are demonstrated by application to a state estimation case study of a CSTR process. The proposed method exhibits 78% improvement in estimation error and takes 95% less time than moving horizon estimation to solve the problem.

Multivariate Analysis of Process Data using Robust Statistical Analysis and Variable Selection

L. H. Chiang, R. J. Pell, M. B. Seasholtz, *Dow Chemical Company*

Historical plant data are useful in developing multivariate statistical models for on-line process monitoring, soft sensors, and process troubleshooting. For the first two purposes, historical data are used to build a model to capture the normal characteristics of the process. However, the presence of outliers can adversely affect the model. Various robust statistical techniques are investigated in this paper for outlier identification. For process troubleshooting and fault identification, it is crucial to identify the key process variables that are associated with the root causes. Genetic algorithms (GA) are incorporated with Fisher discriminant analysis (FDA) for this purpose. These techniques have been successfully applied at The Dow Chemical Company.

PCA with Efficient Statistical Testing Method for Process Monitoring

F.-P. Mu, V. Venkatasubramanian, *Purdue University*

Principal component analysis (PCA) has been used successfully for fault detection and identification in processes with highly correlated variables. The fault detection decision used depends solely on the current sample though the results of previous samples are available and is based on a clear definition of normal operation region, which is difficult to define in reality. In the present work, a novel statistical testing algorithm is integrated with PCA for further improvement of fault detection and identification performance. We use the idea to decompose the scores space and residual space generated by PCA into several subsets so chosen that in each subset the detection problem can be solved with an efficient recursive change detection algorithm based on c2-generalized likelihood ratio (GLR) test.

Computation of the Performance of Shewhart Control Charts

E. B. Martin, P. Mulder, J. Morris, *University of Newcastle*

The performance of a control chart in statistical process control is often quantified in terms of the Average Run Length (ARL). The ARL enables a comparison to be undertaken between various monitoring strategies. These are often determined through Monte Carlo simulation studies. Monte Carlo simulations are time consuming and if limited runs are performed, the results will be inaccurate. Furthermore Monte Carlo simulations do not provide any theoretical understanding of the ARL. An alternative approach using analytical computation is proposed. It is shown how, based on the in-control probability at individual points in the control chart, the density function of the run length can be determined. The density function can consequently be used to calculate the ARL and enable a comparison to be undertaken between various monitoring strategies. The analytical approach is faster, more generic than previous approaches and will also provide a theoretical understanding of the ARL. The analytical results are compared with those of the Monte Carlo simulations for three case studies, independent data, the residuals of AR(1) models and serially correlated data. The theoretical results correspond to the ARL's obtained through Monte Carlo simulations.

Combined Multivariate Statistical Process Control

M. Kano, S. Tanaka, S. Hasebe, I. Hashimoto, *Kyoto University*
H. Ohno, *Kobe University*

Multivariate statistical process control (MSPC) based on principal component analysis (PCA) has been widely used in chemical processes. Recently, the use of independent component analysis (ICA) was proposed to improve monitoring performance. In the present work, a new method, referred to as combined MSPC (CMSPC), is proposed by integrating PCA-based SPC and ICA-based SPC. CMSPC includes both MSPC methods as its special cases and thus provides a unified framework for MSPC. The effectiveness of CMSPC was demonstrated with its applications to a multivariable system and a CSTR process.

Batch Monitoring through Common Subspace Models

J. Morris, S. Lane, E. B. Martin, *University of Newcastle*

The multivariate statistical projection techniques of Principal Component Analysis (PCA) and Projection to Latent Structures (PLS) are popular methods for on-line process monitoring for the detection of changes and malfunctions in process operation. The extension of these methodologies to multi-way PCA and multi-way PLS has enabled the monitoring of batch processes but typically the applications have been limited to single-group applications, i.e. a single product, grade or recipe. Consequently many potential applications have been missed because of the resulting large number of process models required to monitor multi-product and multi-recipe production. This limitation can be overcome through the use of common sub-space multi-way PCA and multi-way PLS models (or groups) constructed by pooling the individual product / recipe variance-covariance matrices. A second issue with the multi-way approaches is the issue of diagnosing the possible source of the batch process malfunction due to the multi-way contribution plot being difficult to interpret. Within the paper an extension to the U2 statistic is proposed which allows the cumulative contribution of each individual variable, or groups of variables, at each sample point to be assessed. The methodologies are illustrated through their application to a metal etcher process and a polymer films production line.

Application of PLS-Based Regression for Monitoring Bitumen Recovery in a Separation Cell

H. Raghavan, S. L. Shah, *University of Alberta*
R. Kadali, B. Doucette, *Suncor Extraction*

Partial Least Squares (PLS) is a technique used to perform regression between blocks of explanatory variables and dependent variables. PLS uses projections of original variables along directions which maximize the covariance between these blocks. It has been popular due to its data-reduction property and its ability to handle collinearity within the data blocks. In this paper some issues which arise in the the development of multivariate static models of industrial processes using PLS regression are studied. An industrial example of the application of PLS regression for the development of inferential sensors to predict the Bitumen Recovery in a separation cell is shown. Some of the challenges encountered in the development and online implementation of the inferential sensors and the proposed solutions are presented.

Online Performance Monitoring and Quality Prediction for Batch Processes

A. Cinar, C. Ündey, *Illinois Institute of Technology*

Two different quality prediction techniques are incorporated with online MSPM through PLS modeling in this study. The first technique is based on unfolding a batch data array by preserving variable direction. An MPLS model between this matrix and vector of elapsed local batch times is developed to reflect the batch progress. More data partitions become available as the batch progresses and these partitions are rearranged into a matrix to develop local MPLS models predicting quality online. The second technique uses hierarchical PLS modeling in an adaptive manner resulting in a model that can be used to predict end-of-batch quality online. Neither technique requires estimation of future portions of variable trajectories and both are suitable for online multivariate statistical process monitoring and fault diagnosis. Case studies from a simulated fed-batch penicillin fermentation illustrate the implementation of the methodology.

Design of Sub-Optimal Robust Gain-Scheduled PI Controllers

H. M. Budman, J.-Y. Gao, *University of Waterloo*

A methodology is proposed for the analysis and design of a robust gain-scheduled PI controller for nonlinear chemical processes. The stability and performance tests can be formulated as a finite set of linear matrix inequalities (LMI) and hence, the resulting problem is numerically tractable. Input saturation and model error are explicitly incorporated into the analysis. A simulation study of a nonlinear CSTR (continuous stirred tank reactor) process indicates that this approach can provide useful sub-optimal robust controllers.

Adaptive Extremum Seeking Control of Continuous Stirred Tank Bioreactors

M. Guay, *Queen's University*
D. Dochain, *Université Catholique de Louvain*
M. Perrier, *Ecole Polytechnique de Montréal*

In this paper, we present an adaptive extremum seeking control scheme for continuous stirred tank bioreactors. We assume limited knowledge of the growth kinetics. An adaptive learning technique is introduced to construct a seeking algorithm that drives the system states to the desired set-points that maximizes the value of an objective function. Lyapunov's stability theorem is used in the design of the extremum seeking controller structure and the development of the parameter learning laws. A simulation experiment is given to show the effectiveness of the proposed approach.

Set Stabilization of a Class of Positive Systems

B. A. Foss, L. Imsland, *Norwegian University of Science and Technology*

A specific class of positive systems is considered, where the system structure allows control of the distribution of ``mass" in the system. Some robustness properties of the controller are pointed out, and the applicability of the model class is discussed. An example considering a CSTR modeled by mass- and energy balances illustrates the presented concepts.

Stabilization of Gas Lifted Wells based on State Estimation

B. A. Foss, G. O. Eikrem, L. Imsland, *Norwegian University of Science and Technology*

This paper treats stabilization of multiphase flow in a gas lifted oil well. Two different controllers are investigated, PI control using the estimated downhole pressure in the well, and nonlinear model based control of the total mass in the system. Both control structures rely on the use of a state estimator, and are able to stabilize the well flow with or without a downhole pressure measurement available. In both cases stabilization of gas lifted wells increases total production significantly.

H-Infinity Control of Descriptor Systems: An Application from Binary Distillation Control

A. Rehm, F. Allgöwer, *Universität Stuttgart*

In this paper the H_infinity control problem for descriptor systems is considered. This problem can efficiently be solved by specialization of a recent solution of the general quadratic performance control problem to the H_infinity case. The solution is given in terms of strict linear matrix inequality (LMI) conditions. Contrary to previous solutions of the descriptor H_infinity control problem, these synthesis conditions can easily be evaluated by standard LMI solvers. The presented synthesis result is applied to a S/KS H_infinity control problem from binary distillation control. The process model of the underlying separation process is given by means of a phenomenological descriptor model which describes the movement of concentration profiles in rectifying and stripping section of the distillation column.

Cascade Control of Unstable Systems with Application to Stabilization of Slug Flow

S. Skogestad, E. Storkaas, *Norwegian University of Science and Technology*

The topic of this paper is the effect of stabilizing control on the remaining control problem. In many cases there is no effect. However, stabilization requires the active use of inputs, and the underlying unstable pole will appear as an undesirable unstable zero if we are concerned with input performance. The implications of this are clearly demonstrated on the application to stabilization of severe slugging in two-phase pipeline-riser systems. We find that a controllability analysis gives important information for measurement selection and performance limitations.

Combined Metabolic and Cell Population Modeling for Yeast Bioreactor Control

M. A. Henson, *University of Massachusetts*
D. Müller, M. Reuss, *Universität Stuttgart*

Several investigators recently have explored the use of cell population balance equation (PBE) models for the design of biochemical reactor control strategies. A major disadvantage of the PBE modeling approach is that the incorporation of intracellular reactions needed to accurately describe cellular processes leads to substantial computational difficulties. We investigate an alternative modeling technique in which the cell population is constructed from an ensemble of individual cell models. The average value or the number distribution of any intracellular property captured by the cell model can be computed from ensemble simulation data. To illustrate the basic procedure, a single cell model of yeast glycolytic oscillations is used to construct large cell ensembles for the investigation of cell population synchronization. The potential use of cell ensemble models for bioreactor controller design are discussed.

Optimization of a Fed-Batch Bioreactor using Simulation-Based Approach

J. H. Lee, N. S. Kaisare, *Georgia Institute of Technology*
C. V. Peroni, *Universitat Rovira I Virgili*

We use simulation-based approach to find the optimal feeding strategy for cloned invertase expression in Saccharomyces cerevisiae in a fed-batch bioreactor. The optimal strategy maximizes the productivity and minimizes the fermentation time. This procedure is motivated from Neuro Dynamic Programming (NDP) literature, wherein the optimal solution is parameterized in the form of a cost-to-go or profit-to-go functions. The proposed approach uses simulations from a heuristic feeding policy as a starting point to generate the profit-to-go vs state data. An artificial neural network is used to obtain profit-to-go as a function of system state. Iterations of Bellman equation are used to improve the profit function. The profit-to-go function thus obtained, is then implemented in an online controller, which essentially converts infinite horizon problem into an equivalent one-step-ahead problem.

Glucose Control in Type I Diabetic Patients: A Volterra Model-Based Approach

R. S. Parker, J. D. Rubb, *University of Pittsburgh*

Glucose concentration controllers for Type I diabetic patients are synthesized using model-based methods. A physiologically-based model of the insulin-dependent diabetic is employed as the patient. For modeling and control purposes, the patient is approximated using nonlinear Volterra series models. These data-driven models are then employed in two nonlinear controller synthesis strategies: internal model control using partitioned inverses (Doyle III et al., 1995), and model predictive control.

Biomass Reconstruction in a Wastewater Treatment Biofilter

A. Vande Wouwer, C. Renotte, *Faculté Polytechnique de Mons*
N. Deconinck, P. Bogaerts, *Université Libre de Bruxelles*

This paper is concerned with a pilot-scale fixed-bed biofilter used for nitrogen removal from municipal wastewater. Process dynamics is described by a set of mass balance partial differential equations, which allow the evolution of the several component concentrations along the biofilter axis to be reproduced. Based on sets of experimental data collected over a several-month period, unknown model parameters are estimated by minimizing an output error criterion. The resulting distributed parameter model and a few pointwise measurements of nitrate, nitrite, and ethanol concentrations can be used to design observers, which allow the unmeasured biomass concentrations to be reconstructed on-line. First, it is demonstrated that asymptotic observers are unsuitable for the model structure. Then, a receding-horizon observer is designed and tested, which shows very satisfactory performance.

An Optical Operating Strategy for Fed-Batch Fermentations by Feeding the Overflow Metabolite

S. Valentinotti, C. Cannizzaro, B. Srinivasan, D. Bonvin, *Ecole Polytechnique Fédérale de Lausanne*

Optimization of the fed-batch fermentation of S. cerevisiae is analyzed. Due to the limited oxygen uptake capacity of the cells, the overflow metabolite ethanol is formed when the substrate concentration is above some critical value. This value decreases during the course of an experiment due to the reduction in dissolved oxygen concentration resulting from biomass formation. Optimal operation corresponds to regulating the substrate concentration along this time-varying critical value. This paper proposes a novel strategy to implement this optimal solution, whereby ethanol is fed along with the substrate and its concentration in the reactor regulated around the inlet concentration value. Sub-optimal strategies of practical interest are also discussed and simulation results are presented.

