List of Abstracts

Tip: all blue highlighted paper identifiers are a direct link to the corresponding papers; for the black identifiers there is no full paper available.

MoPlenary-MT5 Room ZVH
Plenary Session 1 (Plenary Session)
Chair: Georgakis, Christos Tufts Univ.

09:00-10:00 MoPlenary-MT5.1
Architectures, Modularity and Robustness in Networked Control Systems
Baras, John S. Univ. of Maryland

Networked control systems have become ubiquitous. The proliferation of information technology components and in particular networked embedded systems, has opened up new ways to connect systems, processes and agents, for better performance in many applications including manufacturing processes, chemical and biochemical processes, aerospace and automotive systems, communication, sensor and actuator networks. These distributed systems pose fundamentally new challenges as they collaborate to execute the basic "sense-decide-actuate" cycle of control systems, because the sensing, decision-making and actuation elements are not collocated and because they coordinate their activities through a network in a distributed asynchronous (at least partially) manner. Networked control systems are essentially distributed hybrid systems with multiple space-time scales and feedback loops. We review recent advances in this challenging and emerging area. We first describe a novel framework for modeling and analysis of dynamic networked systems that utilizes several interacting dynamic hypergraphs. The simplest of the new class of models utilizes two hypergraphs: the collaboration one and the communication one. The collaboration hypergraph describes the time varying relation of collaboration between the systems. That is it answers the question: who has to collaborate with whom and when. The communication hypergraph describes the time varying communications that occur between the systems. That is it answers the question: who has to communicate with whom and when. We describe a novel path-oriented characterization of these activities in networked control systems. We describe how multi-criteria optimization problems can be formulated and solved within this framework using a combination of algebraic and analytic tools. We next present a new fundamental way for analyzing networked control systems as networks of collaborating agents. The new fundamental view is that agents in such a network are dynamic entities that collaborate because via collaboration they can accomplish objectives and goals much better than working alone, or even accomplish objectives that they cannot achieve alone at all. Yet the benefits derived from such collaboration require some costs (or expenditures), for example due to communications. Or in equivalent terms, the collaboration is subject to constraints such as energy,

communication, trust, organizational relations and structures. Understanding and quantifying this tradeoff between the benefits versus the costs of collaboration, leads to new methods that can be used to analyze, design and control/operate networked control systems. We develop a dynamic constrained coalitional games mathematical framework, which results in dynamic processes characterizing the evolution of the network over time, the so-called network formation process. We demonstrate how the metrics of benefit and cost control the dynamics, their convergence or divergence, and the structure of the resulting equilibria (i.e., generated networks). We demonstrate how system architectures emerge from these considerations and show that some special network topologies are efficient from these benefits versus costs tradeoffs. Next we describe recent advances in model based systems engineering as a most promising new methodology for managing system complexity and for the development of quantitative methods and toolset frameworks for system synthesis so as to meet requirements. We will show how components and compositional system architectures emerge from these considerations. We combine these three fundamental methodologies for the analysis of distributed optimization problems, the emergence of modules and components, characterizing networked systems robustness, investigating compositionality and distributed algorithm performance versus network topologies. Applications in various areas including process control, biology, swarm optimization will illustrate the basic ideas and algorithms.

MoKeynoteT6 Room ZVH
Keynote Session 1 (Semi-Plenary Session)
Chair: Parker, Robert S. Univ. of Pittsburgh

10:20-10:50 MoKeynoteT6.1
Modeling, Control and Inversion of Multi-Phase Equilibrium Reactor Systems
Aggarwal, Mohit Air Products
Sukumar, Balaji Carnegie Mellon Univ.
Ydstie, B. Erik Carnegie Mellon

We propose a simplified modeling approach for multi-phase reactor systems. The model can be used to determine system characteristics, explore parameter sensitivity and test control strategies. The model is based on the thermodynamic equilibrium assumption and invariant inventories to make it computationally inexpensive. We show that the control approach based on the overall inventories of the system can be effectively used for improved performance of such reactor systems. A multi-phase reactor system - the vapor recovery reactor used in carbothermic aluminum reduction process is considered to demonstrate the efficacy of the proposed modeling and control approach.

MoKeynoteT7 Room A
Keynote Session 2 (Semi-Plenary Session)
Chair: Patwardhan, Sachin Indian Inst. of Tech. Mumbai

10:20-10:50 MoKeynoteT7.1

Partial Enumeration MPC: Robust Stability Results and Application to an Unstable CSTR

Pannocchia, Gabriele Univ. of Pisa
Rawlings, James B. Univ. of Wisconsin at Madison
Wright, Stephen Joseph Univ. of Wisconsin-Madison

We revise in this paper the Partial Enumeration (PE) method for the fast computation of a suboptimal solution to linear MPC problems. We derive novel robust exponential stability results for difference inclusions to show that the existence of a continuous Lyapunov function implies Strong Robust Exponential Stability (SRES), i.e. for any sufficiently small perturbation. Given the fact that the suboptimal PE-based control law is non-unique and discontinuous, i.e. a set-valued map, we treat the closed-loop system, appropriately augmented, as a difference inclusion. Such approach allows us to show SRES of the closed-loop system under PE-based MPC. Application to a simulated open-loop unstable CSTR is presented to show the performance and timing results of PE-based MPC, as well as to highlight its robustness to process/model mismatch, disturbances and measurement noise.

MoMT1 Room ZVH

Batch Process Modeling and Control (Regular Session)

Chair: Garcia-Munoz, Salvador Pfizer Inc.

10:50-11:10 MoMT1.1

Latent Variable Modeling of Batch Processes for Trajectory Tracking Control

Golshan, Masoud McMaster Univ.
Macgregor, John McMaster Univ.

Latent Variable Modeling (LVM) of batch processes is explored from the view point of its application to trajectory tracking model predictive controller design. The ability of the models to capture nonlinearity and time-varying properties of batch processes and to provide a well-behaved description of the process are important characteristics to be considered. Furthermore, the importance of requiring as few batches as possible in the modeling step is considered in the discussion of different models. Two previously proposed approaches for batch process modeling (Golshan et al., 2009b) are investigated from the above points of view and benefits of them as well as their drawbacks are specified. Then, a new approach is proposed to overcome the major shortcoming of each previous approach while capturing their major benefits. The impact of the different latent variable modeling approaches on MPC for trajectory tracking is illustrated using a simulation of a Nylon polymerization process.

11:10-11:30 MoMT1.2

Pre-Analysis of Multi-Batch Bioprocesses Data with Finite Mixture Models in the Reduced Feature Subspace

Lin, Weilu East China Univ. of Science and Tech.
Martin, Elaine Univ. of Newcastle Upon Tyne
Montague, Gary Newcastle Univ.

Multi-batch bioprocesses data, unlike the data from other industries, are highly correlated due to the operation characteristics of the industry. In this work, pairwise Fisher discriminant analysis (FDA) is successfully utilized to reveal the similarity between two batches. In order to handle the mixture pattern for the data projected into the reduced feature subspace represented by the first several generalized eigenvectors, the finite Gaussian mixture model is adopted here to calculate the confidence region of each mixture. There are several challenges facing application engineers when estimate finite mixture models (FMMs), such as initialization of the expectation-maximization (EM) algorithm and determination of number of mixtures. In this work, an initialization method based on the uniform prior distribution assumption and a new method to determine the number of components of FMMs based on estimated density histogram are proposed. The utility of the proposed method has been demonstrated in simulation studies. Combined with the pairwise FDA, the method has been successfully applied to a large scale multi-batch bioprocess data set.

11:30-11:50 MoMT1.3

Latent Variable MPC and Its Consistency in Temperature Control of Batch Processes

Shamekh, Awad The Univ. of Manchester, UK
Lennox, Barry Univ. of Manchester

In this work, further investigation has been made to verify the consistency of the latent variable MPC (L-MPC) in reactor temperature control of an exothermic batch process. The paper analyzes the LV-MPC control law derivation and its performance within batch process applications. The article considers both constrained and unconstrained applications.

11:50-12:10 MoMT1.4

Optimizing Batch Crystallization Cooling Profiles: The Design of Dynamic Experiments Approach

Fiordalis, Andrew Tufts Univ.
Georgakis, Christos Tufts Univ.

A new data-driven methodology for optimizing time-variant profiles in batch processes without the need for a first-principles model is applied to a batch cooling crystallization to find the optimum cooling trajectory that minimizes the total amount of nucleation during the crystallization. The method, Design of Dynamic Experiments (Georgakis, 2009), is an extension of the classical Design of Experiments approach and can be applied to any process where time-variant profiles, typically batch and semi-batch operations, are important for optimizing key aspects of the process. As a data-driven approach with no first-principles model required for process optimization, this methodology may be particularly useful for complex processes for which no knowledge-driven model exists.

12:10-12:30 MoMT1.5

Data Fusion for Enhanced Fermentation Process Tracking

Yu, Shengnan Newcastle Univ.
Montague, Gary Newcastle Univ.
Martin, Elaine Univ. of Newcastle Upon Tyne

Near-infrared spectroscopy along with process control variables, such as integral of airflow rate and the integral of alkali addition rate can be used as the basis for the monitoring of key analyte concentrations on a fermentation process. Within this paper, sequential data fusion modeling is applied first, embracing both physical and chemical information. Aiming to overcome the limitations of sequential modeling and to compare model accuracy, a novel data fusion methodology based on Partial Least Squares, weighted multivariate calibration, is introduced. The methodologies are applied to data from an industrial fermentation process and it is shown that the data fusion method results in a 50% improvement in the Root Mean Square Error of Cross Validation (RMSECV) compared to more traditional calibration approaches. An optimisation procedure was then considered in association with spectral window selection (SWS) to attain more accurate data fusion models.

MoMT2 Room A

Modeling and Control of Chemical Processes I (Regular Session)

Chair: Gao, Furong — Hong Kong Univ. of Sci & Tech.
Co-Chair: Kano, Manabu — Kyoto Univ.

10:50-11:10 MoMT2.1

Modelica Based Grade Change Optimization for a Polyethylene Reactor

Larsson, Per-Ola — Lund Univ.
Andersson, Niklas — Lund Univ.
Akesson, Johan — Lund Univ.
Haugwitz, Staffan — Borealis AB / Lund Univ.

This paper presents a dynamic optimization procedure of grade changes of polyethylene production. The optimization is built upon a novel modular Modelica library containing e.g., non-linear DAE models for polyethylene reactors based on models currently used in nonlinear MPC of industrial reactors at Borealis AB. Using Optimica, which extends the Modelica language with constructs for optimization problems, and JModelica.org, a novel framework to translate such optimization problems into NLP problems, grade transition optimization problems can be solved. The solution procedure and a transition example with optimal inputs and outputs are given in the paper showing promising results.

11:10-11:30 MoMT2.2

Rigorous Dynamic Simulator for Control Study of the Large-Scale Benchmark Chemical Plant

Yumoto, Takamasa — Omega Simulation Co., Ltd.
Ootakara, Shigeki — Mitsui Chemical Inc.
Seki, Hiroya — Tokyo Inst. of Tech.
Hashimoto, Yoshihiro — Nagoya Inst. of Tech.
Murata, Hisashi — Toyo Engineering Corp.
Kano, Manabu — Kyoto Univ.
Yamashita, Yoshiyuki — Tokyo Univ. of Agriculture and Tech.

A dynamic simulator for the benchmark vinyl acetate (VAc) monomer production process is introduced. Rigorous first-principles dynamic models of the VAc process are implemented on the commercial software package Visual Modeler (Omega Simulation Co.,Ltd.). The simulator employs pressure flow calculations and considers non-idealities in the process equipment, so that more realistic simulations are made possible, compared with the conventional simulators. The simulator's high performance calculation provides an environment where feasibility and performance of designed control systems can be efficiently evaluated without sacrificing high fidelity of the process model.

11:30-11:50 MoMT2.3

Two-Point Lyapunov Control of Binary Distillation Columns with Four Temperature Measurements

Castellanos-Sahagun, Eduardo — Centro de Investigación en Pol. SA de CV
Alvarez, Jesus — Univ. Autonoma Metropolitana
Baratti, Roberto — Univ. degli Studi di Cagliari
Frau, Andrea — Univ. degli Studi di Cagliari

The problem of controlling binary distillation column effluents by the manipulating the reflux and vapor flow rates on the basis of four temperature measurements is addressed. The problem is motivated by the need of understanding and systematizing two-point control industrial schemes driven by two ad hoc combinations of four temperature measurements (two per section). First, the associated robust nonlinear SF control problem is addressed with passivation by backstepping. Then, on the basis of observability arguments, the behavior of the nonlinear SF controller is approximated with a pair of linear-decentralized OF controllers where: (i) the heat injection (or reflux) rate is adjusted on the basis of a temperature measurement pair in the stripping (or rectifying) section, (ii) the per-section controller consists of a standard PI cascade scheme augmented with P and I elements which enable tuning without primary-secondary dynamic separation via a Lyapunov control design, improving the closed-loop behavior in the sense of an adequate compromise between regulation speed, robustness and control effort. The proposed control design is tested with a representative example through simulations, finding a behavior which outperforms the ones of previous TP control schemes.

11:50-12:10 MoMT2.4

MIQP Formulation for Controlled Variable Selection in Self Optimizing Control

Yelchuru, Ramprasad — NTNU, Trondheim
Skogestad, Sigurd — Norwegian Univ. of Science and Tech.
Manum, Henrik — Norwegian Univ. of Science and Tech.

In order to facilitate the optimal operation in the presence of process disturbances, the optimal selection of controlled variables plays a vital role. In this paper, we present a Mixed Integer Quadratic Programming methodology to select controlled variables c=Hy as the optimal combinations of fewer/all measurements of the process. The proposed method is evaluated on a toy test problem and on a binary distillation column case study with 41 trays.

12:10-12:30 MoMT2.5

Enhanced IMC-Based Load Disturbance Rejection Design for Integrating Processes with Slow Dynamics

Liu, Tao Hong Kong Univ. of Science & Tech.
RWTH Aachen Univ.
Gao, Furong Hong Kong Univ. of Sci & Tech.

By revealing the deficiency of existing internal model control (IMC) based methods for load disturbance rejection for integrating processes with slow dynamics, a modified IMC design is proposed to deal with step or ramp type load disturbance as often encountered in practice. The controller parametrization is based on a two-degree-of-freedom (2DOF) control structure which allows for independent regulation of load disturbance rejection from the setpoint tracking. Analytical controller formulae are given based on classification of the ways by which such load disturbance seeps into the process. It is an obvious merit that there is only a single adjustable parameter in the controller design, which in essence corresponds to the time constant of the closed-loop transfer function for load disturbance rejection, and can be monotonically tuned to meet a trade-off between disturbance rejection performance and closed-loop robust stability. Robust tuning constraints are given correspondingly to accommodate for process uncertainties. An illustrative example is given to show the effectiveness and merits of the proposed method.

MoMT3 Room B

Design, Optimization and Control of Network Systems (Regular Session)

Chair: Gudi, Ravindra IIT Bombay

Co-Chair: Lee, Jay H. Georgia Inst. of Tech.

10:50-11:10 MoMT3.1

Simultaneous Design and Operation Decisions for Biorefinery Supply Chain Networks: Centralized vs. Distributed System

Kim, Jinkyung Georgia Inst. of Tech.

Realff, Matthew J. Georgia Inst. of Tech.

Lee, Jay H. Georgia Inst. of Tech.

We propose an optimization model that enables the selection of biofuel conversion technologies, processing capacities and locations, and the logistics of transportation from the locations of forestry resources to the conversion sites and then to the final markets. A mixed integer linear program (MILP) model is built to solve for (1) the optimal number, locations, and sizes of various types of processing plants, and (2) the amounts of biomass, intermediate products, and final products to be transported between the selected locations, with the goal of maximizing the overall profit under present constraints. It also outputs the cost and profit data associated the selected network in a convenient form for further analysis. The model is tested in the context of designing both distributed and centralized processing system networks based on an industry-representative data set covering the South-eastern region of the United States. We investigate: 1) Which parameters have major effect on the overall economics, and 2) benefits of going to more distributed types of processing networks, in terms of the overall economics and the robustness to demand variations.

11:10-11:30 MoMT3.2

Multi-Objective Optimization Based Robust Sensor Network Design

Kotecha, Prakash Indian Inst. of Tech. Bombay

Bhushan, Mani Indian Inst. of Tech. Bombay

Gudi, Ravindra IIT Bombay

In this article, we propose an explicit integer optimization formulation for the design of reliable and robust (to uncertainty in reliability data) sensor networks. The robustness is achieved by incorporating simultaneous occurrence of different kinds of uncertainty in the failure rate data in the optimization formulation. We show the use of constraint programming to solve these combinatorial problems to global optimality and also evaluate the globally optimal pareto front between robustness and cost of these sensor networks. Such tradeoffs help the designer in making informed choices for the selection of sensor networks. The applicability of the proposed work has been demonstrated on a case study taken from literature.

11:30-11:50 MoMT3.3

Networked Plantwide Process Control with Asynchronous Communication and Control

Xu, Shichao — Univ. of New South Wales
Bao, Jie — The Univ. of New South Wales

The need for economic efficiency and safety has driven the development of large and complex chemical plants. Due to the presence of interactions, controlling such plants are often difficult. This paper aims to address this issue by developing a networked-based process control approach. In this framework, a plantwide process is modeled as network of process units which is controlled by a network of autonomous controllers. The controllers within the network operate with different sampling rates and communicate with each other asynchronously, to allow flexibility and better utilization of communication bandwidth. A key feature of controller network is the connective stability among controllers, which ensures plantwide stability when communication problems such as data packet drop-outs occur. Using the concept of dissipativity, plantwide connective stability and global performance is translated into conditions for which each controller has to satisfy. The controllers are then designed individually to form an autonomous and distributed control system.

11:50-12:10 MoMT3.4

Target Identification in Biological Systems Using Network Connectivity Information from Literature Mining Databases

Guner, Ugur — Georgia Inst. of Tech.
Lee, Jay H. — Georgia Inst. of Tech.
Francone, Omar — Pfizer
Leyfer, Dmitriy — Brandeis Univ.

We address the automated drug target identification problem for pharmaceutical research. It is often the case in pharmaceutical industry to bring a new promising target to clinical trials only to find that it has serious safety concerns or lack of efficacy. A gene downstream or upstream in the pathway can be a remedy, however, finding such an alternative target using existing in-silico or bench tools can be extremely labor-intensive. Recently, increasing amounts of information and observations have been compiled from different areas of biological research and deposited on databases. In this work we propose a novel computational method to quantify indirect relationships between the objects of biological research of interest by using existing relationships from text mining databases to automate the search for novel biological targets. We applied our method to analyze 9575 proteins in Ariadne database and create a rank-ordered list of proteins that are most similar to the original query. We also compared our method with the Jaccard similarity index for link prediction performance. Our method outperformed the Jaccard method in predicting the existing links for 9575 proteins in the database.

12:10-12:30 MoMT3.5

Operational Controllability of Heat Exchanger Networks

Escobar, Marcelo Univ. Federal do Rio Grande do Sul
Trierweiler, Jorge Otávio Federal Univ. of Rio Grande do Sul

Process integration is motivated from economic benefits, but it also impacts on the plant behavior introducing interactions and in many cases making the process more difficult to control and operate. During the operation utility flow rates and bypasses are widely used for effective control of process stream target temperatures, but the number of utility units is usually less than the number of process streams in the network and some bypasses should be selected. This paper addresses the optimal bypass design for heat exchanger networks. It consists in a model-based iterative procedure considering controllability metrics and worst-case disturbance rejection with minimum economic penalty. This is essentially a piecewise linearization approach producing excellent results. The methodology proposed is demonstrated using a case study with 3 different structures, making possible a comparison among different options on a quantitative basis, taking into account the optimal operation attainable with minimum total annual cost. These results clearly point out for the need of a simultaneous framework for design with controllability and profitability. The main goal of this work is to contribute within the field of optimal operation and control of HENs and the definition of the operational controllability concept.

MoMT4 Room C

Fault Detection, Supervision & Safety of Technological Processes (Regular Session)

Chair: Cao, Yi — Cranfield Univ.
Co-Chair: Garcia, Claudio — Pol. School of The Univ. of Sao Paulo

10:50-11:10 MoMT4.1

Fault Detection and Isolation for Multimode Processes with Recursive Principal Component Analysis

Liu, Jialin — Fortune Inst. of Tech.

Contribution plots of the monitored statistics, Q and T2, are investigated to locate faulty variables when the statistics are out of their control limits. It is a popular method for fault isolation; however, it is well known that the smearing out of contributions leads to misdiagnose the faulty variables. Alternatively, the reconstruction-based contribution approach is claimed to guarantee correct diagnosis. It has been examined in this paper that the approach fails to precisely locate faulty variables when encountering multiple sensor faults. A fault isolation chart on principal component (PC) subspace is provided to locate faulty variables for a process with multiple operating regions. The results of the quadruple-tank process simulation show the proposed approach successfully locate faulty variables in a case of multiple sensor faults, as long as the process behavior can be depicted by the scores on the PC subspace.

11:10-11:30 MoMT4.2

Fault Detection Using CUSUM Based Techniques with Application to the Tennessee Eastman Process

Bin Shams, Mohamed — Univ. of Waterloo
Duever, Thomas — Univ. of Waterloo
Budman, Hector M. — Univ. of Waterloo

In this paper, a cumulative sum based statistical method is used to detect faults in the Tennessee Eastman Process (TEP). The methodology is focused on three particular faults that could not be observed with other fault detection methodologies previously reported. Hotelling's-T2 charting based on the cumulative sums of the faults' relevant variables was successful in detecting these faults, however, with significant delay. The speed of detection is further enhanced by retuning the fault's relevant controller at the expense of closed loop performance.

11:30-11:50 MoMT4.3

Valve Friction Quantification and Nonlinear Process Model Identification

Romano, Rodrigo Alvite — Univ. of São Paulo
Garcia, Claudio — Pol. School of The Univ. of Sao Paulo

This paper extends existing methods that jointly estimate the process and friction model parameters, so that a nonlinear process model structure is considered. In

addition, nonlinear optimization is applied to estimate the friction model parameters. The developed estimation algorithm is tested with data generated by a hybrid setup (composed of a real valve and a simulated pH neutralization process), in which the influences of the excitation signal magnitude and of the controller tuning on estimated models are investigated. The results demonstrate that the friction is accurately quantified, as well as "good" process models are estimated in several situations. In addition, the proposed extension presents the advantage of providing reasonable estimates of the nonlinear steady-state characteristics.

11:50-12:10 MoMT4.4

A Branch and Bound Method for Fault Isolation through Missing Variable Analysis

Kariwala, Vinay — Nanyang Tech. Univ.
Odiowei, Pabara-Ebiere — Cranfield Univ.
Cao, Yi — Cranfield Univ.
Chen, Tao — Nanyang Tech. Univ.

Fault detection and diagnosis (FDD) is a critical approach to ensure safe and efficient operation of manufacturing and chemical processing plants. Multivariate statistical process monitoring (MSPM) has received considerable attention for FDD since it does not require a mechanistic process model. The diagnosis of the source or cause of the detected process fault in MSPM largely relies on contribution analysis, which is ineffective in identifying the joint contribution of multiple variables to the occurrence of fault. In this work, a missing variable analysis approach based on probabilistic principal component analysis is proposed for fault isolation. Furthermore, a branch and bound method is developed to handle the combinatorial nature of the problem involving finding the variables, which are most likely responsible for the occurrence of fault. The efficiency of the method proposed is shown through a case study on the Tennessee Eastman process.

12:10-12:30 MoMT4.5

Complete Fault Diagnosis of Uncertain Polynomial Systems

Rumschinski, Philipp — Univ. of Magdeburg
Richter, Jan — Siemens AG
Savchenko, Anton — Inst. for Automation Engineering
Borchers, Steffen — Max Planck Inst. for dynamics of complex Tech. systems
Lunze, Jan — Ruhr-Univ. Bochum
Findeisen, Rolf — Otto-von-Guericke-Univ. Magdeburg

The increase in complexity in process control goes along with an increasing need for complete and guaranteed fault diagnosis. In this contribution, we propose a set-based method for complete fault diagnosis for polynomial systems. It is based on a reformulation of the diagnosis problem as a nonlinear feasibility problem, which is subsequently relaxed into a semidefinite program. This is done by exploiting the polynomial/rational structure of the discrete-time model equations. We assume the measurements of the output and the input to be available as uncertain, but bounded

convex sets. The applicability of the method is demonstrated considering a two-tank system subject to multiple faults.

MoPlenary-AT5 Room ZVH

Plenary Session 2 (Plenary Session)

Chair: Tade, Moses O. Curtin Univ. of Tech.

14:00-15:00 MoPlenary-AT5.1

Solid Oxide Fuel Cell: Perspective of Dynamic Modeling and Control

Huang, Biao Univ. of Alberta

MoPostersT6 Room ZVH
Interactive/Poster Session 1 (Poster Session)
Co-Chair: Alamir, Mazen Gipsa-Lab. (CNRS-Univ. of Grenoble)

15:00-15:30 MoPostersT6.1
Dynamic Behaviour of an HMR Pre-Combustion Gas Power Cycle
Zhao, Lei NTNU
Michelsen, Finn Are SINTEF ICT
Foss, Bjarne A. Norwegian Univ. of Science & Tech.
Aasen, Knut Ingvar Statoil ASA

This paper explores dynamics for control design of a Hydrogen Membrane Reformer (HMR) pre-combustion gas power cycle. For this type of reforming to be competitive to power generation with carbon capture, low costs and emission of CO2 and NOx is required. Further, high operability and robustness is also required. This is achieved through an understanding of the system dynamics and robust control structure design. The paper presents a new dynamic model of the system which is validated against a static model and is the first analysis of dynamic behaviour of the HMR pre-combustion gas power cycle. The paper identifies important dynamic features of the reformer unit and focuses on the responses in outlet temperature and hydrogen concentration of the HMR unit to changes in important candidate inputs. An initial control study explores a simple control scheme for handling important disturbances like feed changes and load changes.

15:00-15:30 MoPostersT6.2
Multi-Resolution Fuzzy Clustering Approach for Image-Based Particle Characterization
Zhang, Bing Louisiana State Univ.
Mukherjee, Rajib Louisiana State Univ.
Abbas, Ali The Univ. of Sydney
Romagnoli, Jose Louisianna State Univ.

This paper presents a novel technique based on combing wavelet transform and Fuzzy C-means Clustering (FCM) for particle image analysis. Through performing wavelet transform on images, the noise and high frequency components of images can be eliminated and the textures and features can be obtained. FCM is then used to divide data into two clusters to separate touching objects. To quantitatively evaluate this method, a case study involving a particle image is investigated. The procedure of selecting optimum wavelet function and decomposition level for this image is presented. 'Fuzzy range' is used as a derived feature for segmentation. The amounts of particles, particle equivalent diameters, and size distribution before and after partition are discussed. The results show that this method is effective and reliable.

15:00-15:30 MoPostersT6.3

Comparison of Nonlinear State Estimation Techniques for Chemical Processes

Shenoy, Arjun V Univ. of Alberta
Prasad, Vinay Univ. of Alberta
Shah, Sirish Univ. of Alberta

Estimation theory finds a wide variety of applications in process engineering. Most chemical processes exhibit highly nonlinear dynamics, and the extended Kalman Filter (EKF)has been widely used to solve the estimation problem in chemical processes. However, it is claimed that the EKF performs poorly when the noise sequences are non-Gaussian(NG). Owing to high nonlinearity of chemical process dynamics, it is likely that innovation sequences are non- Gaussian. Nonlinear estimators such as the unscented Kalman Filter (UKF) and particle filters (PF) have been developed to address the theoretical limitations of the EKF. In this paper, we study the effect of filter assumptions on their practical performance. Different estimation algorithms are applied onto a methyl methacrylate (MMA) continuous stirred tank reactor (CSTR) under different scenarios of state and measurement noise and plant-model mismatch.

15:00-15:30 MoPostersT6.4

Multivariate Process Monitoring Using Classical Multidimensional Scaling and Procrustes Analysis

Mohd Yunus, Mohd Yusri Newcastle Univ. UK
Zhang, Jie Newcastle Univ.

This paper presents a new process monitoring framework using multidimensional scaling. The traditional method of multivariate process monitoring is generally base on principal component analysis (PCA) and is carried out by monitoring the fault detection parameters Hotelling's T2 and squared prediction errors (SPE). Both indexes are derived directly from multivariate scores in the observation sample configurations. This conventional system was found inappropriately used especially in monitoring highly nonlinear multivariate processes leading to a great number of principal components being selected. Alternatively, classical multidimensional scaling (CMDS) is another technique which can be used in compressing multivariate data by using dissimilarity measures for process monitoring. The proposed process monitoring system is developed based on variable relationships and the dissimilarity measures in terms of variable profiles are used in projecting the multivariate scores. A new monitoring index, which is the resultant vector length different between the new and the normal variable profiles, is introduced. Procrustes analysis (PA) is implemented for on-line process monitoring through a moving-window mechanism. The proposed monitoring method is demonstrated on a simulated continuous stirred tank reactor (CSTR) with recycle system. The results show that the proposed system was efficient as well as effective in detecting various abrupt and incipient faults compared to the linear PCA-based scheme.