Target-set Control

R. K. Pearson, *Thomas Jefferson University*
B. A. Ogunnaike, *University of Delaware*

To survive in the face of uncontrollable natural variations, biological organisms have developed adaptation mechanisms that make them remarkably insensitive to variations in certain variables. Conversely, outside these ranges of admissible variation, biological function may change dramatically, usually in undesirable ways (e.g., the organisms die). As a consequence, a set-theoretic control strategy seems quite appropriate for biologically-based processes like fermentation reactors: many variables do not have to be controlled to precise setpoints, but they do have to be maintained within viable operating ranges. This paper proposes a strategy for this kind of set-theoretic control based on {\em zonotopes}, which are the images of n-dimensional cubes under affine transformations. This approach is well-suited to the control of linearized fundamental models or linear empirical models over a specified range of validity. In addition, the results presented here establish strong connections with classical linear control theory. Finally, these results are extended to positive linear systems, a class that includes many biological system models (e.g., compartmental models arising in pharmecokinetics) and that are inherently harder to control than unconstrained linear systems.

Process Monitoring Based on Nonlinear Wavelet Packet PCA

Y. Qian, X.-X. Li, J.-F. Wang, Y.-B. Jiang, *South China University of Technology*

For using process operational data to realize process monitoring, kinds of improved PCA are applied to cope with complexity of industrial processes. In this paper, a novel nonlinear wavelet packet PCA (NLWPPCA) method, which combines input training network with wavelet packet PCA, is proposed. Wavelet packet PCA integrates ability of PCA to de-correlate the variables by extracting a linear relationship with what of wavelet packet analysis to extract auto-correlated measurements. Then the paper gives the methodology of process monitoring based on NLWPPCA. Finally, the proposed approach is successfully applied to an eight variables nonlinear process with noise and Tennessee Eastman process for process monitoring.

Application of Statistical Process Monitoring with External Analysis to an Industrial Monomer Plant

M. Kano, I. Hashimoto, *Kyoto University*
T. Yamamoto, A. Shimameguri, M. Ogawa, *Mitsubishi Chemical Corporation*

The main objective of this industry-university collaboration is to develop an on-line process monitoring system that can detect a particular malfunction in an industrial monomer plant. The most serious malfunction is a blockage caused by an accumulation of polymers inside a cooling unit. Since the blockage requires shutdown maintenance, it is crucial to detect its symptom as early as possible and properly adjust the operating condition to avoid further polymer accumulation. The developed on-line monitoring system can detect the symptom of the blockage by using multivariate statistical process control, distinguish it from normal changes in operating conditions by using external analysis, and persuade operators to take appropriate action.

On-Line Monitoring of a Copolymer Reactor: A Cascade Estimation Design

T. Lopez, *Instituto Mexicano del Petróleo*
J. Alvarez, *Universidad Autonoma Metropolitana - Iztapalapa*
R. Baratti, *Universita' di Cagliari*

In this work the problem of on-line monitoring of product quality and production rate in a copolymer reactor is addressed, using an estimation scheme with secondary measurements of density, refractive index, temperature, and volume. Three different estimator structures are studied: (a) the nominal detectability structure that underlines the extended Kalman filter and Luenberguer observers, (b) a passive estimation structure with estimation degrees equal to one, and (c) a hybrid structure that combines the detectability and passive structures in low and high gain, respectively. The nominal detector maximizes the reconstruction rate, the passive estimator maximizes the robustness, and the cascade (hybrid) design achieves a suitable compromise between them. The approach is illustrated with a copolymer reactor case and simulations.

A Robust PCA Modeling Method for Process Monitoring

D. Wang, J. A. Romagnoli, *University of Sydney*

A robust method for dealing with the gross errors in the data collected for PCA model is proposed. This method, using M-estimator based on the generalized t distribution, adaptively transforms the data in the score space in order to eliminate the effects of the outliers in the original data. The robust estimation of the covariance or correlation matrix is obtained by the proposed approach so that the accurate PCA model can be obtained for the process monitoring purpose. Comparisons with the conventional PCA modeling and other robust outlier's replacement approaches are illustrated through a chemical engineering example.

A Framework for On-Line Trend Extraction and Fault Diagnosis

V. Venkatasubramanian, M. R. Maurya, *Purdue University*
R. Rengaswamy, *Clarkson University*

Qualitative trend analysis (QTA) is a process-history-based data-driven technique that works by extracting important features (trends) from the measured signals and evaluating the trends. QTA has been widely used for process fault detection and diagnosis. Recently, Dash et al. (2001) proposed an interval-halving-based algorithm for automatic trend extraction, which can extract both linear and non-linear primitives. Thus no concatenation is required. Dash et al. (2003) also developed a fuzzy-logic-based framework for trend-matching and fault diagnosis. While the interval-halving algorithm, the trend-matching methodology and their application for FD have been discussed in detail, on-line implementation has not been discussed. In this article, we discuss most of the important issues that are involved in on-line fault diagnosis. We present an algorithm for on-line trend extraction using the interval-halving technique to achieve computational efficiency and robustness. Essentially, the interval-halving algorithm is applied on the data in a window, the window is slid as more data becomes available and, the size of the window (or the starting point of the window) is changed adaptively. A framework for on-line FD using QTA is also presented. The issues addressed are: (1) development of a robust and computationally efficient QTA-knowledge-base, (2) fault detection, (3) estimation of the fault occurrence time, (4) on-line trend matching and, (5) updating the QTA-knowledge-base when a novel fault is diagnosed manually. The Tennessee Eastman process has been used as a case study to illustrate the application of the framework.

Application of Software Sensors for Monitoring and Prediction in Fermentation Processes

M. Thaysen, S. B. Jørgensen, *Technical University of Denmark*

To improve monitoring and control of industrial fermentation processes it is desirable to include information of dynamic responses of relevant biological and chemical species to changes in process conditions whenever possible. Fulfilling this desire is however not trivial, since measurements of relevant species often is difficult to conduct and impossible to obtain at the desired rate. An alternative approach to direct measurement is the development of process software sensors based on mathematical models correlating measurable variables to the desired variables.

The development of two process software sensors for monitoring a) biomass concentration and b) product concentration in fedbatch and continuous yeast fermentations is presented, followed by a validation of the sensors using data from industrial fermentations. The effects of including the software sensors in multivariate statistical process monitoring (MSPM) based on multiway projection to latent structures (MPLS) are investigated with the aim of predicting the product concentration at a certain time point in the fermentation.

Developments in Multi-Rate Predictive Control

J. A. Rossiter, *Sheffield University*
T.-W. Chen, S. L. Shah, *University of Alberta*

Much of the work on predictive based multi-rate control has been based on the GPC algorithm. However academic practitioners in single rate predictive control tend to favour approaches with better stability and performance guarantees. This paper demonstrates how those approaches might be deployed in a multi-rate framework and discusses some issues that arise.

Nonlinear Predictive Control in the LHC Accelerator

C. de Prada, S. Cristea, *University of Valladolid*
E. Blanco, J. Casas, *CERN*

This paper describes the application of a nonlinear model-based control strategy in a real challenging process. A predictive controller based on a nonlinear model derived from physical relationships, mainly heat and mass balances, has been developed and commissioned in the Inner Triplet Heat Exchanger Unit (IT-HXTU) prototype of the LHC particle accelerator being built at CERN, operating at a temperature of about 1.9 K. The development includes a state and disturbances estimator with a receding horizon procedure to improve the regulator predictions.

Disturbance Attenuation with Actuator Constraints by Moving Horizon H-Infinity Control

H. Chen, *Jilin University*
C. W. Scherer, *Delft University of Technology*

Exploiting the moving horizon strategy, we provide in this paper a solution of the constrained L_2-gain attenuation control problem that is less conservative than a recently suggested switching approach based on off-line controller computations. The main advantage of the presented scheme is its capability of automatically relaxing or tightening the performance specification in order to obey hard control constraints while achieving the best possible performance in a suitable class of LMI-generated control gains.

An LMI-based Constrained MPC Scheme with Time-Varying Terminal Cost

B. Pluymers, L. Roobrouck, J. Buijs, J. A. K. Suykens, B. De Moor, *ESAT-SCD-SISTA*

Modelbased Predictive Control (MPC) is a control technique that is widely used in chemical process industry. In the past decade, stability of MPC has been an intensive research area, resulting in the general acceptance of a theoretical MPC stability framework introducing a terminal cost and terminal constraint to the classic MPC formulation. Although guaranteeing stability, issues regarding optimality and feasibility remain. In this paper, an LMI-based constrained MPC scheme for linear systems is introduced which guarantees stability by use of a time-varying terminal cost and terminal constraint. The online calculation of the terminal cost results in improved performance and feasibility compared to MPC schemes with fixed terminal cost. Finally, the technique is illustrated on a copolymerization reactor.

Computational Delay in Nonlinear Model Predictive Control

R. Findeisen, F. Allgöwer, *University of Stuttgart*

By now a series of NMPC schemes exist that lead to guaranteed stability of the closed-loop. However, in these schemes the computation time to find a solution of the open-loop optimal control problem is often neglected. In practice the necessary computation time is often not negligible, and leads, since not explicitly considered, to a delay between the state information and the input signal implemented on the system. This delay can lead to a drastic performance decrease or even to instability of the closed-loop. In this paper we outline a simple approach how the computational delay can be considered in nonlinear model predictive control schemes and provide conditions under which the stability of the closed-loop can be guaranteed. This allows to employ nonlinear model predictive control even in the case that the necessary numerical solution time is significant. The presented approach is exemplified considering the control of a continuous reactor.

Investigation of Calibration-Free Resolution Techniques and Independent Component Analysis

E. B. Martin, S. Triadaphillou, I. Wells, J. A. Morris, *University of Newcastle*

In the case of a reaction, most control systems need to be calibrated to give a quantitative result. A number of issues are associated with the development of calibration models to predict the concentration of a product in a reaction. Model development in terms of data collection can be time consuming, a model will be sensitive to changes in process conditions and it will only provide quantitative information about the property of interest – with no information about side reactions and intermediates. Calibration-free resolution techniques provide an alternative approach to the development of a calibration model. They combine spectroscopic measurement coupled with retrospectively mathematical and statistical assumptions and yield spectral profiles and concentration profiles for the unknown mixture. In this paper, a number of calibration free techniques including VARIMAX, ITTFA, Evolving Factor Analysis, Fixed Window Evolving Factor Analysis, SIMPLISMA are described and applied to a synthetic spectral data set. The results are compared with the complementary technique of Independent Component Analysis (ICA) in particular FastICA and JADE. The results were comparable with ICA separating the signal from the constituent components successfully.

Stage-Based Multivariate Statistical Analysis for Injection Molding

F.-R. Gao, N.-Y. Lu, Y. Yang, *Hong Kong University of Science & Technology*
F.-L. Wang, *Northeastern University*

A multi-stage based PCA modelling and monitoring approach is demonstrated in this paper to injection molding process, a typical multi-stage batch process. Analysing the changes of process correlation can lead to effective division of a batch process into several "operation" stages, in good agreement with process knowledge. This shows that multi-stage based sub PCA model can be employed not only for effectively process monitoring and fault diagnosis, but also to enhance process understanding.

Nonlinear Control of a Batch Reactor in the Presence of Uncertainties

Y. Samyudia, H. Sibarani, *McMaster University*
P. L. Lee, *Curtin University of Technology*

In this paper, we propose new control design strategies within the Generic Model Control (GMC) framework for tracking the pre-determined temperature profiles of a batch reactor. It is shown by simulation studies that the designed robust GMC controller is able to track the temperature reactor profile reasonably well, and its optimal performance is maintained in spite of large uncertainties.

Modeling and Model Based Feeding Control for *Pichia pastoris* fed-batch cultivation

J.-Q. Yuan, H.-T. Ren, *Shanghai Jiao Tong University*
J.-H. Deng, B.-K. He, L.-M. Ren, *North China Pharmaceutical Company*

A structured kinetic model, which takes account of major metabolic pathways of glycerol and methanol in Pichia pastoris, is presented. Based on the combined kinetic and bioreactor model, feeding profiles of methanol are determined with the aim of maintaining constant specific growth rate during production stage. Compared with the decreasing type of specific growth rate resulted from constant feeding profile in the standard protocol, the constant specific growth rate is believed to be advantageous for improving the productivity. Experimental results indicate that simulations of biomass and protein concentration agree well with the measured data, and the specific growth rates were successfully controlled at various set points.

Feedforward Control of Batch Crystallisers - an Approach based on Orbital Flatness

U. Vollmer, J. Raisch, *Max-Planck-Institut Magdeburg*

This contribution addresses the problem of feedforward control design for batch crystallisers based on moment models. Moment models, which are standard in the crystallisation literature, are shown to be orbitally flat, i.e. they are flat after an appropriate time scaling. The reciprocal of the crystal growth rate serves as the time scaling function such that a new notion of `time' is defined by the increase in crystal length. For any desired final crystal size distribution (CSD) which is compatible with the crystalliser model it is possible, exploiting flatness, to analytically compute the corresponding temperature trajectory.

Combined Real-Time and Iterative Learning Control Technique with Decoupled Disturbance Rejection for Batch Processes

S. J. Qin, I. S. Chin, *University of Texas at Austin*
K. S. Lee, M. Cho, *Sogang University*

A novel stochastic control framework for batch and repetitive processes is proposed. The framework provides a pertinent means to incorporate real-time feedback control (RFC) into iterative learning control (ILC) so that the performance of ILC is virtually decoupled from that of RFC. This is a new advancement since the currently practiced methods for combined RFC and ILC have suffered from the problem that RFC has undesirable effects on ILC such as digression from its convergent track along the run index when there occur run-independent real-time disturbances. Performance of the proposed technique has been demonstrated in two numerical processes.

Results Analysis in a Constrained Real-Time Optimization (RTO) System

T. E. Marlin, W. S. Yip, *McMaster University*

This paper presents a new results-analysis strategy for uncertain real-time optimization (RTO) systems. The key contributions of this paper are in 1) developing a mathematical formulation describing the confidence region of a partially constrained optimum and 2) applying that formulation in deciding whether the optimizer results should be implemented. The confidence region of the unconstrained optimum is mapped to the feasible region defined by the inequality constraints to obtain the confidence region of the constrained optimum. The confidence regions of successive predicted optima are compared to decide if the difference between two optima is statistically significant. The proposed approach is applied to a reactor case study with controlled inequality constraints, substantial reduction in performance was achieved.

Predictive Scheduling of a Penicillin Bioprocess Plant

S. Lau, M. J. Willis, G. A. Montague, J. Glassey, *University of Newcastle*

In this paper a predictive strategy for the reactive scheduling of a multi-stage bioprocessing plant is outlined. In the procedure, the various batch stages of the bioprocess are dynamically re-allocated to the appropriate processing units in response to the biological variability inherent in each stage. Forecasts of the process productivity and consequent completion times for the tertiary stages of industrial penicillin fermentations are used in conjunction with a genetic algorithm to solve the scheduling problem. Initial results using data from a commercial penicillin plant demonstrate that the predictive scheduling framework could deliver increased production and, consequently, major financial benefits.

Modeling and Optimization for High-Throughput-Screening Systems

E. Mayer, J. Raisch, *Max-Planck-Institut Magdeburg*

The problem of cyclic scheduling under the requirement of throughput maximization is considered for a special class of cyclically repeated batch processes. All batches have to follow an identical time scheme. The same resource may be visited more than once by the same batch and time window constraints may be stated by the user. It is shown that the cyclic scheduling problem can be transformed into a mixed integer linear optimization problem. The method's application to High-Throughput-Screening processes is demonstrated.

Variance-Constrained Filtering for Uncertain Stochastic Systems with Missing Measurements

Z.- D. Wang, *Brunel University*
W. C. Ho, *City University of Hong Kong*

In this paper, we consider a new filtering problem for linear uncertain discrete-time stochastic systems with missing measurements. The parameter uncertainties are allowed to be norm-bounded and enter into the state matrix. The system measurements may be unavailable (i.e., missing data) at any sample time, and the probability of the occurrence of missing data is assumed to be known. The purpose of this problem is to design a linear filter such that, for all admissible parameter uncertainties and all possible incomplete observations, the error state of the filtering process is mean square bounded, and the steady-state variance of the estimation error of each state is not more than the individual prescribed upper bound. It is shown that, the addressed filtering problem can effectively be solved in terms of the solutions of a couple of algebraic Riccati-like inequalities or linear matrix inequalities. The explicit expression of the desired robust filters is parameterized, and an illustrative numerical example is provided to demonstrate the usefulness and flexibility of the proposed design approach.

Robust Tuning of Feedback Linearizing Controllers via Bifurcation Analysis

J. Hahn, M. Mönnigmann, W. Marquardt, *RWTH Aachen*

Feedback linearization is a nonlinear controller design strategy that results in an explicit formulation of the feedback control law. This method can result in excellent performance if an accurate dynamic process model is available. However, feedback linearization suffers from a lack of robustness if plant-model mismatch exists. The approach presented in this work analyzes the robustness properties of the closed-loop process with specific regard to the controller tuning parameter. Due to this, it is possible to tune the controller such that robustness over the entire operating region is guaranteed even under the assumption of certain types of model mismatch. This method is illustrated with an example and conclusions about its applicability to more general model and controller formulations are presented.

Closed Loop Properties and Block Relative Gain

J. F. Forbes, V. Kariwala, E. S. Meadows, *University of Alberta*

Block Relative Gain (BRG) is a useful method for screening alternatives for block decentralized control at the design stage. In this paper, we establish the connection between the BRG and closed loop properties like stability, input output controllability, block diagonal dominance and interactions. Based on these results, simple rules for pairing of variables for block decentralized control are proposed.

A Tool to Analyze Robust Stability for Constrained MPC

L. O. Santos, J. A. A. M. Castro, *Universidale de Coimbra*
L. T. Biegler, *Carnegie Mellon University*

A sufficient condition for robust stability of nonlinear constrained Model Predictive Control (MPC) with respect to plant/model mismatch is derived.

This work is an extension of a previous study on the unconstrained nonlinear MPC problem, and is based on Nonlinear Programming sensitivity concepts. It addresses the discrete time state feedback problem with all states measured.

A strategy to estimate bounds on the plant/model mismatch is proposed, that can be used off-line as a tool to assess the extent of model mismatch that can be tolerated to guarantee robust stability. These results are illustrated with a simple nonlinear system.

Relationship between Control-Relevant Nonlinearity and Performance Objective

N. Hernjak, *University of Delaware*
F. J. Doyle III, *University of California, Santa Barbara*
F. Allgöwer, T. Schweickhardt, *Universität Stuttgart*

In this work, the relationship between performance objective and control-relevant nonlinearity is investigated for Hammerstein and Wiener systems with polynomial nonlinearities. Nonlinearity assessment of the systems' inverses augmented with first-order linear filters using a numerical measure of nonlinearity shows that the degree of nonlinearity varies depending on the relative magnitude of the filter time constant as compared to the open-loop time constant, but generally shows increasing nonlinearity with decrease in time constant. Similar assessment of the respective nonlinear internal model control (IMC) structures indicates that the Hammerstein nonlinearity is weakly dependent on the filter time constant while the Wiener nonlinearity is strongly dependent. In regards to IMC design, the results show that the examined systems are representative of two different cases: (i) highly nonlinear open-loop systems that require highly nonlinear control for optimal performance (Hammerstein); (ii) mildly nonlinear open-loop systems that require highly nonlinear control only when high levels of performance are desired (Wiener).

Effect of Process Nonlinearity on Linear Quadratic Regulator Performance

M. Guay, R. Dier, P. J. McLellan, *Queen's University*

The control of linear systems has been extensively studied and the literature provides a very`complete and well--characterized collection of tools for their analysis, monitoring, optimization,and control. As a result, process control engineers focus on linear system presentations to`solve a wide range of control problems. Unfortunately, the reality is that few processes are linear, and therefore the effectiveness of using linear control strategies can be questioned. Nonlinear control strategies have advanced greatly, and are becoming more widely accepted; however, their implementation is impeded by the necessity to either find a suitable Lyapunov function or compute the solution of a nonlinear partial differential equations (PDE). Since the solution of nonlinear PDEs is unviable in most applications, linear approximations are often used to develop a control law that is locally optimum with respect to a user--defined cost functional. In order to test the effectiveness of this approach, it would desirable to develop an index that measures the effect of process nonlinearity on linear controller performance. From a design point of view, such a measure would indicate whether sufficient benefit is available to warrant investment in a nonlinear controller. The objective of this paper is to introduce a new local measure of linear controller performance for linear controllers operating on a nonlinear plant. The measure, called the performance sensitivity measure, quantifies the departures from optimality of a locally linear quadratic regulators. The measure applies to nonlinear systems that admit a controllable and observable linearization. It is shown that the measure can be related to standard minimum variance benchmarking techniques and can therefore be assessed using closed-loop process data in an operating region of interest.

Lower Limit on Controller Gain for Acceptable Disturbance Rejection

S. Skogestad, *Norwegian University of Science and Technology (NTNU)*

The objective of almost all controller tuning rules found in the literature, going back to the classic PID rules of Ziegler an Nichols (1942), is to get the ``fastest'' possible closed-loop response, subject to maintaining stability with reasonable robustness margins. This gives a maximum limit on the controller gain. In practice, however, we often want control to be as smooth and ``slow'' as possible, subject to satisfying some minimum performance requirements. This gives a minimum limit on the controller gain, and the goal of this paper is to derive this minimum limit, when the performance requirements is to achieve a specified level of disturbance rejection. Together with the more traditional tunings rules this results in a range for the acceptable controller gain.

Modified Subspace-Identification Method for Building a Long-Range Prediction Model for Inferential Control

Y.-D. Pan, J. H. Lee, *Georgia Institute of Technology*

In a chemical plant involving a series of processing units, it is beneficial to have a model that can accurately forecast the behavior of downstream variables based on upstream measurements. Such a model can be useful in feedforward and inferential control of the downstream variables to compensate for various upstream disturbances. However, creating such a dynamic model can be very difficult. The conventional multivariable identification approach based on minimizing single-step-ahead prediction error, can result in models leading to poor prediction and control in the described context. To alleviate this difficulty, we propose a modification to the conventional subspace identification method geared towards accurate k-step-ahead prediction, where k is a number chosen according to the estimated dead time. It is shown that the modified subspace identification method can be used in conjunction with the k-step prediction error minimization (PEM). Using an illustrative examples involving six mixing units with a recycle loop, we demonstrate the improvement that is possible from adopting the suggested modification.

Model Identification and Error Covariance Matrix Estimation from Noisy Data using PCA

S. L. Shah, *University of Alberta*
S. Narasimhan, *Indian Institute of Technology*

Principal Components Analysis (PCA) is increasingly being used for reducing the dimensionality of multivariate data, process monitoring, model identification, and fault diagnosis. However, in the mode that PCA is currently used, it can be statistically justified only if measurement errors in different variables are assumed to be i.i.d. In this paper, we develop the theoretical basis and an iterative algorithm for model identification using PCA, when measurement errors in different variables are unequal and are correlated. The proposed approach not only gives accurate estimates of both the model and error covariance matrix, but also provides answers to the two important issues of data scaling and model order determination.

Nonlinear Subspace Model Identification

A. Cinar, J. DeCicco, *Illinois Institute of Technology*

Canonical variates state space (CVSS) modeling is a popular subspace linear model identecation technique. A nonlinear extension of CVSS modelling approach was proposed (DeCicco and Cinar, 2000). The modeling procedure consists of two steps: development of a multivariable nonlinear model for a set of latent variables and the linking of the latent variables to outputs of the process. The nonlinear model is structured like a Generalized Additive Model (GAM) and is estimated with CANALS, a nonlinear canonical variate analysis algorithm. This communication presents the methodology and an illustrative example of chemical reactor modeling using data generated from a detailed polymerization reactor model.

Semi-Batch Trajectory Control in Reduced Dimensional Spaces

J. Flores-Cerrillo, J. F. MacGregor, *McMaster University*

A novel inferential strategy for controlling end-product quality properties using complete trajectories of manipulated variables is presented. Control through complete trajectory manipulation using empirical models only is possible by controlling the process in the reduce space (scores) of a latent variable model rather than in the real space of the manipulated variables. Model inversion and trajectory reconstruction is achieved by exploiting the correlation structure in the manipulated variable trajectories captured by a Partial Least Squares (PLS) model. The approach is illustrated with a condensation polymerisation example for the production of nylon. The data requirements for building the model are shown to be modest.

A Subspace Approach to MIMO Control Performance Monitoring and Diagnosis

S. J. Qin, *University of Texas at Austin*
C. A. McNabb, *Boise Paper Solutions*

In this paper we begin with a state space model of a generally non-square process and derive the minimum achievable variance in a state feedback form. We propose a simple control performance calculation which uses orthogonal projection of filtered output data onto past closed-loop data. Finally, we propose a control performance monitoring technique based on the output covariance and diagnose the cause of suboptimal control performance using generalized eigenvector analysis. The proposed methods are demonstrated on an industrial wood waste burning power boiler.