15:00-15:30 MoPostersT6.5

A New Cost-Optimal and Fault-Tolerant Instrumentation Sensor Network Design Methodology for Chemical Plants

Mohammadnia, Vahid Petroleum Univ. of Tech.
Salahshoor, Karim Tehran Petroleum Univ. of Tech.
Salehi, Shabnam Petroleum Univ. of Tech.

In this paper, an optimal redundant instrumentation sensor network design methodology is presented for complex chemical process plants using a combinatorial particle swarm optimization search (CPSO) engine. The approach, which is more flexible and general in comparison with previous works, aims to minimize cost as a main design factor, similar to the usual trend in the literature. Besides, it caters for fault-tolerance issue as a crucially important feature in the design procedure which has not been addressed sufficiently in the reported research works. For this purpose, weak redundancy degree (WRD) and sensor network reliability (R) are incorporated in the proposed design scheme as three evaluating measures. This enables the designer to maintain a desired fault-tolerant redundancy in the proposed sensor network to cope with a possible set of sensor failures. Thus, the developed CPSO engine searches in a diverse variety of sensor networks to adopt the most fitted one based on the imposed fault-tolerant design constraints. This facilitates the network realization of the fault-tolerance as the most attractive feature which is practically very demanding. Implementation of the proposed design methodology is illustrated in a simulated continuous stirred tank reactor (CSTR) as a benchmark process plant used in a large-scale design to show its effective capabilities.

15:00-15:30 MoPostersT6.6

Closed Loop System Identification Using Virtual Control Approach

Racoski, Bruna Federal Univ. of Rio Grande do Sul
Trierweiler, Jorge Otávio Federal Univ. of Rio Grande do Sul

The identification of closed loop systems has played an important role in the current context, since it reduces the operational costs of the identification process in the testing stage, reducing, for instance, off-spec production. However, in order to obtain the models, special care for treating the data is required. In this work, is presented a study on identification of linear models from closed loops operational data, based on the application of a virtual closed loop in the real loop. It consists of the virtual addition and removal of a controller to the analyzed loop, so as to filter the input of the system in a completely off-line procedure. This paper also proposes modifications on this methodology resulting in an simplification of the virtual filter and in the ways to recover the open loop model.

15:00-15:30 MoPostersT6.7

CLPP: A User-Friendly Platform for Nonlinear Robust Observer Design

Alamir, Mazen — Gipsa-Lab. (CNRS-Univ. of Grenoble)
Bellemain, Pascal — Univ. of Grenoble
Boillereaux, Lionel — ENITIAA
Queinnec, Isabelle — LAAS-CNRS
Titica, Mariana — Univ. of Nantes
Othman, Nida — Univ. Claude Bernard Lyon 1
Cadet, Catherine — GIPSA-Lab. Automatic department
Besancon, Gildas — Ense3, Grenoble INP

In this paper, a new user-friendly platform for robust observer design is presented. The aim of this software is to render the process of observer design as simple as possible for process practitioners and researchers involved in control or supervision tasks. The platform is dedicated to laboratory scale processes in which key variables are not directly measured and therefore need to be estimated. Moreover, model mismatches and uncertainties can be potentially recovered. The tool can also be used to analyze the feasibility of the related inverse problem for a given choice of the sensors, the sampling time, the observation window, etc. making it a precious tool to design the instrumentation of the process. A particularly useful feature for researchers is the possibility to automatically generate a MATLAB S-function that may be connected to the user's own control/diagnosis modules to perform the estimation task. The software is intended to be freely available (by simple request) for research and educational purposes by mid 2010.

15:00-15:30 MoPostersT6.8

A Simple Identification Technique for Second-Order Plus Time-Delay Systems

dos Santos, Joăo B. M. — Univ. Federal de Campina Grande
Barros, Péricles R. — Univ. Federal de Campina Grande

Second-Order plus Time-Delay (SOPTD) models are commonly used to approximate systems in order to tune PID controllers. Simple models are dominating for control design in industrial applications. Several estimation techniques have been developed and applied to controller design. Most estimation techniques are based on least-squares and excitations such as step, square waves and pseudo-random signals. In order to speed up the experiments, simple and short excitations have also been considered. In this paper alternatives are proposed to robustify the estimates in order to obtain a better model around important frequencies. Simulation results are presented to illustrate the techniques.

MoPostersT7 Room A
Interactive/Poster Session 2 (Poster Session)
Co-Chair: Nagy, Zoltan K. Loughborough Univ.

15:00-15:30 MoPostersT7.1
A Continuous Regression Function for the Delaunay Calibration Method
Corona, Francesco Helsinki Univ. of Tech.
Liitiäinen, Elia Helsinki Univ. of Tech.
Lendasse, Amaury HUT
Baratti, Roberto Univ. degli Studi di Cagliari
Sassu, Lorenzo Sartec SpA

The Delaunay tessellation and topological regression is a local simplex method for multivariate calibration. The method, developed within computational geometry, has potential for applications in online analytical chemistry and process monitoring. This study proposes a novel approach to perform prediction and extrapolation using Delaunay calibration method. The main property of the proposed extension is the continuity of the estimated regression function also outside the calibration domain. To support the presentation, an application in estimating the aromatic composition in Light Cycle Oil by Near Infrared spectroscopy is discussed.

15:00-15:30 MoPostersT7.2
Improvements on Model Predictive Control for a Pulp Mill Process
Luppi, Patricio Alfredo Cifasis
Basualdo, Marta S. GIAIP-CIFASIS- CONICET- FRRo-Univ. Tecnológica Nacional
García, Maximiliano P. GIAIP-CIFASIS-CONICET

This work constitutes a contribution to the previous one presented by Castro and Doyle (2004a). They decided the incorporation of four Model Predictive Control (MPC) for specific parts of the complex chemical Pulp and Paper plant to improve its global dynamic and economic performance. Meanly the authors supported the decision of including MPC based on the RGA information. In this paper, a deep analysis about each MPC implementation is performed so as to test if the used methodology could guide efficiently for adopting this kind of decisions. Initially, the study begins with a systematic procedure for adjusting the key MPC tuning parameters. The economic and dynamic performance indexes are evaluated to demonstrate for which specific cases a real benefit can be achieved. The results presented here were obtained through dynamic simulations using the computational benchmark model of 8200 states for the same scenarios evaluated by Castro and Doyle (2004b).

15:00-15:30 MoPostersT7.3

An Explicit/Multi-Parametric Controller Design for Pressure Swing Adsorption System

Khajuria, Harish Imperial Coll.
Pistikopoulos, Efstratios N. Imperial Coll.

Pressure swing adsorption (PSA) is a flexible, albeit complex gas separation system. Due to its inherent nonlinear nature and discontinuous operation, the design of a model based PSA controller especially with varying operating conditions, is a challenging task. This work focuses on the design of an explicit/multi-parametric model predictive controller for a PSA system. Based on a system involving four adsorbent beds separating 70 % H2, 30 % CH4 mixture into high purity hydrogen, the key controller objective is to fast track H2 purity to the set point value of 99.99 %. To perform this task, a rigorous and systematic framework is employed. First, a high fidelity PDAE based model is built to mimic the real operation and understand its dynamic behavior. The same model is also used to derive a linear approximate model by applying suitable system identification techniques. Then a model predictive control step is formulated for the reduced model where latest developments in multi-parametric programming are applied to derive a suitable explicit MPC controller. To test the performance of the designed controller and further refine the tuning parameters, closed loop simulations are performed where the PDAE model developed in earlier step act as virtual plant. Comparisons studies of the derived explicit MPC controller are also performed with conventional PID controllers.

15:00-15:30 MoPostersT7.4

Robust Explicit/Multi-Parametric Model Predictive Control for Box-Constrained Linear Dynamic Systems

Panos, Christos Imperial Coll. London
Kouramas, Konstantinos Imperial Coll. London
Pistikopoulos, Efstratios N. Imperial Coll.

Robust explicit/multi-parametric controllers are designed for constrained, linear discrete--time systems with box-constrained states and inputs, involving uncertainty in the left--hand side (LHS) of the Model Predictive Control (MPC) optimization model. Based on previous results, this work presents a new algorithm that features: (i) a dynamic programming reformulation of the MPC optimization, (ii) a robust reformulation of the constraints that accounts for uncertainty and (iii) a multi--parametric programming solution step where the controls are obtained as an explicit function of the states.

15:00-15:30 MoPostersT7.5

Simplified Modelling and Validation of an Industrial Diesel Hydrodesulfurization Plant

Gomez Sayalero, Elena — Univ. of Valladolid
Sarabia, Daniel — Univ. of Valladolid
Cristea, Smaranda — Univ. of Valladolid
Gutierrez, Gloria — Univ. of Valladolid
de Prada, Cesar — Univ. of Valladolid

A dynamic reduced model of an industrial diesel hydrodesulfurization plant has been developed and validated against plant data. Its purpose is the prediction of the rate of hydrogen consumption, as well as some other critical variables, as a function of the hydrocarbon feed, so as to be integrated in a decision support system aimed at the operation optimization in real time of the refinery hydrogen network. A model which combines first physical-chemical principles with black box elements is proposed. The structure of the model and the calibration procedure are described and validation results are presented.

15:00-15:30 MoPostersT7.6

Control of PM10 Concentrations Over a Regional Domain

Carnevale, Claudio — Univ. of Brescia
Filisina, Veronica — Univ. of Brescia
Finzi, Giovanna — Univ. degli Studi di Brescia
Pisoni, Enrico — Univ. of Brescia
Volta, Marialuisa — Univ. of Brescia

The air quality control is a challenging task, due to nonlinear processes that brings to pollution formation and accumulation in the troposphere. Control theory provides useful methodologies and tools to solve this problem. In this paper we propose a two-objective problem to control particulate matter exposure in the troposphere. The approach is based on the minimization of two objectives, namely the Air Quality Index and the emission abatement costs, depending on the decision variables (precursor emission reductions). In particular, this paper focuses on a novel source-receptor model structure able to describe the link between emission and concentration needed by the optimization procedure to describe the Air Quality Index. The methodology has been applied to Northern Italy, a region affected by PM10 levels, often exceeding the EU limit value established for health protection.

15:00-15:30 MoPostersT7.7

Output-Feedback Stabilization of Continuous Bioreactors in the Presence of Biomass Decay

Savoglidis, Georgios — Univ. of Patras
Kravaris, Costas — Univ. of Patras
Lyberatos, Gerasimos — Univ. of Patras

This paper studies the problem of designing output feedback controllers for enlarging the stability region of continuous stirred microbial bioreactors, in the

presence of biomass decay. A specific application is in anaerobic digestion, where the stability region can be very small if the operating steady state is selected to maximize the methane production rate. A proportional output feedback control law is proposed and the size of the stability region of the closed-loop system is estimated using Lyapunov methods. The results show that, even though stability is not global, the guaranteed stability region is large enough to ensure proper operation of the reactor in the presence of physically realistic disturbances.

15:00-15:30 MoPostersT7.8

A Novel Integrated Ecological Model for the Study of Sustainability

Kotecha, Prakash — Vishwamitra Res. Inst.
Diwekar, Urmila — Vishwamitra Res. Inst.
Cabezas, Heriberto — U.S. Environmental Protection Agency
Templeton, Joshua — U.S. Environmental Protection Agency

In recent years, there has been a growing interest among various sections of the society in the study of sustainability. Recently, a generalized mathematical model depicting a combined economic-ecological-social system has been proposed to help in the formal study of sustainability. This model was based on an assumption of non-limiting supply of energy thereby limiting its applicability to real-world scenarios in which energy plays a very crucial role. In this work, we propose an enhanced model which considers various factors related to energy in an integrated economic-ecological-social framework. As a preliminary use of the proposed model, it has been used to conduct various scenario studies to help understand the complex dynamic relationships between the different entities of the ecosystem and to identify any potential catastrophes or trends.

MoAT1 Room ZVH
Control of Biomedical and Pharmaceutical Processes (Regular Session)
Chair: Parker, Robert S. Univ. of Pittsburgh
Co-Chair: Jorgensen, John Bagterp Tech. Univ. of Denmark

16:30-16:50 MoAT1.1
A Dynamic Model with Structured Recurrent Neural Network to Predict Glucose-Insulin Regulation of Type 1 Diabetes Mellitus
Huang, Hsiao-Ping National Taiwan Univ.
Liu, Shih-Wei National Taiwan Univ.
Chien, I-Lung National Taiwan Univ. of Science and Tech.
Lin, Chia-Hung Chang Gung Memorial Hospital

An artificial neural network (ANN) model for the prediction of glucose concentration in a glucose-insulin regulation system for type 1 diabetes mellitus is developed and validated by using the Continuous Glucose Monitoring System (CGMS) data. This network consists of structured framework according to the compartmental structure of the Hovorka-Wilinska model (HWM), and an additional update scheme is also included, which can improve the prediction accuracy whenever new measurements are available. The model is tested on a real case, as well as long term prediction has been carried over an extended time horizon from 30 minutes to 4 hours, and the quality of prediction is assessed by examining the values of the four indexes. For instant, the overall Clarke error grid (CEG) Zone A value is up to 100% for the 30-min-ahead prediction horizon with update. Therefore, for practical purpose, our results indicate that the promising prediction performance can be achieved by our proposed structured recurrent neural network model (SRNNM).

16:50-17:10 MoAT1.2
Optimal Insulin Administration for People with Type 1 Diabetes
Boiroux, Dimitri Tech. Univ. of Denmark
Finan, Daniel Tech. Univ. of Denmark
Poulsen, Niels Kjřlstad Tech. Univ. of Denmark
Madsen, Henrik Tech. Univ. of Denmark
Jorgensen, John Bagterp Tech. Univ. of Denmark

In this paper we apply receding horizon constrained optimal control to the computation of insulin administration for people with type 1 diabetes. The study is based on the Hovorka model, which describes a virtual subject with type 1 diabetes. First of all, we compute the optimal insulin administration for the linearized system using quadratic programming (QP) for optimization. The optimization problem is a discrete-time problem with soft state constraints and hard input constraints. The computed insulin administration is applied to the nonlinear model, which represents the virtual patient. Then, a nonlinear discrete-time Bolza problem is stated and solved using sequential quadratic programming (SQP) for optimization and an explicit Dormand-Prince Runge-Kutta method (DOPRI54) for numerical integration

and sensitivity computation. Finally, the effects of faster acting insulin on the postprandial (i.e., post-meal) blood glucose peak are discussed.