Multivariate Controller Performance Assessment without Interactor Matrix – a Subspace Approach

B. Huang, R. Kadali, *University of Alberta*

Several methods for multivariate control performance assessment (MPA) with or without using the interactor matrix have been proposed in the literature. They are all equivalent, one way or other, by certain transformations. In this paper a subspace framework for MPA is proposed for the estimation of MVC-benchmark variance for feedback multivariate systems. The merit of the new approach is that we start straight from data, and a performance index is calculated directly from subspace matrices without relying on a parametric dynamic model. In addition, a proof that the proposed solution is exactly the same as that of the conventional approaches is provided. We do not claim that the subspace approach as proposed in this paper requires less a priori knowledge than other methods. In fact, the equivalent information of the interactor matrix or Markov parameters is implicitly buried in the subspace matrices. However, avoiding direct use of the interactor matrix and/or Markov parameter matrices does have an advantage of easier acceptance in practice and reduces an intermediate dynamic modeling procedure.

Nonlinear Feedback Control of a Coupled Kinetic Monte Carlo-Finite Difference Code

R. D. Braatz, E. Rusli, T. O. Drews, D. L. Ma, R. C. Alkire, *University of Illinois at Urbana-Champaign*

Product quality variables for many electronics and materials processes are set at the nanoscale and smaller length scales. Although the control of these processes is of scientific and industrial interest, there is a shortage of feedback controller design methods based on the noncontinuum models that describe such nanoscopic phenomena. In this study, linear, gain-scheduled, and nonlinear feedback controllers are designed for a coupled kinetic Monte Carlo-finite difference code that simulates the manufacture of copper interconnects. The feedback controller designs incorporate a low order stochastic model constructed from the coupled noncontinuum-continuum code.

Optimal Control of Transient Enhanced Diffusion

R. D. Braatz, R. Gunawan, M. Y. L. Jung, E. G. Seebauer, *University of Illinois at Urbana-Champaign*

Moore's law requires a continued shinkage of feature sizes in microelectronic devices such as junction depth. The current technology for the formation of ultrashallow junctions depends on ion implantation. The effectiveness of this method is limited by the need to anneal out the point and/or extended defects generated by ion implantation. Silicon self-interstitial defects can mediate the dopant diffusion during the annealing process, which leads to a significant increase of the junction depth. This phenomenon is known as "transient enhanced diffusion" (TED).

The state-of-the-art in post-implant annealing employs rapid thermal annealing. There exists conflicting experimental evidence on the efficacy of using high heating rates in the annealing process to reduce TED. Recent results tend to confirm the benefit of using high heating rates, which also show that the reduction in the junction depth comes at the expense of an undesired increase in the sheet resistance. The tradeoff in reducing the junction depth without sacrificing the sheet resistance motivates a careful optimization of the post-implant annealing temperature program. This paper focuses on the design of such an annealing program using model-based optimization. Worst-case analysis of the resulting optimal trajectory quantifies the performance degradation with respect to control implementation inaccuracies and model uncertainties.

Application of Reduced-Rank Multivariate Methods to the Analysis of Spatial Uniformity of Silicon Wafer Etching

P. Misra, M. Nikolaou, *University of Houston*
A. D. Bailey III, *Lam Research Corporation*

We provide a smooth introduction to reduced-rank multivariate analysis, and show how it can be used to monitor images of etched silicon wafers. Results from two industrial case studies are presented and discussed.

Real-Time Feedback Control of Carbon Content of Zirconium Dioxide Thin Films Using Optical Emission Spectroscopy

P. D. Christofides, N. Dong, Y. Lou, S. Lao, J. P. Chang, *University of California, Los Angeles*

In this work, we present a methodology for real-time carbon content feedback control of a plasma-enhanced metal organic chemical vapor deposition process using optical emission spectroscopy. Initially, an estimation model of carbon content of ZrO_{2} thin films based on real-time optical emission spectroscopy data is presented. Then, a feedback control scheme, which employs the proposed estimation model and a proportional-integral controller, is developed to achieve carbon content control. Using this approach, a real-time control system is developed and implemented on an experimental electron cyclotron resonance high density plasma-enhanced chemical vapor deposition system at UCLA to demonstrate the effectiveness of real-time feedback control of carbon content. Experimental results of the deposition process under both open-loop and closed-loop operations are shown and compared. The advantages of operating the process under real-time feedback control in terms of higher productivity, reduced process variation and lower carbon content are demonstrated.

Design, Simulation, and Experimental Testing of a Spatially Controllable CVD Reactor

R. A. Adomaitis, J.-O. Choo, G. W. Rubloff, L. Henn-Lecordier, Y.-J. Liu, *University of Maryland*

Most conventional chemical vapor deposition systems do not have the spatial actuation and sensing capabilities necessary to control deposition uniformity, or to intentionally induce nonuniform deposition patterns for single-wafer combinatorial CVD experiments. In an effort to address this limitation, a research program is underway focusing on developing a novel CVD reactor system that can explicitly control the spatial profile of gas-phase chemical composition across the wafer surface. This paper discusses the development of a simulator for the three-segment prototype that has recently been constructed and the results of preliminary experiments performed to evaluate the performance of the prototype in depositing tungsten films.

Model-Based Trajectory Control of Pressure Swing Adsorption Plants

M. Bitzer, K. Graichen, M. Zeitz, *Universität Stuttgart*

Pressure swing adsorption (PSA) plants consist of several fixed-bed adsorbers and are operated as cyclic multi-step processes. PSA processes are used for the separation and purification of gas mixtures. Based on a rigorous distributed parameter model of the considered 2-bed PSA plant, a process control scheme is derived which is composed of a nonlinear feedforward and a linear feedback controller. For the design of the feedforward control, a numerical approach for the inversion of the rigorous plant model is presented. The designed trajectory control is evaluated by use of the PSA plant simulation model.

Control of Gasholder Level by Trend Prediction based on Time-Series Analysis and Process Heuristics

C. Han, Y.-H. Chu, J. H. Kim, *Pohang University of Science and Technology*
S. J. Moon, I. S. Kang, *Pohang Iron and Steel Company*
S. J. Qin, *University of Texas at Austin*

A novel method to control gasholder levels in an iron and steel company with accurate prediction of future trend is presented. Although various gasholders are used to recycle by-product gases generated during iron-making, coke-burning and steel-making process, the capacity of the gasholders are insufficient to handle large amount of the gases. To overcome this problem, tight control of the gasholder level should be conducted by predicting their anticipated changes. However, the current prediction logic cannot show satisfactory results due to the lack of characterization of relevant processes. In the proposed method, time-series modeling and heuristics of industrial operators are used to correctly reflect the process characteristics and deal with unexpected process delays. By applying the proposed method to an off-line data set, a significant reduction of discrepancy between predicted values and actual values has been observed. The method is expected to be adopted in the prediction system of POSCO.

Setting of Injection Velocity Profile via an Iterative Learning Control Approach

F.-R. Gao, Y. Yang, *The Hong Kong University of Science and Technology*

Injection velocity is an important variable that affects the quality of injection molded products. Profiling the injection velocity to keep a constant melt-front-velocity inside the mold throughout the filling to ensure a uniform part is the purpose of this work. Based on a transducer designed in a previous work, the melt-front-position is measured online. An iterative learning control system, designed as the outer loop controller in a cascade fashion, is used to search for optimized injection velocity profile. Experiments show that proposed system works well in ensuring a uniform melt-front-velocity when filling molds with varying geometrical shapes, without the necessity of developing a physically based process model.

Dynamics of Process Networks with Recycle and Purge: Time Scale Separation and Model Decomposition

P. Daoutidis, M. Baldea, *University of Minnesota*
A. Kumar, *GE Corporate Research and Development*

Process networks with recycle are well-known to exhibit complex dynamics and to present significant control challenges, due to the feedback interactions induced by the recycle streams. In this paper, we address the dynamic analysis and control of process networks with recycle and small purge streams used for removal of light inert components (feed impurities and/or reaction byproducts) from the recycle loop. We establish, through a singular perturbation analysis, that such networks exhibit a time scale separation in their dynamics, with the slow dynamics induced by the small amount of inert purged from the recycle loop. We also present a model reduction method for deriving a nonlinear low-order model of this slow dynamics which can be used to rationally address the control of the level of inerts in the network.

Youla-Kučera Parametrisation in Self-Tuning LQ Control of a Chemical Reactor

J. Mikleš, L. Čirka, M. Fikar, *Slovak University of Technology in Bratislava*

One of the most important control problems in the chemical industry is a control of chemical reactors. Chemical reactors represent a typical class of plants with nonlinear behavior. For the most part of theoretical works reference signal is assumed to be from a class of stochastic functions. However, in technologic practice, references belong always to a class of deterministic functions. Moreover, practical needs of control show, that it is not always sufficient to restrict the output and control signals only. Very often, the manipulated variable derivatives should be restricted as well. The solution of such a control problem represents then a non-conventional LQ problem. The contribution deals with the application of self-tuning LQ control of a laboratory continuous stirred tank reactor. The strategy of the linear control system is based on a recursive identification of the dual YK (Youla-Kucera) parameter of the plant and subsequent calculation of a new YK parameter of the controller. This YK parameter is determined via a non-conventional LQ control design where squared derivative of the manipulated variable and control error are considered.

Feedback Control of Industrial Solution Polymerization of Acrylic Acid using NIR Measurements

G. Févotte, N. Othman, *Université Lyon 1*
J. B. Egraz, J. M. Sau, *COATEX*

In situ Near Infrared spectroscopy is used to monitor and control the concentration of monomer in solution polymerization processes. The Partial Least Square optimization technique is used to correlate the NIR spectrum with the concentrations of monomer and polymer in the reactor. Non linear input-output linearizing geometric control is then designed to control the concentration of monomer in the reactor. Controlling the concentration of monomer has a direct influence on the product quality and is very important to ensure the process safety. The control strategy is validated on-line during the solution polymerization of acrylic acid in an industrial pilot-scale reactor.

Data-Driven Modeling of Batch Processes

D. Bonné, S. B. Jørgensen, *Technical University of Denmark*

A one dimensional grid of interdependent linear models obtained from operation data is proposed for modeling repeated finite horizon, nonlinear and non-stationary process operations. Such finite horizon process operations include start-ups, grade transitions, shut-downs, and of course batch, semi-batch and periodic processes. The model grid is identified from data using a novel interpretation of generalized ridge regression that penalizes weighted discrepancies between one linear model and the models in its neighborhood. It is furthermore outlined how different representations of such a model grid may be used off-line as well as on-line, for prediction, monitoring, control, and optimization. Among these representations is a linear time-varying state space model which may be used for design in established linear monitoring and control methodologies.

Two-dimensional Population Balance Modelling of Semi-Batch Organic Solution Crystallization

G. Févotte, F. Puel, *Université Lyon 1*

A population balance model simulates the time variations of two characteristic sizes of hydroquinone particles during crystallization. The population balance equations combined with kinetic models and mass balance equations allowed the simulation of the crystallization of hydroquinone characterized by a rod-like habit. Semi continuous isothermal operations were performed at the lab-scale in the presence of various additive concentrations. Both the experimental supersaturation trajectory and the final bi-dimensional Crystals Size Distribution (CSD) were correctly predicted by the model. The simulated elongation factor characterizing the crystal shape was therefore in agreement with the experimental one. For secondary nucleation, indirect effects were assumed to occur and satisfactory predictions of the final number of fine particles were obtained. A major interest of the two-dimensional model lies in its ability to relate the time variations of the crystal habit : the particles lengthen in the first moments of their growth and then progressively get thicker until the end of the process.

Calorimetric Estimation of Viscosity and Acid Number in Alkyd Reactors

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T. Lopez, S. Pérez, J. Alvarez, *Universidad Autónoma Metropolitana-Iztapalapa*

In the industrial operation of batch alkyd polymerization reactors, the process evolution, and the product quality and variability are monitored by measuring the acidity and the viscosity of a cold (possibly diluted) samples withdrawn from the reactor. The batch is stopped at the maximum yield allowed by the gelation point of the cold product, and this is decided on the basis of these C(cold)-viscosity measurements in conjunction with a plot of C-viscosity versus acid number. In this work is designed and experimentally tested a software sensor that estimates the C-viscosity and the conversion of acid groups on the basis of the continuous measurement of the heat exchange rate between a continuous stirred vessel appended to the reactor and a cooling coil. The identification of the underlying time-varying observability property yields the designs of the heat exchange devise and of the corresponding robust nonlinear geometric observer. The resulting software sensor is experimentally tested in a pilot plant reactor.

State Estimation in Batch Crystallization using Reduced Population Models

S. Motz, S. Mannal, E. D. Gilles, *Universität Stuttgart*

This contribution deals with the design of an observer for state estimation of a batch crystallizer, which is described by a detailed population balance model. Therefore, the rigorous model containing (partial) integro-differential equations is first reduced by applying an integral approximation technique to a model of moments that consists of only a few ordinary differential equations. This reduced model serves then as the basis for the design of a Luenberger type observer. The performance of the observer is finally demonstrated by using the rigorous population balance model for the simulation of the crystallizer plant.