17:10-17:30 MoAT1.3

Testing PFC Controller on a Well Validated in Silico Model of a Type I Diabetic Patient

Campetelli, German GIAIP-CIFASIS
Zumoffen, David Alejandro CIFASIS-CONICET
Basualdo, Marta S. GIAIP-CIFASIS- CONICET- FRRo-Univ. Tecnológica Nacional
Rigalli, Alfredo aa

Diabetes technology has been focused since three decades ago on developing the artificial pancreas through several closed-loop control algorithms linking glucose measurements and insulin delivery. This work is focused on rigorously analyzing the Predictive Functional Control (PFC) algorithm capabilities for deciding about the correct insulin dosage under everyday circumstances. The study is done by applying the PFC in a recently developed model of the endocrine system, approved by the FDA in 2008, as a substitute to animal trial. The platform used here consists only of a limited number of patients: 10 children, 10 adolescents, and 10 adults. To realistically represent the full closed loop system, a model of a subcutaneous glucose sensor was added and the constraints related to the insulin pump were taken into account by the predictive controller. The performance of the controller, with and without the sensor model, was evaluated by means of the Control Variability Grid Analysis (CVGA) technique and the results were satisfactory in all patients.

17:30-17:50 MoAT1.4

Dynamic Optimization of a Batch Pharmaceutical Reaction Using the Design of Dynamic Experiments (DoDE): The Case of an Asymmetric Catalytic Hydrogenation Reaction

Makrydaki, Foteini Tufts Univ.
Georgakis, Christos Tufts Univ.
Saranteas, Kostas Sepracor, Inc.

The present research work aims to demonstrate the effectiveness of the new methodology of Design of Dynamic Experiments (DoDE) in optimizing an important pharmaceutical reaction. An easily developed response surface model (RSM) is used instead of a hard to develop knowledge-driven process model. The DoDE approach allows the experimenter to introduce dynamic factors in the design, which during the RSM optimization are treated as all the other factors, simplifying the analysis significantly, leading to the rapid optimization of batch processes with respect to time-varying decision variables. The DoDE approach enables the discovery of optimal time-variant operating conditions that are better than the optimal time-invariant conditions discovered by the classical Design of Experiments (DoE) approach. In the present case of the asymmetric catalytic hydrogenation, 24 experiments are conducted for the DoDE approach and the best run results in a

45% improvement comparing to the best run of 17 runs of the DoE approach. This is achieved by applying a decreasing temperature profile during the batch reaction. Optimization of the economic performance index of the process through the respective response surface models defines an optimum operation. The DoDE optimum operation is better than the respective one through the DoE. The DoDE advantage increases as the required quality level for the final product is higher. For the medium quality, the DoDE approach results in an improvement of 30% over the DoE one.

17:50-18:10 MoAT1.5

Experiences in Batch Trajectory Alignment for Pharmaceutical Process Improvement

Garcia-Munoz, Salvador Pfizer Inc.
Polizzi, Mark Pfizer Inc.
Prpich, Andrew Pfizer Inc.
Strain, Cathal Pfizer Inc.
Lalonde, Adam Pfizer Inc.
Negron, Vilmary Pfizer Inc.

In multivariate analysis of batch data, the step known as trajectory alignment (or synchronization) is not solely intended to homogenize the number of samples across batch data. Its primary objective is to standardize the data according to the evolution of the process, irrespective of the number of samples per run. The use of an indicator variable performs both objectives well. Two examples from the pharmaceutical sector are discussed to illustrate the different ways to deal with uneven samples across batches and across variables in the same batch (multi-rate data). Since trajectory alignment is not necessarily trivial, a simple approach based on the covariance matrix of the scores from a variable-wise unfolded data set is used to assess the need to analyze the dynamics of a given process (and hence perform alignment). The presented examples are representative of a broad variety of batch processes that are operated by recipe in the pharmaceutical sector. In our experience, the variables associated with the automation triggers in these recipes are the best indicator variables to use since the resulting alignment scheme can be performed in real-time for monitoring applications.

18:10-18:30 MoAT1.6

Acute Inflammation Treatment Via Particle Filter State Estimation and MPC

Hogg, Justin Univ. of Pittsburgh
Clermont, Gilles Univ. of Pittsburgh
Parker, Robert S. Univ. of Pittsburgh

Models of acute inflammatory disease may have the potential to guide treatment decisions in critically ill patients. Model Predictive Control (MPC) leverages the predictive capacity of a model to determine a control strategy that guides a system to a target trajectory. As applied to acute inflammation, MPC might be used to guide a patient from disease to health by monitoring the patient state, computing and applying an optimal intervention strategy, and updating the strategy if the patient

state diverges from predictions. A key challenge to the application of MPC is mapping the observable patient state into the complete state space of the model. We propose that a Particle Filter (PF) is a suitable algorithm for state estimation in nonlinear models of acute inflammation. As a proof of concept, we apply MPC and PF to the administration of hemoadsorption (HA) treatment in an 8-state model of endotoxemia in rats. In silico tests demonstrate that the PF generates accurate state estimates from limited observations in the presence of noise and parameter uncertainty. Furthermore, we explore the maximal predicted benefits of HA treatment with a standard single column configuration and hypothetical multi-column configurations, where each column has a specificity for a target cytokine. Simulations suggest that two column HA will improve treatment efficacy, but physiological restrictions on HA will limit benefits from higher order configurations.

MoAT2 Room A

Model Predictive Control (Regular Session)

Chair: Christofides, Panagiotis D. Univ. of California at Los Angeles

Co-Chair: Palazoglu, Ahmet N. Univ. of California at Davis

16:30-16:50 MoAT2.1

Lightweight Model Predictive Control Intended for Embedded Applications

Currie, Jonathan AUT Univ.

Wilson, David I. Auckland Univ. of Tech.

The computational demands of Model predictive control (MPC) are well known, and due to its internal constrained optimiser, historically has been ill-suited for embedded controllers designed to tackle high-speed applications. This paper explores the options of developing a low-cost lightweight MPC controller destined for micro-controller or FPGA architectures for modest applications demanding reasonable controller horizons. An object based MPC development tool is introduced and applied to an experimental 4-tank level system to explore the performance of the algorithm.

16:50-17:10 MoAT2.2

Application of IHMPC to an Unstable Reactor System: Study of Feasibility and Performance

Gonzalez, Alejandro, Hernan Inst. of Tech. Development for the Chemical Industry

Adam, Eduardo Inst. of Tech. Development for the Chemical Industry

Marcovecchio, Marian INGAR- Inst. de Desarrollo y Diseńo

Odloak, Darci Univ. of São Paulo – Brazil

Almost all the theoretical aspects of Model Predictive Control (MPC), such as stability, recursive feasibility and even the optimality are now well established for both, the nominal and the robust case. The stability and recursive feasibility are usually guaranteed by means of additional terminal constraints, while the optimality is achieved considering closed-loop predictions. However, these significant improvements are not always applicable to real processes. An interesting case is the control of open-loop unstable reactor systems. There, the traditional infinite horizon MPC (IHMPC), which constitutes the simplest strategy ensuring stability, needs to include an additional terminal constraint to cancel the unstable modes, producing in this way feasibility problems. The terminal constraint could be an equality or an inclusion constraint, depending on the local controller assumed for predictions. In both cases, however, a prohibitive length of the control horizon is necessary to produce a reasonable domain of attraction for real applications. In this work, we propose an IHMPC formulation that has maximal domain of attraction (i.e. the domain of attraction is determined by the system and the constraints, and not by the controller) and is suitable for real applications in the sense that it accounts for the case of output tracking, it is offset free if the output target is reachable, and minimizes the offset if some of the constraints become active at steady-state.

17:10-17:30 MoAT2.3

Two-Stage Multivariable Antiwindup Design for Internal Model Control

Adegbege, Ambrose Adebayo The Univ. of Manchester
Heath, William Paul Univ. of Manchester

Multivariable plants under input constraints such as actuator saturation are liable to performance deterioration due to problems of control windup and directional change in control action. In this paper, we propose a two-stage internal model control (IMC) antiwindup design which guarantees optimal closed loop performance both at transient and at steady state. The two-stage IMC is based on the solution of two quadratic programs (QP). The first QP addresses the transient behaviour of the system and ensures that the constrained closed-loop response is as close as possible to the unconstrained closed-loop response. The second QP guarantees optimal steady-state behaviour of the system. Simulated examples show that the two-stage IMC has superior performance when compared to other existing optimization-based antiwindup methods. We consider a scenario where the proposed two-stage IMC competes favourably with a long prediction horizon model predictive control (MPC).

17:30-17:50 MoAT2.4

Handling Communication Disruptions in Distributed Model Predictive Control

Christofides, Panagiotis D. Univ. of California at Los Angeles
Heidarinejad, Mohsen Univ. of California, Los Angeles
Liu, Jinfeng Univ. of California, Los Angeles
Muńoz de la Peńa, David Univ. de Sevilla

In this work, we deal with distributed model predictive control (DMPC) of nonlinear systems with communication disruptions between the distributed controllers. Specifically, we focus on the design of DMPC systems that take into account communication channel noise and data losses between the distributed controllers explicitly. In contrast to most of the existing DMPC methods which assume flawless communication, we employ a specific channel model to consider a number of realistic data transmission scenarios. In order to ensure the stability of the closed-loop system under communication disruptions, each model predictive controller utilizes a stability constraint which is based on a suitable Lyapunov-based controller. The theoretical results are demonstrated through a nonlinear chemical process example.

17:50-18:10 MoAT2.5

Application of Soft Constrained MPC to a Cement Mill Circuit

Muralidharan, Guru Prasath Tech. Univ. of Denmark
Jorgensen, John Bagterp Tech. Univ. of Denmark

In this paper we develop a Model Predictive Controller (MPC) for regulation of a cement mill circuit. The MPC uses soft constraints (soft MPC) to robustly address the large uncertainties present in models that can be identified for cement mill

circuits. The uncertainties in the linear predictive model of the cement mill circuit stems from large variations and heterogeneities in the feed material as well as operational variations. These sources of variations give rise to very nonlinear behavior and variations in the dead-times of the cement mill circuit. The uncertainties may be characterized by the gains, time constants, and time delays in a transfer function model. The developed soft MPC is compared to a normal MPC. The comparison is conducted using a rigorous cement mill circuit simulator used for operator training. The simulations reveal that compared to normal MPC, soft MPC regulate cement mill circuits better and in a plant friendly way by using less variations in the manipulated variables (MVs).

18:10-18:30 MoAT2.6

Short-Term Planning Model for Petroleum Refinery Production Using Model Predictive Control

Yuzgec, Ugur Bilecik Univ.
Palazoglu, Ahmet N. Univ. of California at Davis
Romagnoli, Jose Louisianna State Univ.

A model predictive control (MPC) strategy is developed to determine the optimal solution of the short-term refinery production planning problem. The main objective of the proposed algorithm is to maximize the total profit and to minimize the costs regarding the refinery process over a planning horizon. The refinery planning problem is solved in discrete time over a pre-determined prediction horizon and this prediction horizon is shifted by one time interval at each subsequent step where the optimization is repeated. To demonstrate the performance of this receding horizon strategy, two literature examples are introduced where the refinery process comprises the oil fields, crude oil vessels, the storage, charge and production tanks, as well as the crude distillation units (CDU). The performance of the strategy for different moving horizon lengths is presented and discussed.

MoAT3 Room B

Systems Biology I (Invited Session)

Co-Chair: Ionescu, Clara — Ghent Univ.

Organizer: Jacobsen, Elling W. — Automatic Control, KTH

16:30-16:50 MoAT3.1

Mixed-Integer Non-Linear Optimal Control in Systems Biology and Biotechnology: Numerical Methods and a Software Toolbox

Hirmajer, Tomas — Slovak Univ. of Tech. in Bratislava

Balsa-Canto, Eva — CSIC

Banga, Julio R. — IIM-CSIC (Spanish Council for Scientific Res.

Here we consider the problem of optimal manipulation of biological or biotechnological systems, formulated as a class of mixed-integer optimal control problems. We describe the current state of the art regarding the numerical solution of these problems, and a software implementation developed in our group (DOTcvp toolbox, based on Matlab).

DOTcvp combines the control vector parameterization approach with a number of local deterministic and global stochastic and hybrid (mixed-integer) non-linear programming solvers and suitable dynamic process simulation methods so as to cover the solution of a wide class of problems. The performance of DOTcvp is illustrated considering representative set of benchmark problems, including the problem of drug displacement in a patient, the optimal operation of a fed-batch bioreactor, and the optimal control of intracellular calcium oscillations.

The DOTcvp toolbox is freely available to academic users.

16:50-17:10 MoAT3.2

Density-Based Modeling and Identification of Biochemical Networks in Cell Populations

Hasenauer, Jan — Univ. Stuttgart

Waldherr, Steffen — Univ. of Stuttgart

Doszczak, Malgorzata — Univ. of Stuttgart

Scheurich, Peter — Univ. of Stuttgart

Allgower, Frank — Univ. of Stuttgart

In many biological processes heterogeneity within cell populations is an important issue. In this work we consider populations where the behavior of every single cell can be described by a system of ordinary differential equations. Heterogeneity among individual cells is accounted for by differences in parameter values and initial conditions. Hereby, parameter values and initial conditions are subject to a distribution function which is part of the model specification. Based on the single cell model and the considered parameter distribution, a partial differential equation model describing the distribution of cells in the state and in the output space is derived.

For the estimation of the parameter distribution within the model, we consider experimental data as obtained from flow cytometric analysis. From these noise-corrupted data a density-based statistical data model is derived. Employing this model of the data the parameter distribution within the cell population is computed using convex optimization techniques.

To evaluate the proposed method, a model for the caspase activation cascade is considered. It is shown that for known noise properties the unknown parameter distributions in this model are well estimated by the proposed method.

17:10-17:30 MoAT3.3

Modelling of Detailed Insulin Receptor Kinetics Affects Sensitivity and Noise in the Downstream Signalling Pathway

Luni, Camilla — Univ. of California, Santa Barbara
Sanft, Kevin — Univ. of California, Santa Barbara
Petzold, Linda — Univ. of California Santa Barbara
Doyle III, Francis Joseph — Univ. of California at Santa Barbara

Insulin resistance is a primary defect underlying the development of type II diabetes. In healthy conditions, insulin stimulates glucose uptake from the blood stream, but in diseased conditions the normal metabolic response is impaired. Identifying specific drug targets to restore insulin sensitivity at the cellular level and developing an effective treatment strategy require insight into both the biochemical mechanisms involved and the whole signalling network response to external cues. This study focuses on the consequences of integrating a detailed biochemical description of the insulin receptor trafficking compartment within a phenomenological model of the downstream signalling pathway. While the description of the experimental data is preserved by an iterative procedure of parameter fitting, the dynamic response of the network is highly modified, as shown by analyzing the complementary information derived from studying both connection sensitivities and node noise in the network. This is crucial considering the importance of network dynamics for identifying effective drug targets.