Robust Iterative Learning Control Design based on Gradient Method

S. Liu, T.-J. Wu, *Zhejiang University*

An iterative learning control (ILC) method using both feedback and feedforward actions is proposed for a class of uncertain linear systems to achieve precise tracking control. A sufficient condition for the plant uncertainty and feedback controller, which guarantees the robust convergence of the learning, is given. The procedure of designing the robust algorithm has two steps: At first, the feedback controller with robust performance is synthesized based on H-infinite optimal approach according to the request of the sufficient condition; secondly, the incremental feedforward input signal is derived by gradient method with fixed step size. It is shown that the feedforward action has relation to the adjoint system of the closed nominal system.

Compensator for Internet-based Advanced Control

S.-H. Yang, X. Chen, *Loughborough University*

Internet-based control is becoming next generations of control systems, in which time delay and data loss in Internet transmission are the major obstacles for bringing this control system into a reality. This paper proposes new control architecture in cooperated with two compensators to attack this major difficulty. These two compensators are located in the feedback and feed-forward channels in the architecture in order to compensate the control action and assure the stability of the control system. The novel compensators and control system architecture are illustrated and evaluated through a simulation example by using the DMC control algorithm.

Model-Based Auto-Tuning System Using Relay Feedback

H.-P. Huang, K.-Y. Luo, *National Taiwan University*

An on-line model based autotune system that employes conventional ATV test is proposed. The ATV responses from normalized FOPDT and SOPDT processes are grouped into two zones in a space, which has normalized amplitude and normalized period as coordinates. In terms of the amplitude and the period of constant cycles of an ATV test, model-based tuning rules are also prepared for two types of process, one for FOPDT in one zone and one for under-damped SOPDT in the other zone. Thus, from an ATV test, the amplitude and period of constant cycles are used in an identification step to select tuning rules to be applied to a given process. Then, PID controller settings are computed according to the selected tuning rules. The system can be inplemented as simple as the conventional autotune system, and the resulting control performance is compatible to that from a model-based controller design.

The Explicit Model-Based Tracking Control Law via Parametric Programming

E. N. Pistikopoulos, V. Sakizlis, J. D. Perkins, *Imperial College London*

In this paper two methods are presented for deriving the explicit model-based tracking optimal control law for constrained linear dynamic systems subject to persistent disturbances. The first scheme augmentes explicitely the model dynamics with a set of integral states that are then readily inroporated with a positive definite penalty in the system performance measure. The second scheme employs a state observer for estimating the value of the disturbance and then computes the new state target. Then it shifts accordingly the state and control values to ensure asymptotic tracking. The controller underlying structure in both approaches is derived off-line via parametric programming before any actual process implementation takes place. The proposed control schemes guarantee steady-state offset elimination and optimal performance in the presence of unknown constant uncertainties. Keywords: Model predictive control, parametric programming, process control, integral action, observer.

Discrete Control of Nearly Integrable Two-Dimensional Continuous Systems

S. Blouin, M. Guay, K. Rudie, *Queen's University*

Many manufacturing processes involve an interplay of logical and continuous objectives. Hybrid Control Systems are well-suited for studying interaction between continuous and logical control goals. Here a technique for generating the interfaces of a family of Hybrid Control Systems is presented. This amounts to extracting (untimed and speci ﬁcation-independent) abstractions for a class of non-linear continuous systems satisfying an integrability property. A two-dimensional example illustrates an extension of the technique to a larger class of systems.

Variance Estimation in Multisensor Fusion Algorithm

C.-Q. Zhong, X.-L. Dong, L.-Y. Zhang, Y. Cao, *Dalian University of Technology*

In weighted fusion algorithm for multisensor, the weights are only determined by noise variance and the precision of the variance estimation will affect the performance of the fusion algorithm. An approach of variance estimation for multisensor is presented and proves unbiased in this paper. The recurrence formula for the algorithm is also proposed, and moreover, there is no need for initial values, for which the approach is adaptive and can be used in real-time estimation. A numerical example is given to show the usefulness of the approach.

Respirometry Estimations Based Monitoring of Biological Wastewater Treatment Processes

D.-C. Yuan, L.-P. Fan, H.-B. Yu, *Shenyang Institute of Automation*

A method is presented to monitor wastewater treatment processes by incorporating multivariable principal component analysis (PCA) with the knowledge of respirometry estimations. Respirometry is the measurement of an activated sludge respiration which reflects the oxygen rate consumed by biomass, and can be estimated from dissolved oxygen concentrations. Because dissolved oxygen concentrations which are available at most plants have the quick response time and easy maintenance, respirometry estimations based monitoring strategy has advantages for the fault detection. The improvement of some fault detection indexes are demonstrated through IWA's Benchmark simulations.

Wavelet Packet Images Matching Applied to Noise Faults Diagnosis

C. Lu, G.-Z. Wang, *Tsinghua University*
Q.-G. Qiu, *Dalian University of Technology*

In order to avoid the difficulty of installing vibration sensors and extracting characteristic frequency vectors on the traditional vibration-based abrasion faults diagnosis of main bearing of diesel engine, this paper presents a new approach based on the noise signal of diesel engine and wavelet packet images processing. Based on that, the standard time-frequency distribution images of all fault conditions, including the gap abrasion information of main bearing, can be defined. Correspondingly, a gap abrasion fault diagnosis model of main bearing with images matching is set up. Through comparing the Euclid Distance values between standard fault images and the test image, the model can recognize the gap abrasion condition. The result shows that this method is simple and effective, and makes the best use of fault information.

Performance Monitoring based on Characteristic Subspace

M. Guo, S.-Q. Wang, *Zhejiang University*

In the operation and control of chemical process, automatic data logging systems produce large volumes of data. It is important for supervising daily operation that how to exploit the valuable information about normal and abnormal operation, significant disturbance and changes in operational and control strategies. In this paper, principal component analysis (PCA) is clarified its essence from the view of space, and every different subspace represents different operational mode and process performance. Based on that, distance between two subspaces is calculated to evaluate the difference between them.The method is illustrated by a case study of a fluid catalytic cracking unit (FCCU) reactor-regenerator system.

Abstracts

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Soft-Sensing of the Dry Point of Benzene using PCA and DRBFN

Y.-Q. Chang, F.-L. Wang, *Northeastern University*
F.-R. Gao, *The Hong Kong University of Science and Technology*

Measurements of temperatures and flows and pressures are used to estimate the dry point of the product for the distillation column. The Problem is characterized by the model complication and the strong colinearity between the measurements. In this article, the distributed RBF neural network (DRBFN) and principal component analysis (PCA) are used to develop the soft sensor (PCA-DRBFN model), and PCA is also used for data compressing and validation. Another two models, principal component regression (PCR) soft sensor model and DRBFN soft sensor model, are used to compare the performance with the proposed soft sensor. Simulation shows that the proposed model can be of the specialties of the better estimation quality and the simplified structure.

A Fault Diagnosis Method for Fermentation Process

L.-L. Ma, F.-L. Wang, Y.-B. Jiang, *Northeastern University*
F.-R. Gao, *The Hong Kong University of Science and Technology*

Process fault diagnosis requires the on-line information on process state variables that are often inaccessible in real-time for the processes like a fermentation process. A composite model is proposed, combining a kinetic model of the first principles and a neural network model that models the kinetic model parameters changes, to estimate on line the states . This composite model can retain and enhance the process knowledge, at the same time, avoid the complexity of modeling the entire process by kinetics. The estimated process states from the composite model are then fed to a wavelet network for fault detection and diagnosis. The proposed system is successfully applied to a glutamic acid fermentation process, demonstrating the feasibility and effectiveness of the proposed system.

Multi-PCA Models for Process Monitoring and Fault Diagnosis

L.-L. Ma, Y.-B. Jiang, F.-L. Wang, *Northeastern University*
F.-R. Gao, *The Hong Kong University of Science and Technology*

Multivariate statistical approaches have been proved effective for reducing the dimension of highly correlated process variables and subsequently simplifying the tasks of process monitoring and fault diagnosis. However, for the process with distinctive stages, a single statistical model is not sufficient or even incapable to map the substantive process information. In this paper, multi-PCA models are proposed for promptly detecting faults and improving the exactness of the diagnosis as well. The effectiveness of the approach is demonstrated on a complicated fermentation process.

A Fault Accommodation Control For Nonlinear Processes

Y.-W. Zhang, F.-L. Wang, G. Yu, *Northeastern University*
F.-R. Gao, *The Hong Kong University of Science & Technology*

An active fault accommodation control law is developed for a class of nonlinear processes to guarantee the closed-loop stability in the presence of a fault, based on a neural network representation of the dynamics due to faults. Applications of the proposed design indicate that the fault accommodation control law is effective for a typical nonlinear fermentation process.

A Novel Detection of Vessel Liquid Level based on Echo Identification

Z.-H. Zhang, J.-M. Yuan, *University of Science and Technology Beijing*
W.-Y. Huang, *Southeast University*

A novel non-invasive level detection is developed in the paper for application to processes where high pressure, high temperature, high viscosity, strong corrosion liquid may be involved. The theoretical analysis and experiment suggest that the proposed echo method can measure level well. The key to the success of this detection is the proper extraction of the echo information from noisy waves by using a proper Wavelet Transform.

Multi-Site Performance Monitoring in Batch Pharmaceutical Production

C. W. L. Wong, A. J. Morris and E. B. Martin, *University of Newcastle*
R. E. A. Escott, *GlaxoSmithKline Chemical Development*

A challenge facing the pharmaceutical and chemical industries is how to understand and identify differences in process behaviour where the same product is manufactured at two different sites. A number of approaches based on multi-way principal component analysis are investigated. Pre-screening of the data was initially performed to remove any abnormal data. Batch length equalisation was then achieved through the application of multivariate Dynamic Time Warping (DTW) to the process data. Batch duration was then further reduced by cutting in order to focus on the time period of particular interest. The first approach analysed the data from each site individually. Two combined models were then investigated. In the first model, the global mean and standard deviation for the two sites were removed to give the new data matrix. In the second study, the local mean and standard deviation were removed. The multi-group model approach of Lane et al. (2001) based on the pooled sample variance-covariance matrix was shown to be appropriate for the development of a joint model between the two sites by removing site differences. This development provides a powerful approach for handling the differences between sites, through a data based approach, thus enabling a better understanding of the subtle behaviours in performance between two manufacturing sites.

Process Monitoring of an Electro-Pneumatic Valve Actuator Using Kernel Principal Component Analysis

S.-O. Song, G. Lee, E. S. Yoon, *Seoul National University*

In this paper, an approach for monitoring using a multivariate statistical technique, namely kernel principal component analysis is studied. Kernel principal analysis has recently been proposed as a new method for performing a nonlinear form of principal component analysis (PCA). The basic idea of kernel PCA is to first map the input space into a feature space via a nonlinear map and then compute the principal components in that feature space. For the process monitoring application, reconstructed input patterns can be obtained by approximating the pre-image of scores in feature space. An application study of an electro-pneumatic valve actuator in a sugar factory is described. The results show that the kernel PCA approach can detect several actuator faults earlier than linear PCA This study indicates the great potential of Kernel PCA for process monitoring.

Real-Time Application of Scheduling Quasi-Minmax Model Predictive Control to a Bench-Scale Neutralization

Y.-H. Lu, *Georgia Institute of Technology*
Y. Arkun, *KOC University*
A. Palazoglu, *University of California at Davis*

Scheduling quasi-minmax model predictive control is an MPC algorithm developed initially for linear parameter varying (LPV) system, then developed for nonlinear systems. In this paper, real-time application of the scheduling quasi-minmax MPC algorithm onto a bench-scale pH neutralization reactor is presented. The control performance is compared with multi-linear model based MPC with terminal constraint and scheduling PID controller in which tuning parameters are from IMC design.

Fault-Tolerant Control of Process Systems: Integrating Supervisory and Feedback Control over Networks

N. H. El-Farra, A. Gani, P. D. Christofides, *University of California*, *Los Angeles*

This work proposes a methodology for the design of fault-tolerant control systems for nonlinear processes with actuator constraints. The proposed approach is predicated upon the idea of integrating supervisory and feedback control over networks. Initially, a family of candidate control configurations, characterized by different manipulated inputs, are identified. For each control configuration, a bounded nonlinear feedback controller, that enforces asymptotic closed-loop stability in the presence of constraints, is designed, and the constrained stability region associated with it is explicitly characterized. A switching policy is then derived, on the basis of the stability regions, to orchestrate the activation/deactivation of the constituent control configurations in a way that guarantees closed loop stability in the event of control system failures. The switching laws are implemented by a higher-level supervisor that constantly monitors the process and communicates with the various control configurations over a network. The effects of delays in fault detection, network communication and actuator activation are taken explicitly into account in executing the switching logic. The efficacy and implementation of the proposed approach are demonstrated through a chemical process example.

Real-Time Optimization of Distillation Column via Sliding Modes

A. Y. Torgashov, K.-C. Park, H.-C. Choi, Y.-K. Choe, *Samsung Fine Chemicals Co., Ltd.*

The real-time optimization (RTO) system of distillation column has been proposed using sliding modes. On the basis of formulated optimization problem, the parameters for the distillate composition controller are so selected that the condition for the occurrence of sliding modes holds in order to provide a search procedure. An investigation of the transient performance of RTO-system under feed composition disturbances indicated a stable tracking for the shifted optimal distillation operating points.

A Receding Optimization Control Policy for Production Systems with Quadratic Inventory Costs

C.-Y. Song, H. Wang, P. Li, *Zhejiang University*

For stochastic disturbance, such as stochastic demands and breakdown of the system, the production systems is presented as a piecewise deterministic process model. At any given time only one type of product can be produced by the system. A setup (with setup time and cost) is required if production is to be switched from one type of product to another. Preventive maintenance activity is performed for reducing the aging of the system, and the jump rates of the system state depend on the aging of the system. The objective of the problem is to minimize the costs of setup, production, maintenance and the quadratic costs of inventory. The decision variables are a sequence of setups and the production and preventive maintenance plan. According to two time horizons, the original problem is decomposed into two sub-problems. The asymptotic optimality solution of the original problem is constructed via receding optimize the sub-problems. Simulation results show the feasibility of the proposed approach in practice.

Hard Real-Time CORBA (HRTC) for Process Control Systems

S. Galán, M. Rodríguez, R. Sanz, *Universidad Politécnica de Madrid*

Control systems for process plants are complex applications running in several interacting computers with varying degrees of integration. The construction, deployment and maintenance of the software system is a difficult problem and distributed object oriented technology offers a good way to deal with it. The open standard CORBA provides flexible middleware capable of integrating complex applications in heterogeneous environments, but was originally designed with large business applications in mind and is not perfectly suited for the construction of control systems. Even with recent advances in the real-time specification for CORBA, it is only suitable for soft real-time applications and do not deal with the tight requirements of closed control loops. In this paper, the building of a process control testbed to unveil the hurdles toward the goal of CORBA control systems, with both predictable and event-driven transports, is presented. The benefits of such emergent technology are discussed.

A Disaggregation Technique for the Optimal Planning of Offshore Platforms

M. C. A. Carvalho, *University of Sao Paulo*
J. M. Pinto, *Polytechnic University*

There is a great incentive for developing systematic approaches that effectively identify strategies for planning oilfield complexes. This paper proposes an MILP that relies on a reformulation of the model proposed by Tsarbopoulou (UCL M.S. Dissertation, London, 2000). Moreover, a disaggregation technique is applied to the MILP. A master problem determines the assignment of platforms to wells and a planning subproblem calculates the timing for fixed assignments. Results show that the decomposition approach generates optimal solutions for instances of up to 145 wells and 64 platforms in 10 discrete time periods that otherwise could not be solved with a full-scale model.

Analysis and Modeling of Industrial Purified Terephthalic Acid Oxidation Process

S.-J. Mu, H.-Y. Su, R.-L. Liu, Y. Gu, J. Chu, *Zhejiang University*

A mathematic model to predict the concentration of 4-carboxy-benzaldhyde (4-CBA) for an industrial Purified Terephthalic Acid (PTA) oxidation unit is built in this paper. The model is based on a mechanism model from the results of bench-scale laboratory experiment and chemical reaction principle, which is structured into two series ideal CSTR models. Six plant factors are designed to correct the deviation between the laboratory model and the industrial practice. For the existing of substantial time delays between process variables and quality variable, the weighted moving average method is applied to make each variable be in same time slice. The analysis of process data by projection on latent variables of Partial Least Square (PLS) and analysis of Hotelling's T-squared statistic value of Principal Component Analysis (PCA) are gave to discriminate the operating data into normal operating part and load down and load up operating part. At the each operating part, the typical data are selected to regress the plant factors. The proposed model predictive result follows the tracks of the observed value quite well. Compared with the empirical Amoco model, the proposed model is regarded as to be more suitable to be applied to industrial online soft sensor.

Analyzing the Start-Up of Reactive Distillation Columns

F. Reepmeyer, J.-U. Repke, G. Wozny, *Technical University Berlin*

In this paper a simulation model developed for the start up process of a cold and empty reactive distillation (RD) column is presented. The rigoros model is experimentally validated with data from a pilot plant at the department. The sample reaction is a transesterification of a fatty methylester with isopropanol. With the validated model, different start up strategies, known from conventional distillation have been applied. It was found, that the total reflux strategie cannot be recommended for RD processes. Mathematical optimization of the the control variables heating duty, reflux and feed flowrate did not show significant savings in start up time. Alternative strategies utilizing product recycle flows and initial column charges are presented. With these strategies about 80% of the necessary start up time could be saved.

Plantwide Economical Dynamic Optimization: Application on a Borealis Borstar Process Model

W. Van Brempt, P. Van Overschee, T. Backx, *IPCOS*
Ø. Moen, *Borealis*
C. Kiparissides, C. Chatzidoukas, *Aristotle University of Thessaloniki*

A novel plantwide dynamic optimizer PathFinder has been applied to a dynamic model of a Borealis Borstar process. PathFinder optimizes dynamic paths subject to a merely economical criterion. Introduction of process constraints allows for a gradual migration from the currently used transition towards a more optimal transition. Special care has been taken to integrate the optimizer with on-line control tools. The results show a significant improvement in added value during a grade transition.

Fuzzy Neural Network for Predicting 4-CBA Concentration of PTA Process

R.-L. Liu, Y.-X. Wang, H.-Y. Su, S.-J. Mu, Y.-Y. Hu, W.-Q. Chen, J. Chu, *Zhejiang University*

A fuzzy neural network model has been developed to predict the 4-CBA concentration of the oxidation unit in PTA process. Several technologies are used to deal with the process data before modeling. Suitable input variables set has been selected according to prior knowledge, experience and fuzzy curve method. Dead time delay has been considered in the fuzzy neural network model. The simulation results show that the model of the fuzzy neural network is better than that of AMOCO in prediction precision.

Designing Neurofuzzy System based on Improved CART Algorithm

L. Jia, E.-G. Li, J.-S. Yu, *East China University of Science and Technology*

In this paper, a neuro-fuzzy system based on improved CART algorithm (ICART) is presented, in which the ICART algorithm is used to design neuro-fuzzy system. It is worth noting that ICART algorithm partitions the input space into tree structure adaptively, which avoids the curse of dimensionality (number of rules goes up exponentially with number of input variables). Moreover, it adopts density function to construct the local model for every node in order to overcome the discontinuous boundaries existed in CART algorithm. To illustrate the validity of the proposed method, a practical application are done.

Hybrid Control of a Four Tanks System

C. de Prada, S. Cristea, *University of Valladolid*
D. Megías, J. Serrano, *Universitat Autónoma de Barcelona*

Many processes, even being of a continuous nature, involve in its operation signals or rules different from the classical continuous variables represented by real variables and modelled by DAE. In practice they include on/off valves or other binary actuators, are subjected to logical operational rules, or are mixed with sequential operations. As a result, classical control does not fit very well with the overall operation of the plant. In this paper we consider the problem of hybrid control from a predictive control perspective, showing in a practical non trivial example with changing process structure, how the problem can be stated and solved. The process to be controlled has four interconnected tanks. The system operates in different modes according to the value of a set of on/off valves. The paper describes the process, the hybrid model and its associated MPC controller, showing some experimental results.

Temperature Control of Butyl Propionate Reactive Distillation

S.-G. Huang, *National Taiwan University of Science and Technology*
C.-C. Yu, *National Taiwan University*

In this work, we explore the temperature control of n-butyl propionate reactive distillation. Process characteristics of n-butyl propionate are explored and a systematic procedure is proposed for the design of butyl propionate heterogeneous reactive distillation. Control objective is to product specifications: high purity propionate and ppm level of acid. The control structure design procedure consists of the following steps: (1) selection of manipulated variables, (2) determine temperature control trays, and (3) find controller settings. Since two specifications on the bottoms product have to be met and stochiometric balance has to be maintained, we have a 2x2 control problem with two obvious inputs: reboiler duty and feed ratio. The reactive distillation exhibits unique temperature sensitivities and the non-square relative gain (NRG) successfully identifies temperature control trays. It results in an almost one-way decoupled system. Therefore, decentralized PI controllers are employed. Simulation results indicate good control performance can be achieved with simple control strategy.

Design and Control for Recycle Process with Tubular Reactor

Y.-H. Chen, *National Taiwan University of Science and Technology*
C.-C. Yu, *National Taiwan University*

Interaction between design and control for gas-phase adiabatic tubular reactor with liquid recycle is studied. This generic bimolecular reaction, A+B=C, has two important features: (1) stoichimoetiric balance has to be maintained and (2) reactor temperature plays an important role in design and operability. More importantly, it represents a large class of important industrial processes. Optimal reactant distribution can be obtained directly form the simplified TAC equation and effects of kinetics parameters and relative volatilities on this optimality are also explored. The results show that an increased reactor exit temperature leads to a more controllable optimal design while a high activation energy results in a less controllable one. For the operability analysis, two control structures are proposed with three different combinations of TPM. The control structure using the reactor inlet temperature as TPM gives good control performance when the reactant distribution is held constant. However, potential problem may arise as the result of high reactor exit temperature (Tout). For the case of biased reactant distribution, the reactant redistribution provides an extra degree of freedom and this alleviates the high Tout problem. The results presented in this work clearly indicate that simple material and energy balances provide useful insights in the design and control of recycle processes.

Optimal Control of Fluid Catalytic Cracking Unit

Q.-Y. Jiang, Z.-K. Cao, J. Cai, H. Zhou, *Xiamen University*
Z.-L. Chen, C.-L. Wang, X.-L. Chen, M.-B. Deng, *China Petroleum & ChemicalCorporation Guangzhou Branch*

This paper discusses the problem of on-line optimal control of FCCU. First a new optimal control scheme is put forward. Then some key problems to make up this optimal control system and the solving scheme are discussed. Finally, the on-line industrial running results of this system are given.

Modeling and Advanced Process Control (APC) for Distillation Columns of Linear Alkylbenzene Plant

X.-M. Jin, G. Rong, S.-Q. Wang, *Zhejiang University*

Distillation columns are operated in various sequences in a linear alkylbenzene (LAB) complex to separate multi-component mixtures. The columns are key systems influencing the economic performance of the LAB complex, such as product quality, product rate, and utility usage, etc. This paper introduces industrial application of model predictive control (MPC) for the series of columns in a LAB complex, which involves four distillation columns, HF acid stripper, benzene column, paraffin column, and LAB column. The APC system that is consisted of twelve controlled variables, twelve manipulated variables and eight disturbance variables is used to deal with the constrained multivariable control problem of the distillation columns. Firstly, process modeling that includes experimental test and process identification is presented. Then, the construction and implementation of the APC system for the distillation columns are discussed. Industrial application results show that the APC system can maintain the best operation for a long time and realize ultimate operating potential of the distillation columns by reducing the consumption of energy, improving product purity, and minimizing operating cost.

A Robust Iterative Learning Control with Neural Networks for Robot

C. Shao, J. Nie, *Dalian University of Technology*
F.-R. Gao, *The Hong Kong University of Science and Technology*

Using identification of neural networks, a new robust iterative learning control algorithm is proposed in the paper. Combined with feedback control in real time, the neural network is employed to identify the nonlinear system online and to produce the feed-forward actions of iterative learning control algorithm to realize continuous trajectory tracking task for robot. Simulation results demonstrate that the algorithm can not only overcome uncertainties and external disturbances, but also meet the trajectory command with few iterative learning and network training, and thus possess better robustness and control performance.

Robust Stable Adaptive Control of Uncertain Bilinear Plants and It's Application for Distillation Column

C. Shao, G. Luo, *Dalian University of Technology*
F.-R. Gao, *The Hong Kong University of Science and Technology*

A robust stable adaptive control design is considered for a class of bilinear plants with uncertainties of unmodeled high-order dynamics and bounded disturbances. A basic optimal control law is first introduced by the generalized minimum variance control strategy, followed by a modification of introducing the modeling error estimate to the control law. Modified least-squares scheme with a relative bilinear dead zone is then developed to combine with the modified control law to form a novel robust adaptive control algorithm, with minimum priori knowledge of the plant. The resulting closed loop system is proven theoretically to have a zero average tracking error and robust stability with respect to unmodeled high-order dynamics and bounded disturbances. Furthermore, the proposed algorithm is investigated by several numerical examples, and an application in controlling of a distillation column to demonstrate the effectiveness of the robust stable adaptive controller.

Combined Gain-Scheduling and Multimodel Control of a Reactive Distillation Column

B. H. Bisowarno, Y.-C. Tian, M. O. Tadé, *Curtin University of Technology*

Reactive distillation (RD) is a favourable alternative to conventional series of reaction-separation processes. Control of RD is challenging due to its integrated functionality and complex dynamics. Linear PID algorithm is not satisfactory and needs because of the need for adequate retuning over a wide range of operating conditions. Combined gain-scheduling and multimodel control scheme is proposed to handle the nonlinearities of the process. Simulation results show the superior performance of the proposed method to that of a standard PI control.