17:30-17:50 MoAT3.4

Identifiability of a Hodgkin-Huxley Type Ion Channel under Voltage Step Measurement Conditions

Csercsik, Dávid — Computer and Automation Res. Inst. Hungarian Acad. of
Szederkenyi, Gabor — Computer and Automation Res. Inst. Hungarian
Hangos, Katalin M. — Computer & Automation Rsrch. Inst. of the Hungarian Acad. of S

In this paper, we analyze the identifiability properties of a Hodgkin-Huxley (HH) type voltage dependent ion channel model under voltage clamp circumstances. The elimination of the differential variables is performed, and the identifiability of various parameters is analyzed using the differential algebra approach and the algorithm

based on the Taylor series expansion of the output. It is shown that the model is structurally non-identifiable using certain commonly applied parametrizations, and hidden dependences between physical parameters are unravelled. Using the results of the identifiability analysis, physically meaningful examples are shown when the model parameters are different but the system outputs are identical.

17:50-18:10 MoAT3.5

Robustification As a Tool in Modeling Biochemical Reaction Networks

Nenchev, Vladislav Automatic Control, KTH
Jacobsen, Elling W. Automatic Control, KTH

Biological functions have evolved to become robust against a multitude of perturbations such as gene mutations, intracellular noise and changes in the physical and chemical environment. This robustness should be reflected in models of the underlying biochemical networks, and robustness analysis is frequently employed in validating models of intracellular biochemical reaction networks. However, at present there are no tools or guidelines available to support postulation of model modifications that can serve to improve the robustness. Herein we propose a method based on computing the sensitivity of the robustness with respect to generic dynamic perturbations applied to the individual network edges. To quantify robustness we compute the smallest simultaneous change in the activity of the network nodes that induces a bifurcation in the network, resulting in a qualitative change in the network behavior. The focus is on biological functions related to bistable switches and sustained oscillations, and the proposed methodology is demonstrated through application to metabolic oscillations in white blood cells and bistable switching in MAPK signal transduction.

18:10-18:30 MoAT3.6

Fractal Structure and Storage Dynamics of Glycogen

Ionescu, Clara Ghent Univ.

Fractals are complex structure which can be characterized in a compact form using least amount of information. The fact that nature has applied very simple rules to provide optimal space filling structures and dynamical efficiency is already known to researchers. Glycogen storage is such an example of dynamical efficiency and self-similar structure. This paper provide a model for the storage dynamics of glycogen, suggesting that the fractal structures leads to phase constancy in the growth dynamics.

MoAT4 Room C

Modeling and Identification Methodologies (Regular Session)

Chair: Pannocchia, Gabriele — Univ. of Pisa

Co-Chair: Tangirala, Arun K. — Indian Inst. of Tech. Madras

16:30-16:50 MoAT4.1

Spline Wavelets for System Identification

Mukhopadhyay, Siddhartha — Bhabha Atomic Res. Center

Mahapatra, U — Bhabha Atomic Res. Center

Tangirala, Arun K. — Indian Inst. of Tech. Madras

Tiwari, Akhilanand Pati — Bhabha Atomic Res. Centre

The paper introduces spline wavelets as a modelling tool for system identification and proposes the technique of consistent output prediction using wavelets for estimating system parameters. It suggests that direct weighted summation of projections in approximation space could be used for deriving consistent output prediction in case model structure is built with spline wavelets. This can be viewed as identification using prefiltered input and output. The prefiltering is motivated to decorrelate samples such that local fit can be considered as a possible solution. An iterative algorithm, alternately projecting the solution in time and wavelet domain for penalized minimization of local error in wavelet coefficients could be designed for estimating system parameters. The algorithm is computationally efficient and exhibits excellent performance in cross validation. As a case study, the paper addresses the problem of modelling Liquid Zone Control System (LZCS) in a large Pressurized Heavy Water Reactor (PHWR). In this work, an identification scheme of a single input single output (SISO) linear time invariant (LTI) model of the LZCS system is studied. Excellent approximation is achieved by modelling with Biorthogonal spline wavelets used for deriving consistent output prediction of the LZCS process.

16:50-17:10 MoAT4.2

Improved Phase-Based Calibration Modelling and Quality Prediction by Investigating the Effects of Inter-Phase Correlation

Zhao, Chunhui — The Hong Kong Univ. of Science and Tech.

Gao, Furong — Hong Kong Univ. of Sci & Tech.

Phase-based quality analysis and prediction has been widely addressed by employing different calibration modeling techniques in multiphase batch processes. In this paper, a rational analysis scheme is presented to evaluate and understand the effects of the inter-phase correlation on, such as the extraction of the latent information, model structure and quality prediction. This is performed by combining partial least squares and principal component of predictions and implementing it bi-directionally (Bi-PLS-PCP). Within each phase, it separates the process systematic variation into the common and unique parts respectively based on their changes under the influence of the inter-phase correlation. They can then be quantitatively evaluated and made better use of for enhanced process understanding and

improved quality prediction. The strength and efficiency of the proposed algorithm are verified on a typical multiphase batch process, injection molding.

17:10-17:30 MoAT4.3

Closed-Loop PARSIMonious Subspace Identification: Theory and Application to MPC

Pannocchia, Gabriele Univ. of Pisa
Calosi, Mirco AspenTech S.r.l.

We propose in this paper a novel subspace identification method, based on PARSIMonious parameterization (Qin et al., 2005), and we show that such algorithm guarantees consistent estimates of the Markov parameters with open-loop and closed-loop data. The method uses the predictor form and it effectively exploits in all steps the Toeplitz structure of the Markov parameters' matrices. After evaluation of (AK = A_;KC,C) from the identified observability matrix, the method computes (BK = B_; KD, D, K) and the initial condition by solving a single (well conditioned even for unstable systems) Least Squares problem. We use such method to obtain linear models for MPC design, and we show how the proposed method compares favorably with other existing subspace algorithms in two examples.

17:30-17:50 MoAT4.4

Process Identification Using Nonideal Step Inputs

Ahmed, Salim Univ. of Qatar

Methods to estimate the parameters and the time delay of continuous time transfer function models using different nonideal step inputs are presented. By nonideal step inputs we refer to excitation signals that initially change gradually or in smaller steps to a final value unlike the ideal step that requires a sudden jump equalling the size of the step. Many different forms of such input signals can be designed. We consider four types namely the saturated ramp, the staircase input, the saturated sinusoid and the filtered step input. Two approaches are taken for the parameter estimation. First, estimation equations are directly obtained for the particular inputs and second, equivalent ideal step responses are generated from the nonideal step responses and step response method is used to estimate the parameters. The estimation equations are based on the integral equation approach. The necessary mathematical derivations are provided taking a first order plus time delay model as an example. Simulation results for both first and second order models are presented to demonstrate the efficacy of the proposed methodologies.

17:50-18:10 MoAT4.5

Conditions for Identifiability Using Routine Operating Data for a First-Order ARX Process Regulated by a Lead-Lag Controller

Shardt, Yuri Univ. of Alberta
Huang, Biao Univ. of Alberta

The conditions for closed-loop identifiability using routine operating data are largely unknown. In this paper, the closed-loop identifiability conditions for a first-order

autoregressive process with exogenous input (ARX) that is regulated using a 3-parameter lead-lag controller and that has no external excitation will be examined using an analytical approach. Despite the convoluted nature of the intermediate results, the final conditions for absolute identification of the stable region can be concisely stated. These results suggest that the class of internal model controllers (IMCs) can, despite their aggressive behaviour, successfully identify an ARX model without any external excitation. As well, Monte Carlo simulations performed using MATLAB confirmed the analytical results that were obtained. Future work in this area can focus on extending the results to other model structures, to other types of controllers, and to higher order processes.

18:10-18:30 MoAT4.6

Feasibility of Coupling Dehydrogenation of Ethylbenzene with Hydrogenation of Nitrobenzene in an Autothermal Catalytic Membrane Reactor: Modeling Study

Abo-Ghander, Nabeel S. Univ. of British Columbia
Logist, Filip Katholieke Univ. Leuven
Grace, John R. Univ. of British Columbia
Van Impe, Jan F.M. Katholieke Univ. Leuven
Elnashaie, Said New Mexico Tech. Univ.
Lim, Jim C. Univ. of British Columbia

The coupling of reactions in catalytic membrane reactors provides novel reactor configurations that allow shifting the thermodynamic equilibrium and yields of thermodynamically limited reactions and enhancing significantly the rate of production. An interesting pair to couple is the dehydrogenation of ethylbenzene to styrene and the hydrogenation of nitrobenzene to aniline. Hydrogen produced in the dehydrogenation side diffuses through the membrane and assists in shifting the equilibrium conversion of ethylbenzene and the yield of styrene while the large heat of reaction released from the hydrogenation side is utilized to provide the heat needed on the dehydrogenation side. The feasibility and performance of the co-current integrated catalytic membrane reactor configuration is investigated by means of models based on both homogeneous and heterogeneous fixed bed concepts. The ethylbenzene conversion and styrene yield obtained from the proposed reactor are then compared with those for simple fixed bed reactors without membranes. In the homogeneous modeling, the conversion of ethylbenzene is predicted to be ~39% in the simple fixed bed (without any membrane) compared to ~85% in the proposed catalytic membrane reactor. When intraparticle diffusion resistance is taken into consideration, the integrated reactor is predicted to have an ethylbenzene conversion of ~72% when catalyst pellets are isothermal and ~65% for non-isothermal catalyst pellets. The yields of styrene predicted by the homogeneous modeling are ~35% and ~80% for the simple fixed bed and the catalytic integrated reactor, respectively. The heterogeneous model of the integrated reactor, however, predicts less substantial, though still major gains, than the homogenous model, i.e. a styrene yield of ~70% for the isothermal catalyst pellets compared to ~65% for the non-isothermal catalyst pellets.

TuPlenaryT5 Room ZVH

Plenary Session 3 (Plenary Session)

Chair: Dochain, Denis Univ. Catholique de Louvain

08:30-09:30 TuPlenaryT5.1

Control Theory, Practice and Benefits in the Chemical Industry : Status and Perspectives

Lacroix, Marc SOLVAY, S.A., Brussels, Belgium

TuKeynoteT6 Room ZVH
Keynote Session 3 (Semi-Plenary Session)
Chair: Bonvin, Dominique EPFL

09:50-10:20 TuKeynoteT6.1

A Comparison of Nonlinear State Estimators for Closed-Loop Control of Batch Crystallizers

Mesbah, Ali TU Delft
Huesman, Adrie Delft Univ. of Tech.
Kramer, Herman TU Delft
Van den Hof, Paul M.J. Delft Univ. of Tech.

This study investigates the effectiveness of various nonlinear estimation techniques for output feedback model-based control of batch crystallization processes. Several nonlinear observers developed under deterministic and Bayesian estimation frameworks are applied for closed-loop control of a semi-industrial fed-batch crystallizer. The performance evaluation is done in terms of closed-loop behavior of the control strategy and its ability to cope with model imperfections and process uncertainties such as measurement errors and uncertain initial conditions. The simulation results suggest that the extended and the unscented Kalman filters perform best in terms of fulfilling the control objective. Adopting a time-varying process noise matrix, which is particularly suited for batch processes, further enhances the accuracy of state estimates at the expense of a slight increase in computational burden. The results also indicate that model imperfections and process uncertainties rather significantly deteriorate the closed-loop performance of the controller due to inaccurate state estimation.

TuKeynoteT7 Room A
Keynote Session 4 (Semi-Plenary Session)
Chair: Bernaerts, Kristel Katholieke Univ. Leuven

09:50-10:20 TuKeynoteT7.1
Rapid Design of System-Wide Metabolic Network Modifications Using Iterative Linear Programming
Yang, Laurence Univ. of Toronto
Cluett, William Univ. of Toronto
Mahadevan, Radhakrishnan Univ. of Toronto

Computationally-aided metabolic engineering is an important, complementary strategy to combinatorial strain design for enhanced biochemical production by microbes. Bilevel optimization problems have been formulated for optimal strain design via reaction removal, activation, and inhibition. Deterministic global optimization of the resulting mixed integer linear programs (MILPs) requires extensive computational effort, especially for genome-scale models of metabolism. Improving the computational efficiency of such algorithms is an ongoing challenge. Here, we present Enhancing Metabolism with Iterative Linear Optimization (EMILiO)--a novel bilevel optimization-based algorithm that includes all possible flux modifications and is solved with remarkable computational efficiency via iterative linear programming. The resulting solution is recursively pruned to generate alternate, parsimonious strain designs with maximal biochemical production rates. We demonstrate our algorithm for succinate production using the iAF1260 genome-scale model of Escherichia coli metabolism. Our algorithm identifies aerobic succinate-producing strains with increased glyoxylate shunt activity, which is consistent with experiments in the literature. We also identified novel strain design strategies that may have implications for the control of industrial bioreactors to maximize succinate production.

TuMT1 Room ZVH

Population Balance Modelling (Regular Session)

Co-Chair: Engell, Sebastian TU Dortmund

10:20-10:40 TuMT1.1

Automatic Differentiation Based QMOM for Population Balance Equations

Kariwala, Vinay Nanyang Tech. Univ.
Cao, Yi Cranfield Univ.
Nagy, Zoltan K. Loughborough Univ.

The quadrature method of moments (QMOM) has emerged as a promising tool for the solution of population balance equations in the past few years. The QMOM requires solving differential algebraic equations (DAEs) consisting of ordinary differential equations related to the evolution of moments as well as nonlinear algebraic equations resulting from the quadrature approximation of moments. In this paper, the use of automatic differentiation (AD) technique is proposed for solution of DAEs arising in QMOM. In the proposed method, the variables of interest are approximated using high-order Taylor series. Using AD, the high-order Taylor coefficients can be recursively calculated to obtain high-fidelity solution of the DAE system. Benchmark examples drawn from literature are used to demonstrate the superior accuracy and computational advantage of the AD-QMOM over existing state-of-the-art techniques, such as DAE-QMOM.

10:40-11:00 TuMT1.2

An Inverse Problem Approach to Extract the Growth Kernel in Particulate Processes

Bouaswaig, Ala Eldin Tech. Univ. Dortmund
Engell, Sebastian TU Dortmund

Mathematical models of particulate processes usually include a population balance equation to describe the dynamics of the size distribution. The structure of the population balance equation is the same in all models of particulate processes and the specific physical and chemical interaction of the particles is described by individual kernels. Usually first principles modeling is used to develop the kernels, but in cases in which this is intractable, inverse problem techniques have been proposed in the literature to extract the kernels from experimental data.

In this work we introduce an approach that can be used for extracting the growth kernel. This approach is applicable even when the assumption of separable growth rate that has been made in previous approaches does not hold and when coagulation with known dynamics and growth are taking place simultaneously.

11:00-11:20 TuMT1.3

A Stochastic Formulation for the Prediction of PSD in Crystallization Processes: Comparative Assessment of Alternative Model Formulations

Grosso, Massimiliano — Univ. degli Studi di Cagliari
Baratti, Roberto — Univ. degli Studi di Cagliari
Romagnoli, Jose — Louisianna State Univ.

A stochastic formulation for the description of antisolvent mediated crystal growth processes is discussed. In the proposed approach the crystal size growth dynamics is driven by a deterministic growth factor coupled to a stochastic component. The evolution in time of the particle size distribution is then described in terms of a Fokker-Planck equation. In this formulation the specific form of the stochastic model leads to different shapes for the probability density function. In this work we investigate and assess comparatively the performance of the FPE approach to model the crystal size distribution based on different expressions for the stochastic component. In particular, we consider the Langevin equation with a multiplicative noise term that depends on the crystal size (time and space). It is shown and corroborated via experimentation that the best stochastic model is given by the Geometric Brownian Motion (GBM). Excellent quantitative agreement between experiments and the predictions from the FPE-GBM model were obtained for a range of conditions. Validations against experimental data are presented for the NaCl-water-ethanol anti-solvent crystallization system.

11:20-11:40 TuMT1.4

Forward and Inverse Integration of Population Balance Equations with Size-Dependent Growth Kinetics

Bajcinca, Naim — Max Planck Inst. for Dynamics of Complex Tech. Systems

A method for forward and inverse integration of a class of population balance equations with a size-dependent growth rate is contributed in this article. A unique differential transformation of the independent time and internal coordinates is introduced, leading to straight line characteristics with constant values for the density function. The evolution of the density function is then given by transporting the initial and boundary conditions. For the integration of the temporal behavior of the boundary conditions, a generalization of the standard method of moments is introduced, resulting in integro-differential equations involving convolution integrals. The solution to the inverse integration problem involves a pre-computation of given correlation/convolution integrals. The usability of the method is illustrated in a case study of a batch crystallization process with size-dependent growth rate kinetics. The proposed method is compared to a high resolution finite volume scheme using a numerical example.

11:40-12:00 TuMT1.5

Multi-Scale Modeling and Inventory Control of Particle Growth Processes

Du, Juan Carnegie Mellon Univ.
Sukumar, Balaji Carnegie Mellon Univ.
White, Christy Carnegie Mellon Univ.
Ydstie, B. Erik Carnegie Mellon

In this paper, we develop a multi-scale model to describe the particle growth in a fluidized bed reactor. Population balance model is presented to describe the dynamical behavior of the particle size distribution. Stability analysis is derived to determine the control configuration for the complex particulate process. Inventory control strategy is applied to control the particle size distribution.

TuMT2 Room A

Monitoring, Modeling and Control of Tubular Reactors (Regular Session)

Chair: Tonomura, Osamu Kyoto Univ.

Co-Chair: Wattamwar, Satyajit Tech. Univ. of Eindhoven

10:20-10:40 TuMT2.1

Process Monitoring of Tubular Microreactors Using Particle Filter

Tonomura, Osamu Kyoto Univ.
Kano, Jun-ichi Kyoto Univ.
Kano, Manabu Kyoto Univ.
Hasebe, Shinji Kyoto Univ.

Microreactors consist of tens to hundreds of micrometer-scale channels. The residence time of a fluid can be set exactly and backmixing can be minimized. Particularly, very short residence time can be achieved. In addition, it is possible to precisely control the reaction temperature due to large surface to volume ratio of channels. These features of microreactors make it possible to realize the production of specialty chemicals, which cannot be handled in conventional reactors. The most recognized problem in microreactors is channel blockage. The catalyst deterioration is also an inevitable problem for catalyst reactions in microreactors. To realize stable long-term operation of microreactors, it is necessary to detect such problems as early as possible. Since miniaturized sensors are expensive and their direct installation inside channels may disturb the flow, it is indispensable to develop a process monitoring system using a few indirect measurements. In this research, a state and parameter estimation system for tubular microreactors (TMRs) is developed to detect process faults. In the developed system, a process model is derived from the first-principle model of TMRs. Particle Filter (PF) or Extended Kalman Filter (EKF) or Ensemble Kalman Filter (EnKF) is designed to obtain the unknown parameters such as catalyst efficiency from a single wall temperature sensor. To achieve high estimation performance, the optimal sensor location is determined on the basis of the observability. The numerical examples illustrate that the blockage and the catalyst deterioration of TMRs can be detected more rapidly and accurately by using PF, as compared with EnKF and EKF.

10:40-11:00 TuMT2.2

Conceptual Modelling and Optimization of Jacketed Tubular Reactors for the Production of LDPE

Van Erdeghem, Peter M.M. KU Leuven
Logist, Filip Katholieke Univ. Leuven
Heughebaert, Michiel Katholieke Univ. Leuven
Dittrich, Christoph SABIC Petrochemicals
Van Impe, Jan F.M. Katholieke Univ. Leuven

This paper deals with the model based optimization of tubular reactors for the production of LDPE. Due to the high complexity, solving an optimization problem of an industrial application is not straightforward. Often researchers seek the shortest

way to reach their final goal by going directly to the development of a high-complexity model and optimize this with respect to a certain objective. Although this approach seems the fastest way to success, it can be a bumpy road with a lot of dead ends. Therefore, a divide and conquer strategy is adopted, i.e., first develop a conceptual low-complexity model, set up the optimization problem and then use the obtained knowledge during the optimization of more complex models. The aim of this paper is to give the results of the three steps which have to be accomplished in order to achieve this subgoal. First, the multizone process of LDPE production is modelled as a sequence of conceptual modules which simulate the steady-state characteristics of one reaction and cooling zone. Then, this model is fitted to industrial data such that it quantitatively describes the real process. Finally, a multiple objective design optimization problem is formulated, i.e., where along the reactor and which amount of initiator has to be injected to maximize the profit at different economic situations.

11:00-11:20 TuMT2.3

Identification of Low Order Tensorial Models for Tubular Reactors

Wattamwar, Satyajit — Tech. Univ. of Eindhoven
Backx, Ton — Eindhoven Univ. of Tech.
Weiland, Siep — Eindhoven Univ. of Tech.

In this paper we propose a novel procedure for obtaining a low order model of a large scale, non-linear process. Our approach is based on the combinations of the methods of Proper Orthogonal Decomposition (POD), and non-linear System Identification techniques. It is showed here that the modal coefficient corresponding to the spectral decomposition of the system solutions can be viewed as the states of the reduced model. This has paved a way to propose a novel model reduction strategy for large scale systems. In the first step the spectral decomposition of system solutions is used to separate the spatial and temporal patterns (time varying modal coefficients) and in the second step a reduced model structure and it's parameters; linear and of non-linear tensorial (multi-variable polynomial) type are identified for approximating the temporal patterns obtained by the spectral decomposition. The state space matrices which happens to be the parameters of a black-box to be identified, appears linearly in the identification process. For the same reason, Ordinary Least Square method is used to identify the model parameters. The simplicity and reliability of proposed method gives computationally very efficient linear and non-linear low order models for large scale processes. The method is of generic nature. The efficiency of the proposed approach is illustrated on a benchmark example depicting industrial tubular reactor, which are often used in petrochemical industries. The results show good performance of the proposed method.

11:20-11:40 TuMT2.4

IHMPC and POD to the Control of a Non-Isothermal Tubular Reactor

Marquez, Alejandro National Univ. of Colombia
Espinosa, Jairo IPCOS N.V.
Odloak, Darci Univ. of São Paulo – Brazil

This paper presents the result of applying POD (Proper Orthogonal Decomposition) and IHMPC (Infinite Horizon Model Predictive Control) to the control of a non-isothermal tubular reactor. This paper is based on a previous work of O.M. Agudelo, J.J. Espinosa, B. De Moor Control of a Tubular Chemical Reactor by means of POD and Predictive Control Techniques, in Proceedings of the European Control Conference 2007 (ECC 2007), pp. 1046- 1053, Kos, Greece, 2007, where a finite horizon model predictive control and POD techniques are applied a non-isothermal tubular reactor. In this paper the control objective is to keep the operation of the reactor at a desired operating condition in spite of the disturbances in the feed flow. POD and Galerkins method are used to derive the low order linear model that captures the dominant dynamics of the PDEs, which are subsequently used for controller design. Two IHMPC formulations are constructed on the basis of the low order linear model and are demonstrated, through simulation, to achieve the control objectives.

TuMT3 Room B

Integrated (Plant Wide) Design and Control (Regular Session)

Chair: Bao, Jie — The Univ. of New South Wales

Co-Chair: Van den Hof, Paul M.J. — Delft Univ. of Tech.

10:20-10:40 TuMT3.1

Plantwide Operability Analysis Based on a Network Perspective: A Study on the Tennessee Eastman Process

Setiawan, Ridwan — The Univ. of New South Wales

Hioe, Denny — The Univ. of New South Wales

Bao, Jie — The Univ. of New South Wales

Complex process plants increasingly appear in modern chemical industry due to the considerable economic efficiency that complex and interactive process designs can offer. Interactions between process units (e.g., material recycle and energy integration) often cause significant difficulties in plantwide control. As such, it is important to study plantwide operability (i.e., whether a plantwide process can be effectively controlled) prior to control system design and preferably during the stage of process design. This paper presents such an analysis approach based on a network perspective, where a plantwide process is modelled as a network of process units interconnected with physical mass and energy flow. This approach can be used to determine plantwide stability, stabilizability and disturbance attenuability. The proposed method is illustrated with the Tennessee Eastman Process.

10:40-11:00 TuMT3.2

Plant-Wide Control Based on Minimum Square Deviation

Zumoffen, David Alejandro — CIFASIS-CONICET

Basualdo, Marta S. — GIAIP-CIFASIS- CONICET- FRRo-Univ. Tecnológica Nacional

Molina, Gonzalo Dario — GIAIP-CIFASIS

In this work a new systematic and generalized strategy to solve the MIMO plantwide control problem is proposed. The methodology called Minimum Square Deviation (MSD) considers several points such as the optimal sensor location (OSL) based on sum of square deviation (SSD) and the control structure selection (CSS) based on net load evaluation (NLE) problems simultaneously. Particularly, this work focuses on selecting the best MIMO control structure by using a new steady-state index called NLE. Thus, alternative control structures can be obtained through different interaction levels and defining a corresponding performance improvement. Two well-known chemical processes are proposed here for testing this methodology. In addition, a robust stability analysis applying the classical _-tool is performed by considering both parametric and unmodeled dynamic uncertainties.

11:00-11:20 TuMT3.3

Application of Decomposition Methodology to Solve Integrated Process Design and Controller Design Problems for Reactor-Separator-Recycle System

Abd. Hamid, Mohd. Kamaruddin — Tech. Univ. of Denmark
Sin, Gurkan — CAPEC, Department of Chemical and Biochemical Engineering, Tech.
Gani, Rafiqul — CAPEC, Department of Chemical and Biochemical Engineering, Tech.

This paper presents the integrated process design and controller design (IPDC) for a reactor-separator-recycle (RSR) system and evaluates a decomposition methodology to solve the IPDC problem. Accordingly, the IPDC problem is solved by decomposing it into four hierarchical stages: (i) pre-analysis, (ii) design analysis, (iii) controller design analysis, and (iv) final selection and verification. The methodology makes use of thermodynamic-process insights and the reverse design approach to arrive at the final process-controller design decisions. The developed methodology is illustrated through the design of a RSR system involving consecutive reactions, A <-> B -> C and shown to provide effective solutions that satisfy design, control and cost criteria. The advantage of the proposed methodology is that it is systematic, makes use of thermodynamic-process knowledge and provides valuable insights to the solution of IPDC problems for RSR systems.

11:20-11:40 TuMT3.4

Towards the Systematic Design of Actuation for Process Systems

Huesman, Adrie — Delft Univ. of Tech.
Bosgra, Okko — Delft Univ. of Tech.
Van den Hof, Paul M.J. — Delft Univ. of Tech.

Currently systematic design of actuation (operational degrees of freedom) for process systems is not possible because (i) the required domain knowledge has not been identified and (ii) it is unclear how to explore the relation between actuation and operational improvement. This paper proposes geometry and flux equations as the required domain knowledge. It is explained that the relation between actuation and operational improvement should be explored in an optimal control setting. By means of an example (distillation) it is illustrated that a spatial actuation extension may result in considerable operational improvement.

11:40-12:00 TuMT3.5

Iterative Data-Based Modelling and Optimization for Rapid Design of Dynamic Processes

Chi, Guoyi — Nanyang Tech. Univ.
Yan, Wenjin — Nanyang Tech. Univ.
Chen, Tao — Nanyang Tech. Univ.

We consider an off-line process design problem where the response variable is affected by several factors. We present a data-based modelling approach that iteratively allocates new experimental points, update the model, and search for the

optimal processfactors. A flexible non-linear modelling technique, the kriging (also known as Gaussian processes), forms the cornerstone of this approach. Kriging model is capable of providing accurate predictive mean and variance, the latter being a quantification of its prediction uncertainty. Therefore, the iterative algorithm is devised by jointly considering two objectives: (i) to search for the best predicted response, and (ii) to adequately explore the factor's space so that the predictive uncertainty is small. This method is further extended to consider dynamic processes, i.e. the process factors are time-varying and thus the problem becomes to design a time-dependent trajectory of these factors. The proposed approach has been demonstrated by its application to a simulated chemical process with promising results being achieved.

TuMT4 Room C

Modeling and Control of Biological Processes (Regular Session)

Chair: Jorgensen, John Bagterp — Tech. Univ. of Denmark

Co-Chair: Schaum, Alexander — Univ. Autónoma Metropolitana – Iztapalapa

10:20-10:40 TuMT4.1

Complete Partial Control Design for Extractive Fermentation Process

Nandong, Jobrun — Curtin Univ. of Tech. Sarawak Campus

Samyudia, Yudi — Curtin Univ. of Tech.

Tade, Moses O. — Curtin Univ. of Tech.

In this paper, the methodology for complete partial control design based on a novel PCA-based technique incorporating the inventory and constraint control objectives is described. Brief descriptions on the PCA-based technique, some definitions and criteria are also presented. The application of the methodology is demonstrated using a case study of extractive alcoholic fermentation process. Result shows that good understanding of the interaction among process variables is the key principle for designing partial control strategy. Interestingly the proposed methodology allows the designer to understand this interaction and hence to exploit its benefit in partial control design.