Constructing Takagi-Sugeno Fuzzy Model based on Modified Fuzzy Clustering Algorithm

Z.-Y. Xing, L.-M. Jia, T.-Y. Shi, Y. Qin, Q.-H. Jiang, *China Academy of Railway Science*

Gath-Geva fuzzy clustering algorithm is a nonparallel fuzzy clustering algorithm and is not easy to get a suitable and interpretable fuzzy set. The outputs of the Takagi-Sugeno fuzzy model can influence the input space partition. Neglecting this influence increases the identification error. In this paper, a modified Gath-Geva fuzzy clustering algorithm is introduced to solve these problems. Together with weighted least square method, we construct Takagi-Sugeno model to identify non-linear system. The identification of the glass oven demonstrated the effectiveness of the proposed method.

Nonlinear Predictive Functional Control based on Artificial Neural Network

Q.-L. Zhang, L. Xie, S.-Q. Wang, *Zhejiang University*

An Artificial Neural Network (ANN) is an adequate tool for modeling nonlinear systems and can be applied straightforward in the predictive functional control. New structure of ANN multi-step prediction that is different from cascade or parallel is presented, at the same time, the nonlinear predictive functional control using this ANN model has been developed in this paper. The useful of this control strategy is evaluated by applying it to a Continuous Stirred Tank Reactor (CSTR). The simulation results indicate that it is more effective than PID control.

Computational Intelligence (CI) Self-Adaptive PID (CISAPID)

M.-Z. Yi, Y. Qin, L.-M. Jia, *China Academy of Railway Sciences*

A new method for Computational Intelligence (CI), CI formulated with Analytic Functions and Logics, is given, and a new PID controller ?CISAPID is put forward. CISAPID take the strategy attempt to incarnate but not to realize or imitate the complex thinking and behaviour of human being. The constitution ?principle and qualitative arguments tuning experience of CISAPID are analysed in detail. Simulation and practical application show that the performance of CISAPID is better than that of general PID.

Robust Stability Analysis for Descriptor Systems with State Delay and Parameter Uncertainty

S.-Y. Xu, J. Lam, *University of Hong Kong*
C.-W. Yang, *Nanjing University of Science and Technology*

This paper considers the problem of robust stability analysis for continuous descriptor systems with state delay and structured uncertainties. A computationally simple approach to test the stability of descriptor delay systems is proposed. Based on this, we developed a sufficient condition which guarantees that the perturbed descriptor delay system under consideration is regular, impulse-free and stable for all admissible uncertainties. An example is provided to demonstrate the application of the proposed approach.

Zone Model Predictive Control Algorithm Using Soft Constraint Method

Z.-H. Xu, J. Zhao, J.-X. Qian, *Zhejiang University*

A zone model predictive control algorithm is proposed and developed through the soft constraint method. The estimation of zone violation is avoided; as a consequence the selection of the approximate setpoint when the control variable violates its zone constraint is skipped. To further improve control performance, zone trajectory method is proposed and a parameter is provided to trade off the response performance and model accuracy. The effective performance is proved by the simulation results. The stability of the algorithm is also analyzed.

Evaluation Method and Workbench for APC Strategies

G. Reinig, B. Mahn, M. Boll, *Ruhr University of Bochum*

The large number of various advanced control strategies (e.g. Model Predictive Control, Neural Networks or Fuzzy Control) and the lack of a practically usable selection methodology make it very difficult to choose an appropriate strategy for a given plant. In order to support the selection of proper control strategies and products from the viewpoint of industrial application a set of relevant evaluation criteria is developed. These comprise five groups of items: identification and tuning, implementation, control performance, robustness and integrity, usability. A flexible and expandable test environment (workbench) is created. The workbench is the platform for detailed (rigorous) dynamic models, DCS basic controllers and the APC algorithms / products. OPC is used as the communication standard to link the heterogeneous components. The evaluation approach and workbench are demonstrated for PID based and commercial Model Predictive Controllers at some typical process units and plants (binary distillation, Tennessee Eastman Challenge process, Debutanizer/Depropanizer, Deviding Wall Column).

Non-Fragile PID Stabilizing Controller on Second-Order Systems with Time Delay

J.-M. Xu, L. Yu, *Zhejiang University of Technology*

Based on an extension of the Hermite-Biehler Theorem to the quasipolynomial stability problem, this paper studies the problem of stabilizing a second-order plant with dead time via a PID controller. The region in PID parameters space for the closed-loop stability is given. For a feasible proportional gain (kp), the region of all the admissible integral gains (ki) and derivative gains (kd) is a convex polygon. The PID controller design is formulated as a convex optimization problem of load disturbance rejection with constraints on stability and non-fragility, which can be solved by using existing linear programming techniques.

A Method of Controlling Unstable, Non-Minimum-Phase, Nonlinear Processes

C. Panjapornpon, M. Soroush, *Drexel University*
W. D. Seider, *University of Pennsylvania*

A method of controlling general nonlinear processes is presented. It is applicable to stable and unstable processes, whether non- minimum- or minimum-phase. The control system includes a nonlinear state feedback and a reduced-order nonlinear state observer. The application and performance of the control method are shown by implementing the control method on a chemical reactor with multiple steady states. The control system is used to operate the reactor at one of the steady states, which is unstable and non-minimum-phase.

Design of a Sliding Mode Control System based on an Identified SOPDT Model

C.-T. Chen, S.-T. Peng, *Feng Chia University*

In this paper, we consider the issue of designing a model-based control system for the regulation of chemical processes. Based on an identified second-order-plus-dead-time (SOPDT) model, a designed optimal sliding surface and the use of a delay-ahead predictor, a novel and systematic sliding mode control system design methodology is proposed. The convergence property of the closed-loop system is guaranteed theoretically through satisfying a sliding condition and the system performance is examined with some typical chemical processes. Besides, with the concept of delay equivalent, a simple technique is presented such that the proposed sliding mode control scheme can be utilized directly to handle with the regulation control of non-minimum phase processes. Extensive simulation results reveal that the proposed sliding mode controller design methodology is applicable and promising, which provides robust and high control performance for the regulation of chemical processes.

Nonlinear MIMO Adaptive Predictive Control based on Wavelet Network Model

D.-X. Huang, Y.-H. Wang, Y.-H. Jin, *Tsinghua University*

A MIMO nonlinear adaptive predictive control strategy is presented in which the wavelet neural network based on a set of orthogonal wavelet functions is adopted. A nonlinear mapping from the network-input space to the wavelons output space in the hidden layer is performed firstly. Then, the output layer uses a linear structure. Its weight coefficients can be estimated by a linear least-squares estimation method. The excellent statistic properties of the weight parameter estimation can be obtained. Based on developed recursive algorithm, a MIMO nonlinear adaptive predictive control strategy is implemented. A simulated MIMO nonlinear process example shows that the control scheme is effective.

Input-Output Pairing of Multivariable Predictive Control

L.-C. Chen, *GAIN Tech Co.*
P. Yuan, G.-L. Zhang, *University of Petroleum*

Regardless of what predictive control strategy is used, the predictive horizon is the main design parameter. The stability, control performance and robustness of predictive control system are mainly depended on it. For multivariable predictive controller, selection of predictive horizon is an input-output pairing problem. In this paper, Response Index Array, Dynamic Interaction Index Array and Relative Steady-State Index Array are proposed as the criteria for the selection of predictive horizon and pairing. The design procedure for multivariable predictive controller is summed up. As an example, the pairing of a heavy oil fractionator is given. The design has been successfully implemented on several industrial fractionators.

Generalized Predictive Control for a Class of Bilinear Systems

G.-Z. Liu, P. Li, *Liaoning University of Petroleum & Chemical Technology*

A new generalized predictive control algorithm(BGPC) for a kind of input-output bilinear system is proposed in the paper. The algorithm combines bilinear and linear terms of I/O bilinear system, and constitutes an ARIMA model analogous to linear systems. Using optimization predictive information fully, the algorithm carries out multi-step predictions by recursive approximation. The heavy computation of generic nonlinear optimization is avoided with control law of analytical form being used to the non-minimum phase bilinear systems. Simulation results show the effectiveness of the algorithm and the performance of the algorithm is better than linear generalized predictive control (LGPC).

Nonlinear Model Predictive Control using a Neural Network

R.-D. Zhang, P. Li, *Liaoning University of Petroleum & Chemical Technology*

In this paper, a neural network model-based generalized predictive control for a class of nonlinear discrete-time systems is presented with the local linearization of nonlinear activation function and applied to a nonlinear system. Using the Taylor expansion method, the algorithm converts the nonlinear multi-step predictions into a series of local linear multi-step predictions and uses linear GPC method to gain the control law. Compared to some previous algorithms, the method does not need any assumptions and it also avoids the shortcomings of some past nonlinear multi-step predictive algorithms. For example, it can give a direct and effective multi-step predictive method and avoids the complicated nonlinear optimization. In the algorithm, unlike some other algorithms, only one BP neural network is used, so the computation burden is not very serious. A simulation result is also presented in the article, evidencing that the controller presents a fairly good performance.

Process Optimization and Control under Chance Constraints

P. Li, M. Wendt, H. Arellano-Garcia, G. Wozny, *Technische Universität Berlin*

We propose to use chance constrained programming for process optimization and control under uncertainty. The stochastic property of the uncertainties is included in the problem formulation. The output constraints are to be ensured with a predefined confidence level. The problem is then transformed to an equivalent deterministic NLP problem. The solution of the problem has the feature of prediction, robustness and being closed-loop. In this paper, the basic concepts and solution strategies are discussed to illustrate the potential for optimization and control under uncertainty.

Since the uncertainty properties are taken into account, the solution of the problem is a decision a priori. A predefined probability to satisfy the constraints will be held under the uncertainty and thus the decision is robust. Moreover, the solution provides a comprehensive relationship between the performance criterion and the probability level of satisfying the constraints. Thus one can decide on proper actions which will result in a desired compromise between profitability and reliability. In this way, conservative or aggressive decisions, which may have been made so far, can be prevented. We have solved linear dynamic, nonlinear steady-state and nonlinear dynamic chance constrained problems and applied these approaches to several optimization and control applications.

Adaptive Extremum Seeking Control of Nonisothermal Continuous Stirred Tank Reactors

M. Guay, *Queen's University*
D. Dochain, *Université Catholique de Louvain*
M. Perrier, *Ecole Polytechnique de Montréal*

In this paper, we present an adaptive extremum seeking control scheme for nonisothermal continuous stirred tank reactors. We assume limited knowledge of the reaction kinetics. An adaptive learning technique is introduced to construct an optimum seeking algorithm that drives the system states to optimal equilibrium concentrations of the reaction mixture. Lyapunov's stability theorem is used in the design of the extremum seeking controller structure and the development of the parameter learning laws. Under mild assumptions, the resulting controller is an output-feedback controller. the performance of the technique is demonstrated with the van de Vusse reaction.

On the Use of Controller Parameterization in the Optimal Design of Dynamically Operable Plants

K. G. Dunn, C. L. E. Swartz, *McMaster University*

This paper explores some issues pertaining to the use of Q--parametrization in the optimal design of dynamically operable plants. An optimization--based plant design formulation in which a discrete-time implementation of the controller parametrization is embedded, is described. Its application is demonstrated through a reactor case study in which the resulting design is compared against that obtained using PI control. Differences in results obtained are discussed and related to the design problem formulation. The impact of other assumptions, such as the disturbance dynamics, is also discussed.

Improved Performance of Robust MPC with Feedback Model Uncertainty

A. L. Warren and T. E. Marlin, *McMaster University*

Robust model-predictive controllers use an estimate of model uncertainty in the on-line controller calculation and can be overly conservative for some uncertainty descriptions. This paper discusses the various causes of conservative control with particular emphasis given to the concept of ‘closed-loop’ probabilistic predictions. A multi-input-multi-output MPC is proposed in which an off-line, non-convex calculation is used to characterize the closed-loop uncertainty a priori. This uncertainty information is incorporated into a convex, quadratic program resulting in a MPC formulation that can be efficiently solved on-line. A distillation column case study demonstrates the benefits of the proposed robust MPC.

Adaptive Extremum Seeking Output Feedback Control for a Continuous Stirred Tank Bioreactor

N. I. Marcos, M. Guay, *Queen's University*
D. Dochain, *Université Catholique de Louvain*

An adaptive extremum seeking controller is presented for the optimization of the production rate of a continuous stirred tank bioreactor. This controller is saturated outside a domain of interest and a reduced-order high-gain observer is designed to estimate the substrate concentration of the bioreactor. Semiglobal asymptotic stability is proved and recovery of the performance achieved under state feedback is shown when the gain of the observer is sufficiently high. A simulation experiment is given to illustrate the proposed approach.