10:40-11:00 TuMT4.2

Output-Feedback Control for a Class of Biological Reactors

Schaum, Alexander — Univ. Autónoma Metropolitana – Iztapalapa

López-Arenas, Teresa — Univ. Autónoma Metropolitana

Alvarez, Jesus — Univ. Autonoma Metropolitana

Moreno, Jaime A. — Univ. Nacional Autonoma de Mexico-UNAM

The problem of regulating the biomass growth rate at its maximum value in an open-loop unstable, continuous, non-monotonic biological reactor using biomass measurement and manipulation of substrate feed rate is considered. An Output-Feedback controller is designed exploiting the reactor open-loop stability and inherent observability properties and the relative degree structure to obtain robust and non-wasteful closed-loop performance. The resulting controller has a high degree of independency with respect to the kinetic growth rate expression, thus ensuring robustness against typical model uncertainties. A representative case example with non-monotonic Haldane kinetics is employed to test the proposed controller, in absence and presence of modeling and measurement errors.

11:00-11:20 TuMT4.3

Modelling Lipid Production in Microalgae

Mairet, Francis Inria
Bernard, Olivier Inria
Masci, Pierre INRIA
Lacour, Thomas LOV
Sciandra, Antoine LOV

Microalgae offer potentially great opportunities for producing biofuel. In order to optimize triglycerid production, this article proposes a dynamical model of microalgal lipid production. In this model, intracellular carbon is divided between a functional pool and two storage pools (sugars and neutral lipids). The various intracellular carbon flows between these pools lead to a complex dynamic with a strong discrepancy between accumulation and mobilization of neutral lipids. This generates an hysteresis which has been observed experimentally. The model has been validated with experiments of *Isochrysis affinis galbana* (T. iso) culture under various nitrogen limitation conditions.

11:20-11:40 TuMT4.4

Optimal Operating Points for SCP Production in the U-Loop Reactor

Jorgensen, John Bagterp Tech. Univ. of Denmark
Jřrgensen, Sten Bay Tech. Univ. of Denmark

The microorganism *Methylococcus capsulatus* can grow on cheap carbon sources such as methane and methanol. *M. capsulatus* has a protein content of approximately 70% and can be used for production of so-called Single Cell Protein (SCP). Static simulations of SCP production using *Methylococcus capsulatus* in an U-loop reactor have been used to determine the optimal operation. The optimal operating point is located close to both washout and oxygen limitation. With oxygen being the most expensive reactant, the U-Loop reactor is operated in the oxygen limited mode and substrate feed is controlled according to the oxygen feed. The maximum oxygen feed is determined by the maximum biomass concentration that can be tolerated in the reactor. Higher biomass concentration is believed to give a more viscous fluid that requires more pumping energy for circulation in the U-loop and has a lower gas-liquid oxygen transfer rate. The optimal dilution rate is relative constant around 0.2 1/hr. This operating strategy gives the highest SCP productivity.

11:40-12:00 TuMT4.5

Comparison of Two Model Predictive Control for the Ethanol Production Optimization of a Two-Stage Bioreactor with Cellular Recycling

Aceves-Lara, Cesar-Arturo INSA
Bideaux, Carine Univ. de Toulouse; UPS, INSA, INP, LISBP
Molina-Jouve, Carole Univ. de Toulouse; UPS, INSA, INP, LISBP
Roux, Gilles LAAS

This paper addresses the problem of dynamic optimization of ethanol production. This process is described by a nonlinear model. A Model Predictive Control (MPC)

has been implemented in order to optimize the bioprocess dynamically. Two algorithms were used together with a MPC: the Pattern Search (PS) and the Iterative Ant Colony Algorithm (IACA). They were compared with an open-loop control experimentally implemented. The MPC with the PS algorithm showed a better performance than the MPC with IACA and than the open-loop control.

13:30-13:50 TuAT2.1

On-Line PI Controller Tuning Using Closed-Loop Setpoint Response

Mohammad, Shamsuzzoha aNorwegian Univ. of Science and Tech.
Sigurd, Skogestad Norwegian Univ. of Science and Tech.
Trondheim, Norway
Halvorsen, Ivar J. SINTEF ICT

A simple method has been developed for PI controller tuning of an unidentified process using closed-loop experiments. The proposed method is similar to the Ziegler-Nichols (1942) tuning method, but it is faster to use and does not require the system to approach instability with sustained oscillations. The method requires one closed-loop step setpoint response experiment using a proportional only controller with gain Kc0. From the setpoint response one observes the overshoot, the corresponding time to reach the peak (tp) and the steady-state change (b=y(_;)/ys). Based on simulations for a range of first-order with delay processes, simple correlations have been derived to give PI controller settings similar to those of the SIMC tuning rules (Skogestad, 2003). The controller gain (Kc/Kc0) is only a function of the overshoot observed in the setpoint experiment whereas the controller integral time (Ä;I) is mainly a function of the time to reach the peak (tp). Importantly, the method includes a detuning factor F that allows the user to adjust the final closed-loop response time and robustness. The proposed tuning method, originally derived for first-order with delay processes, has been tested on a wide range of other processes typical for process control applications and the results are comparable with the SIMC tunings using the open-loop model.

13:50-14:10 TuAT2.2

Analysis and Performance Comparison of PID and Fractional PI Controllers

Gude, Juan J. Univ. of Deusto
Kahoraho, Evaristo Univ. of deusto

This paper compares the frequency domain performance criterion (Jv) of PI, fractional PI, and PID controllers when a step load disturbance is applied at the plant input. Process information is available in form of first-order plus dead-time (FOPDT) model. In addition, the controllers were compared using the Hinf–norm of the sensitivity function as a measure of robustness, and some comments on industrial practice are offered in this context.

14:10-14:30 TuAT2.3

Adaptive Step Size Control in Implicit Runge-Kutta Methods for Reservoir Simulation

Völcker, Carsten Tech. Univ. of Denmark
Jorgensen, John Bagterp Tech. Univ. of Denmark

This paper concerns predictive stepsize control applied to high order methods for temporal discretization in reservoir simulation. The family of Runge-Kutta methods is presented and in particular the explicit singly diagonally implicit Runge-Kutta (ESDIRK) methods are described. A predictive stepsize adjustment rule based on error estimates and convergence control of the integrated iterative solver is presented. We try to improve the predictive stepsize control by smoothing the stepsize sequence through combining the control of error with the control of convergence.

14:30-14:50 TuAT2.4

Design of a Control Lyapunov Function for Stabilizing Specified States

Yang, Yu Univ. of Alberta
Lee, Jong Min Univ. of Alberta

This paper focuses on the design of control Lyapunov function for control affine systems to guarantee the stability for the states of interest in a specified region. Without restrictive assumptions found in previous approaches, a min-max optimization problem is formulated to solve for a quadratic Lyapunov function. A derivative-free coordinate search method is employed to optimize a non-differentiable objective function. Approximation of the objective function as a piecewise linear function gradually reduces search space, leading to an effective Lyapunov function. A CSTR example with actuator saturation is illustrated to demonstrate the efficacy of the proposed approach.

14:50-15:10 TuAT2.5

Thermal Budget Control for Rapid Thermal Processing Systems with Spike-Shaped Temperature Profile

Jeng, Jyh-Cheng National Taipei Univ. of Tech.
Lee, Bor-Chi National Taiwan Univ.
Su, An-Jhih National Taiwan Univ.
Yu, Cheng-Ching National Taiwan Univ.

Rapid thermal processing (RTP) systems with spike-shaped temperature profile are widely used in IC industry for providing precise thermal budgets. This thermal budget control issue gets more crucial as the technology node progressively shrinking. With its exceptionally stringent performance requirements (for example, high temperature uniformity and high temperature ramp-up/down rate), temperature control in RTP systems is a challenging task. In this study, we present the methodology of designing a control system for providing precise thermal budget. By tuning controller parameters and designing the set-point profile, the method targets thermal budget indices instead of temperature servo control. Two types of controllers, PI and PI2D,

are considered. Practical issues, such as the feasibility range for temperature ramp-up/down rate and the effect of model mismatch, are also discussed. The results show the simple PI controller performs well in spike RTP systems.

TuAT3 Room B

Modelling, Control and Optimization of Energy Systems I (Invited Session)

Chair: Budman, Hector M. Univ. of Waterloo

Organizer: Budman, Hector M. Univ. of Waterloo

13:30-13:50 TuAT3.1

Receding Horizon Experiment Design with Application in SOFC Parameter Estimation

Jayasankar, Barath Univ. of Alberta
Huang, Biao Univ. of Alberta
Ben-Zvi, Amos Univ. of Alberta

In this work the problem of optimal input design (OID) in a receding-horizon framework for online parameter estimation is solved. The designed optimum input is used for dynamic experiment and subsequent estimation of parameters. A fuel cell experiment design and parameter estimation problem is investigated through the proposed approach. Some of the issues related to the application of the proposed method are examined and guidelines for selecting appropriate experimental settings are provided.

13:50-14:10 TuAT3.2

Performance Analyses of Microbial Fuel Cells Operated in Series

Pinto, Roberto Pires École Pol. de Montréal
Tartakovsky, Boris National Res. Council of Canada
Perrier, Michel Ec. Pol.
Srinivasan, B. Ec. Pol. Montreal

Microbial Fuel Cells (MFCs) are capable of producing electricity while cleaning wastewater. This novel technology can replace energy-consuming aerobic treatment even if low effluent concentrations are demanded. The goal of this work is to optimize a MFC-based wastewater treatment process. A MFC mathematical model, which accounts for co-existence of methanogenic and anodophilic microbial populations, is used to compare different operating modes and reactor configurations. The following observations are made based on the model analysis: (i) the ratio between the anodophilic and methanogenic populations can be controlled by the electrical load; (ii) co-existence of the two populations decreases reactor performance, and (iii) reactors connected in series always improves treatment efficiency.

14:10-14:30 TuAT3.3

Model Predictive Control of a Kaibel Distillation Column

Kvernland, Martin Reinertsen Engineering
Halvorsen, Ivar J. SINTEF ICT
Skogestad, Sigurd Norwegian Univ. of Science and Tech.

This is a simulation study on controlling a Kaibel distillation column with model predictive control (MPC). A Kaibel distillation column has several advantages

compared with conventional binary column setups. The Kaibel column separates a feed stream into four product streams using only a single column shell. The distillation process is a multivariable process which leads to a multivariable control problem. The objective for optimal operation of the column is chosen to be minimization of the total impurity flow. An offline optimization on a mathematical model leads to temperature setpoints to be used by a controller. An MPC generally obtain less total impurity flow compared to conventional decentralized control when the distillation column is exposed to disturbances. It also counteracts process interactions better than decentralized control.

14:30-14:50 TuAT3.4

Networked Control of Distributed Energy Resources Using an Adaptive Communication Policy

Sun, Yulei Univ. of California, Davis
El-Farra, Nael H. Univ. of California, Davis

This work presents a model-based networked control structure with an adaptive communication policy for managing Distributed Energy Resources (DERs) over a shared, resource-constrained communication network. The central objective is to find a state-dependent strategy for establishing and terminating communication between the supervisor and the DERs in a way that minimizes network resource utilization without jeopardizing the desired stability and performance properties. To this end, a bounded robust Lyapunov-based controller that enforces constrained closed-loop stability in the absence of communication suspension is initially designed for each DER. A dynamic model of each DER is then included within the supervisor to provide estimates of the states of the DER when measurements are not transmitted through the network. To determine when communication between a given DER and the supervisor must be re-established, the evolution of the Lyapunov function is monitored within the DER's stability region such that if it begins to breach a state-dependent stability or performance threshold at any time, the sensor suite is prompted to send its data over the network to update its corresponding model in the supervisor. Communication is then suspended for as long as the Lyapunov function satisfies the specified threshold. The underlying idea is to use the Lyapunov stability constraint for each DER as the basis for adaptively switching on or off the communication with the supervisor. Finally, the results are illustrated through an application to a solid oxide fuel cell example.

14:50-15:10 TuAT3.5

Dynamic Modeling and Control of a Hybrid Vehicle with Onboard Fuel Processor

Nieto Deglioumini, Lucas GIAIP-CIFASIS-CONICET
Feroldi, Diego CIFASIS (UNR-CONICET-UPCAM)
Zumoffen, David Alejandro CIFASIS-CONICET
Basualdo, Marta S. GIAIP-CIFASIS- CONICET- FRRo-Univ. Tecnológica Nacional

The transient behavior of a Fuel Processor System to produce Hydrogen from bio-ethanol with high performance, coupled with a Proton Exchange Membrane Fuel Cell is modeled. The Ethanol Processor is based on a previous steady state design, optimized to work with maximum efficiency around 10 kW of rated power. From the dynamic rigorous model, a linearized model is identified to apply a systematic procedure to synthesize the control structure. The Fuel Cell System is then hybridized with supercapacitors as auxiliary power source, to lower the overall consumption of hydrogen, hence of bio-ethanol too. The entire vehicle is tested using standard driving cycles, widely utilized in related literature and to measure pollutant emissions. The overall behavior reaches the expectations and is capable of fulfilling the requirements of urban and highway scenarios,

TuAT4 Room C

Robust and Reliable Model Identification (Regular Session)

Chair: Gopaluni, Ratna Bhushan — Univ. of British Columbia

Co-Chair: Van Impe, Jan F.M. — Katholieke Univ. Leuven

13:30-13:50 TuAT4.1

A Framework for Model-Based Design of Experiments in the Presence of Continuous Measurement Systems

Galvanin, Federico — Univ. of Padova

Barolo, Massimiliano — Univ. of Padova

Bezzo, Fabrizio — Univ. of Padova

Model based design of experiments (MBDoE) techniques are a useful tool to maximise the information content of experimental trials when the purpose is identifying the set of parameters of a deterministic model in a statistically sound way. When samples are collected in a discrete way, the formulation of the optimal design problem is based on the maximisation of the expected information, usually calculated from discrete forms of the Fisher information matrix. However, if a continuous measurement system is available, information can be acquired gradually in a continuous way, and a new MBDoE approach is required to take into account the specificity of the measurement system. In this paper a novel design criterion is formulated by optimising a continuous measurement of the Fisher information matrix, with the purpose of reaching a statistically satisfactory estimation of model parameters in the easiest and quickest way. The benefits of the proposed strategy are discussed through a simulated case study, where the effectiveness of the design is assessed by comparison to a standard MBDoE approach.