A BMI-Based Design of Switched PID Controllers

J. Aoyama, K. Konishi, T. Yamamoto, T. Hinamoto, *Hiroshima University*

This paper provides a design method for 2DOF PID controllers including switched PD compensator based on bilinear matrix inequalities(BMIs). Two design specifications based on H_2 norm are formulated in BMIs, and PID parameters can be exactly obtained by solving the BMI problems via branch and bound algorithms. A set of PD compensators can be obtained simultaneously using proposing design method. The most effective parameter is selected out of the set of PD compensator based on the switching criterion which obtained from estimated system conditions using recursive least squares algorithms. Numerical example is also shown.

Hybrid Control: Implementing Output Feedback MPC with Guaranteed Stability Region

P. Mhaskar, N. H. El-Farra, P. D. Christofides, *University of California, Los Anglos*

In this work, a hybrid control scheme that employs switching between bounded control and model predictive control (MPC) is proposed for the output feedback stabilization of linear time-invariant systems with input constraints. Initially, we design a bounded output feedback controller for which the region of constrained closed-loop stability is explicitly characterized and an MPC controller that minimizes a given performance objective subject to constraints. Switching laws are derived to orchestrate the transition between the two controllers in a way that reconciles their respective stability and optimality properties, and guarantees asymptotic closed-loop stability for all initial conditions within the stability region of the bounded controller. The hybrid scheme is shown to provide a safety net for the practical implementation of output feedback MPC by providing a priori knowledge, through off-line computations, of a large set of initial conditions for which closed-loop stability is guaranteed. The proposed hybrid control approach is illustrated through a simulation example.

An Internal Model Control for Max-Plus Linear Systems with Linear Parameter Varying Structure

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H. Goto, K. Takeyasu, *Japan Research Institute*

The max-plus-linear (MPL) system is a state-space description for a certain class of discrete-event-systems that are linear in max-plus algebra, and it has remarkable analogous features to the conventional linear state-space description in the modern control theory. Hence, several control techniques in the modern control theory have been extended so that they could be applied to MPL systems. In the research context, the internal model control (IMC) for MPL systems has been proposed by Boimond et al. and it succeeds to realize feedback control techniques for discrete-event-systems described in MPL systems. In this paper, the IMC control for MPL systems is extended to the case where the controlled systems are given as MPL systems with linear parameter varying structure, which is called LPV-MPL systems. In the LPV-MPL systems, the systems parameters are explicitly represented in the systems description. Hence, the obtained IMC control law can utilize the additive information on the parameters variations effectively when the parameters are measured on-line, or the variation of the parameters are scheduled beforehand.

Hybrid strategy for parameter estimation and PID tuning

L. Wang, D.-Z. Zheng, D.-X. Huang, *Tsinghua University*

Parameter estimation and PID tuning are two crucial issues in control engineering. Classical methods either require some prior information or depend on some rules, especially they are short of generality and their performances are not satisfied in many engineering fields. Although genetic algorithm and simulated annealing approaches have gained much attention and applications during the past decades, it may cause the premature convergence of genetic algorithm and prohibitive time-consumption required for simulated annealing if executing them alone. In this paper, reasonably combining the parallel structure of genetic algorithm with the controllable jumping property of simulated annealing, a class of effective and general hybrid optimization strategy is proposed for parameter estimation and PID tuning. The proposed strategy is easy to be understood and implemented, and only a little pre-needed information is required. Numerical simulation results demonstrate that the hybrid strategy is of effectiveness, robustness on initial states, and adaptability on models or plants, and comparisons show that the hybrid strategy can achieve performances greatly better than those of pure genetic algorithm and classical methods.

Integration of Product Quality Estimation and Operating Condition Monitoring for Efficient Operation of Industrial Ethylene Fractionator

H. Kamohara, A. Takinami, M. Takeda, *Showa Denko K.K.*
M. Kano, S. Hasebe, I. Hashimoto, *Kyoto University*

In this industry-university collaboration, a soft sensor for measuring a key product quality and a monitoring system for testing the validity of the soft sensor were developed to realize highly efficient operation of the ethylene production plant. To estimate impurity concentrations in ethylene products from online measured process variables, dynamic partial least squares (PLS) models were developed. The developed soft sensor can estimate the product quality very well, but it does not function well when the process is operated under unexperienced conditions. Therefore, a monitoring system was developed to judge whether the soft sensor is reliable based on the dynamic PLS model. In addition, simple rules were established for checking the performance of a process gas chromatograph by combining the soft sensor and the monitoring system. The soft sensor and the monitoring system have functioned successfully.

On-Line Lower-Order Modeling Using Fuzzy Systems

A. B. Rad, H. F. Ho, Y. K. Wong, W. L. Lo, *The Hong Kong Polytechnic University*

In this paper, we present a novel on-line approximation technique to find the parameters of a First-Order plus Time Delay (FOPTD) model of higher-order systems based on fuzzy reasoning. Based on the information obtained from the model, the parameters of a PID controller can be adjusted on-line. The performance of this algorithm is verified by simulation studies. The simulated examples demonstrate the feasibility and adaptive property of the proposed algorithm.

A Novel Soft Sensor Modeling for Gasoline Endpoint of the Crude Unit

X.-M. Tian, G.-C. Chen, *University of Petroleum*

This paper presents a novel soft sensor model for identifying the gasoline endpoint of a crude unit. A hybrid model was developed, by combining in series a first principal model with a neural network. A nonlinear observer was designed, based on the prior knowledge of the process, to estimate the composition C of the upper unit. The neural network is used to predict the gasoline endpoint with C and other process parameters as its input. The error between real measurement and the network prediction is feedback for the network correction. Industrial applications of the proposed model indicate that the proposed model is accurate and adaptable.

State and Parameter Estimation through Dynamic Bayesian Forecasting

Z. Lu, E. Martin, J. Morris, *University of Newcastle*

Successful application of model based control and optimisation depends on having good estimates for the system dynamic states and parameters. A multivariate dynamic linear model is developed for the estimation of the states from limited measurements in a non-linear system comprising model uncertainties. Since the noise statistics are rarely available a priori, the noise covariance matrix is commonly treated as a tuning parameter and determined through repeated simulations in previous applications on batch process. For non-linear, time varying processes, the assumption of a constant process noise covariance matrix may not be sufficient to provide sufficiently accurate estimation. Using a fixed value of noise statistics can lead to poor estimation or potentially result in filter divergence. In this paper Monte Carlo simulations are used to obtain the time-varying noise covariance matrix from the information drawn from the prediction errors and updating information. The methodology eliminates the need for the tuning of the process noise covariance matrix. The non-diagonal and time-varying covariance matrix is obtained on-line in contrast to a diagonal and constant covariance matrix.

Heat Transfer in a Cable Penetration Fire Stop System

S.-P. Kwon, J. Cho, S.-O. Song, W. Kim, E. S. Yoon, *Seoul National University*

In this work the dynamic heat transfer occurring in a cable penetration fire stop system built in the firewall of nuclear power plants is three-dimensionally investigated to develop a test-simulator that can be used to verify effectiveness of the sealants. The dynamic heat transfer can be described by a partial differential equation (PDE) and its initial and boundary conditions. For the shake of simplicity PDE is divided into two parts; one corresponding to the heat transfer in the axial direction and the other corresponding to the heat transfer on the vertical layers. Two numerical methods, SOR (Sequential Over-Relaxation) and FEM (Finite Element Method), are implemented to solve these equations respectively. The axial line is discretized, and SOR is applied. Similarly, all the layers are separated into finite elements, where the time and spatial functions are assumed to be of orthogonal collocation state at each element. The heat fluxes on the layers are calculated by FEM. It is shown that the penetration cable influences the temperature distribution of the fire stop system very significantly. The simulation results are shown in the three-dimensional graphics for the understanding of the transient temperature distribution in the fire stop system.

Modeling of Metabolic Systems using Global Optimization Methods

E. P. Gatzke, *University of South Carolina*
E. O. Voit, *Medical University of South Carolina*

This paper considers the metabolic engineering problem of dynamic modeling in complex biological systems. New areas under consideration include dynamic system modeling of metabolic systems using a Generalized Mass Action (GMA) representation. The modeling problem will be presented as a nonconvex global optimization problem to be solved using deterministic optimization techniques. Advanced control and estimation methods can be devised based on the input-output model of the nonlinear dynamic system. A ve-state fermentation pathway is considered using global optimization techniques for modeling and a discrete-time GMA formulation.

A State-Shared Modeling Approach to Transition Control

Z.-H. Tian, K. A. Hoo, *Texas Tech University*

A rigorous theoretical derivation of a state-shared model structure for multiple-input multiple-output (MIMO) systems is proposed. When a nonlinear system transitions in a large operating space, this state-shared modeling approach can be used to approximate the nonlinear system, such that effective model-based controllers can be applied. A MIMO nonlinear reactor system illustrates the proposed approach.

Temperature Control of the Batch Polypropylene Reactor by ADRC

Y.-Q. Wang, X.-F. Zhu, *South China University of Technology*

A new control method called Active-Disturbance Rejection Controller (ADRC) is proposed for temperature control of a batch polypropylene reactor in this paper. This controller is mainly composed of three parts, i.e. ¡°extended state observer¡± (ESO), input reference signal tracking-differentiator (TD) and a non-linear state error feedback (NLSEF) control law. The simulation results have shown that ADRC can obtain quite good performances with the process uncertain. As the control algorithm in DCS ADRC is developed and tested for a batch polypropylene reactor in a local Petro-Chemical plant. The experiment results have indicated that the controller can give much better dynamic responses than the other control algorithms conducted several years ago.

Fermentation Batch Process Monitoring by Step-By-Step Adaptive MPCA

N. He, L. Xie, S.-Q. Wang, J.-M. Zhang, *Zhejiang University*

Multi-way principal component analysis (MPCA) has been successfully applied to the monitoring of batch and semi-batch processes in most chemical industry. A new approach is presented to overcome the method MPCA s need for estimating or filling in the unknown part of the process variable trajectory deviations from the current time until the end. The approach is based on the Multi-block PCA method and processes the data in a sequential and adaptive manner. The adaptive rate is easily controlled by a parameter that represents the similarity between current and past data. The method is evaluated on industrial fermentation process data and is compared to the traditional MPCA. The method may have significant benefit when monitoring multi-stage batch process where the latent vector structure can change at several points during the batch.

Improved Operation of a Batch Polymerization Reactor through Batch-To-Batch Iterative Optimization

Z.-H. Xiong, J. Zhang, *University of Newcastle*

A batch-to-batch iterative product quality optimisation control strategy for a batch polymerisation reactor is proposed. Recurrent neural networks are used to model the dynamic behaviour of product quality variables. Model-plant mismatches and unknown disturbances are reflected in the model prediction errors. The repetitive nature of batch processes enables this information being discovered from previous batches and used to improve the current batch operation. Recurrent neural network predictions for the current batch are modified using prediction errors in previous batches. Because modified model errors are gradually reduced from batch to batch, the control trajectory gradually approaches to the optimal control policy and tracking errors also converge. The proposed scheme is illustrated on a simulated batch polymerisation reactor.

Kappa Number Prediction by Hybrid Model for Batch Pulp Cooking Process

Y. Li, J. Zhang, X.-F. Zhu, D.-P. Huang, *South China University of Technology*

In batch pulp cooking process the wood chips are converted into pulp by lignin dissolution in cooking acid. The percentage of non-dissolved lignin is often expressed by so called Kappa number. To obtain desired quality of the pulp, Kappa number of the pulp should be decreased to the desired value at the end of batch cycle. Since reliable on-line commercial sensors of Kappa number are still unavailable, developing the soft sensor for measuring Kappa number in batch pulp cooking process is of practical significance. In this paper, a kinetic hybrid model is developed to predict the Kappa number for the batch cooking process. The effectiveness of the proposed hybrid model can be illustrated by the predicted errors for a actual cooking process.

A Modular Batch Laboratory Process

R. Olsson, K.-E. Årźen, *Lund Institute of Technology*

In this paper a new batch laboratory process is described. The process can be used stand-alone for illustrating the control problems associated with single-unit batch control. It is also possible to connect several processes together to form a multi-purpose batch cell. Used in this way the process can be used in teaching laboratories on recipe-based batch control and scheduling of batch processes. The use of the process in process control education is described in the paper.

The process is inexpensive, modular, and portable. The process is small enough to fit on the desk beside the PC used for the control system. The process can be connected to a laptop using a RS-232 serial line, which makes it easy to use the process at lectures and presentations.

Using Optimization to Detect Snowball Effects

Thomas J. McAvoy, *University of Maryland*

In process plants with recycle streams some level control architectures are inoperable. Their use leads to large excursions in manipulated and/or controlled variables and this behavior has been termed the snowball effect. The snowball effect is a steady state phenomenon and it can be analyzed using steady state process models. In this paper a steady state mixed integer nonlinear programming (MINLP) approach is used to analyze for large excursions in process variables. This MINLP approach can be used to detect the likely occurrence of a snowball effect in a plant and to develop control architectures that can avoid this problem. The optimization-based approach is illustrated on a three-reactor three-distillation column plant taken from the literature.