13:50-14:10 TuAT4.2

Investigating Bayesian Robust Experimental Design with Principles of Global Sensitivity Analysis

He, Fei — Univ. of Strathclyde

Yue, Hong — Univ. of Strathclyde

Brown, Martin — The Univ. of Manchester

The purpose of model-based experimental design is to maximise the information gathered for quantitative model identification. Instead of the commonly used optimal experimental design, robust experimental design aims to address parametric uncertainties in the design process. In this paper, the Bayesian robust experimental design is investigated, where both a Monte Carlo sampling strategy and local sensitivity evaluation at each sampling point are employed to achieve the robust solution. The link between global sensitivity analysis (GSA) and the Bayesian robust experimental design is established. It is revealed that a lattice sampling based GSA strategy, the Morris method, can be explicitly interpreted as the Bayesian A-optimal design for the uniform hypercube type uncertainties.

14:10-14:30 TuAT4.3

A Risk Based Approach to Estimate the Key Uncertainties

Anand, Farminder — Georgia Inst. of Tech.
Realff, Matthew J. — Georgia Inst. of Tech.
Lee, Jay H. — Georgia Inst. of Tech.

Decisions during the early stages of R&D are often made under substantial uncertainty. Evaluation of R&D alternatives under uncertainty generally does not provide a clear choice that is best under all possible scenarios. For optimal investment of R&D resources, it is important to identify the key uncertainty contributors from a decision maker's perspective. Global sensitivity analysis (GSA) is a tool that can be used to determine key uncertainties that contribute the most to the variance of the bottom-line objective. It is often the case, however, that is not able to distinguish between the uncertainties. Motivated by this, we propose a new tool called conditional – global sensitivity analysis (c-GSA), which further considers the decision-maker's risk preference. The conditional sensitivity measures quantify the contributions of different individual uncertainty factors to the upper and lower halves of the distribution function of the objective function. It is argued that the use of may appeal to a risk-aversive decision maker as it leads to a lower rate of false acceptance decisions at the expense of a higher rate of false rejection decisions, whereas the use of does the opposite.

14:30-14:50 TuAT4.4

Nonlinear System Identification from Small Data Sets

Gopaluni, Ratna Bhushan — Univ. of British Columbia
Marshman, Devin James — Univ. of British Columbia

We propose a novel algorithm for identification of structured nonlinear systems using a compressive sampling approach. Compressive sampling is an approach to reconstruct randomly sampled signals from small data sets. The proposed algorithm provides empirical evidence to suggest that parameters can potentially be estimated from small data sets using compressive sampling. This approach is illustrated through simulated examples.

14:50-15:10 TuAT4.5

Effect of Varying Controller Parameters in Closed-Loop Subspace Identification

Bakke, Morten — Norwegian Univ. of Science and Tech.
Johansen, Tor Arne — Norwegian Univ. of Science and Tech.
Skogestad, Sigurd — Norwegian Univ. of Science and Tech.

It is well known that subspace identification methods that assume open loop data without correlations between the input and noise, may give biased estimates when applied to closed loop data. The effect of the controller gain parameters on the quality of the identified model is studied when closed loop data are used. Several subspace identification methods (both open loop and closed loop methods), and different simulated data sets ranging from ideal 2 x 2 linear systems, to a fairly

realistic nonlinear debutanizer process simulator, are considered. The results show that up to a point, higher controller gain during the identification experiment gives more accurate models than with lower controller gain, for both open and closed loop subspace identification methods. It is observed that the sensitivity to the controller gain is very small for the closed loop sub-space method tested for the ideal cases when its assumptions are satisfied. An explanation for this is that in this case there will be no bias, while the open loop methods may have a bias that depends on the controller parameters. Another interesting observation is that for the debutanizer example, the nonlinearities seem to lead to biased estimates also with the closed loop subspace method, and the choice of controller gain appears to be just as important as the use of a closed loop subspace identification method for the accuracy of the estimates.

WeKeynoteT6 Room ZVH

Keynote Session 5 (Semi-Plenary Session)

Chair: Christofides, Panagiotis D. Univ. of California at Los Angeles

09:00-09:30 WeKeynoteT6.1

Optimal Control of Transport-Reaction System with Time Varying Spatial Domain

Dubljevic, Stevan Unversity of Alberta
Ng, James Univ. of Alberta

This paper considers the multiscale optimal control of crystal growth. The optimal control is realized for the crystal pulling arm modeled by the standard rigid body dynamics, while the underlying dynamics of the diffusion of heat in the crystal growth region is given by parabolic partial differential equations (PDEs) with time varying spatial domain. The underlying transport-reaction system is developed from the first principles and the associated dynamics is analyzed in appropriate functional state space setting. The complete description of the evolutionary parabolic domain time varying PDE is provided and explored within the coupled master-slave control setting. Numerical simulations demonstrate an optimal pulling evolution rate and its effects on the temperature profile in the crystal with the time varying domain.

WeKeynoteT7 Room A

Keynote Session 6 (Semi-Plenary Session)

Chair: Gao, Furong Hong Kong Univ. of Sci & Tech.

09:00-09:30 WeKeynoteT7.1

Self-Optimizing Control and NCO Tracking in the Context of Real-Time Optimization

Jäschke, Johannes Norwegian Univ. of Science and Tech. (NTNU)

Skogestad, Sigurd Norwegian Univ. of Science and Tech.

This paper reviews the role of self-optimizing control (SOC) and necessary conditions of optimality tracking (NCO tracking). We argue that self-optimizing control is not an alternative to real-time optimization (RTO), NCO tracking or model predictive control (MPC), but is to be seen as complementary. In self-optimizing control we determine controlled variables (CV), that keep the process close to the optimum when a disturbance enters the process. These CVs are controlled at their setpoints using PID or model predictive controllers. Preferably, the setpoints are kept constant, but they may also be adjusted using RTO or NCO tracking. In any case, a good choice of CVs will reduce the frequency of setpoint changes by RTO or NCO tracking. When selecting self-optimizing CVs, a set of disturbances has to be assumed, as unexpected disturbances are not rejected in SOC. On the other hand, RTO and NCO tracking adapt the inputs at given sample times without any assumptions on what disturbances occur. It is only assumed that they occur on a slower time scale than the sampling. Disturbances with high frequencies or which which do not lead to a steady state are not rejected optimally. By using NCO tracking in the optimization layer and SOC in the control layer below, we demonstrate that the advantages of both methods complement each other. This combination allows fast optimal action for the expected disturbances, while other disturbances are compensated by NCO tracking on a slower time scale.

WeMT1 Room ZVH

Process Analytical Tools (Regular Session) (Joint DYCOPS/CAB Session)

Chair: Morris, Julian Newcastle Univ.

09:30-09:50 WeMT1.1

Towards the Robust Application of PAT in Real Time Control

Morris, Julian Newcastle Univ.
Chen, Zengping State Key Lab. of Chemo/Biosensing & Chemometrics,Hunan Un
Lovett, David Perceptive Engineering, Daresbury Innovation Centre,Daresbury, C

Process Analytical Technologies (PAT) are increasingly being explored and adopted by pharma-chem and bio-pharma companies for enhanced process understanding, Quality by Design (QbD) and Real-time-Release (RTR). To achieve these aspirations there is a critical need to extract the most information, and hence understanding, from complex and often very 'messy' spectroscopic data. A number of new approaches will be shown to overcome the limitations of existing calibration/modelling methodologies and algorithms and their use in some industrial applications will be presented.

09:50-10:10 WeMT1.2

Quality-By-Design Using a Gaussian Mixture Density Approximation of Biological Uncertainties

Rossner, Niko Tech. Univ. Berlin
Heine, Thomas Tech. Univ. Berlin
King, Rudibert Tech. Univ. of Berlin

In this contribution the uncertainties of a biological process model are taken into account explicitly to calculate optimal process trajectories. For this purpose, the initial condition and the uncertainties of the model parameters are described by a weighted sum of normal distributions. Such a so-called Gaussian mixture density (GMD) approximation is propagated through the nonlinear process model to calculate a second order approximation of the statistical properties of the planed process trajectory. A Value@Risk primary objective is used to obtain an optimal process design procedure in presence of uncertainties. In an extensive simulation study a descriptive fermentation process model is used to compare the classical trajectory planning with the robust design approaches. Here, different degrees of approximation complexity and the influence of the weighting factor in the Value@Risk dual objective criterion is investigated.

10:10-10:30 WeMT1.3

Kernel Regression with Correlated Errors

De Brabanter, Kris — Katholieke Univ. Leuven
De Brabanter, Jos — Katholieke Univ. Leuven
Suykens, Johan — K.U. Leuven
De Moor, Bart — K.U.Leuven

It is a well-known problem that obtaining a correct bandwidth in nonparametric regression is difficult in the presence of correlated errors. There exist a wide variety of methods coping with this problem, but they all critically depend on a tuning procedure which requires accurate information about the correlation structure. Since the errors cannot be observed, the latter is a hard goal to achieve. In this paper, we show the breakdown of several data-driven parameter selection procedures. We also develop a bandwidth selection procedure based on bimodal kernels which successfully removes the error correlation without requiring any prior knowledge about its structure. Some extensions are made to use such a criterion in least squares support vector machines for regression.

10:30-10:50 WeMT1.4

Possibilistic Validation of a Constraint-Based Model under Data Scarcity: Application to Pichia Pastoris Cultures

Tortajada, Marta — Biopolis S.L.
Llaneras, Francisco — Univ. Pol. de Valencia
Picó, Jesús — Univ. Pol. de Valencia

Constraint-based modelling allows building structured models of cells without accounting for intracellular kinetics. These models can be combined with experimental data to estimate the (pseudo-steady) state or phenotype exhibited by cells at given conditions, standing out as a useful analytical tool. In this work, a simplified, constraint-based model of *Pichia pastoris*, a widely recognized platform for recombinant protein expression, is derived from its metabolic network. Then, the model is validated against experimental data provided by different research groups: possibility theory is used to analyse the consistency between model and measurements. Afterwards, the biomass growth rate is estimated to illustrate the ability of the model to predict non-measured fluxes. The approach followed in this contribution is particularly useful in scenarios lacking data; it makes it possible to link the extracellular behaviour of *Pichia pastoris* during cultivation with its internal state, being a promising tool for optimization and monitoring industrial processes.

10:50-11:10 WeMT1.5

Possibilistic Estimation of Metabolic Fluxes During a Batch Process Accounting for Extracellular Dynamics

Llaneras, Francisco — Univ. Pol. de Valencia
Sala, Antonio — Univ. Pol. de Valencia
Picó, Jesús — Univ. Pol. de Valencia

Constraint-based models use the available knowledge about the operating constraints (e.g., mass balances and thermodynamic laws) to define a space of feasible states for cell cultures. Predictions can then be obtained incorporating experimental measurements of metabolite concentrations to perform a metabolic flux analysis. Although these predictions are typically static, aimed to study cells at given state, several works accounting for extracellular dynamics can be found in literature. In this work we formulate these predictions of time-varying fluxes and metabolites as possibilistic constraint satisfaction problems. The benefit of the described approach is that richer estimates are obtained —not only point-wise ones—, while considering uncertainty and even in scenarios of data scarcity. The method could also be the basis for on-line fault detection in industrial processes.

WeMT2 Room A

Nonlinear Model Predictive Control (Regular Session)

Chair: Patwardhan, Sachin — Indian Inst. of Tech. Mumbai

Co-Chair: Imsland, Lars — Norwegian Univ. of Science and Tech.

09:30-09:50 WeMT2.1

On Gradient Computation in Single-Shooting Nonlinear Model Predictive Control

Ringset, Ruben — Cybernetica AS

Imsland, Lars — Norwegian Univ. of Science and Tech.

Foss, Bjarne A. — Norwegian Univ. of Science & Tech.

This paper gives an overview of methods for computing derivative information in dynamic optimization with path constraints. Efficiency of forward and adjoint techniques are discussed in a discrete-time setting and some algorithms are derived. Next, the discussion is extended to also include continuous-discrete systems. Dimensions in the model, signal parameterization, horizon length and sampling interval affect each of the methods differently. The key contribution of this paper is to give an overview of these methods, how they can be combined, and how different parameters affect efficiency.

09:50-10:10 WeMT2.2

Adaptive Quasi-Infinite Horizon NMPC of a Continuous Fermenter

Huang, Rui — Carnegie Mellon Univ.

Patwardhan, Sachin — Indian Inst. of Tech. Mumbai

Biegler, Lorenz T. — Carnegie Mellon Univ.

Uncertainties inherent in biological systems make control of continuous fermenters a challenging task. This work proposes to integrate the quasi-infinite horizon nonlinear model predictive control (NMPC) algorithm, with an adaptive state and parameter estimator. As a result, the quasi-infinite horizon NMPC can be applied to systems with only part of the states measured. Moreover, the adaptive parameter estimation can update the uncertainty parameter online in the presence of plant-model mismatch. Two variations of target setting optimization problem are proposed to adjust the equilibrium points when they drift away due to the plant-model mismatch. The proposed method is applied to a fermenter with partial state feedback.

10:10-10:30 WeMT2.3

Sequential and Iterative Distributed Model Predictive Control of Nonlinear Process Systems Subject to Asynchronous Measurements

Christofides, Panagiotis D. — Univ. of California at Los Angeles

Chen, Xianzhong — Univ. of California, Los Angeles

Liu, Jinfeng — Univ. of California, Los Angeles

Muńoz de la Peńa, David — Univ. de Sevilla

In this work, we focus on sequential and iterative distributed model predictive control (DMPC) of large scale nonlinear process systems subject to asynchronous measurements. Assuming that there is an upper bound on the maximum interval between two consecutive asynchronous measurements, we design DMPC schemes that take into account asynchronous feedback explicitly via Lyapunov techniques. Sufficient conditions under which the proposed distributed control designs guarantee that the states of the closed-loop system are ultimately bounded in regions that contain the origin are provided. The theoretical results are illustrated through a catalytic alkylation of benzene process example.

10:30-10:50 WeMT2.4

Offset-Free Nonlinear Model Predictive Control Based on Moving Horizon Estimation for an Air Separation Unit

Huang, Rui — Carnegie Mellon Univ.
Patwardhan, Sachin — Indian Inst. of Tech. Mumbai
Biegler, Lorenz T. — Carnegie Mellon Univ.

Air separation units (ASU) pose a classic problem for nonlinear system control. This paper proposes a framework that integrates nonlinear model predictive control (NMPC) and moving horizon estimation (MHE). We prove that the proposed method achieves offset free regulatory behavior, even in the presence of plant-model mismatches. If the plant uncertainty structure is known, the proposed framework can be modified to estimate the uncertainty parameters. Thus, the model used in the NMPC and MHE can be adaptively modified online. Finally, the proposed method is applied on a large scale air separation unit, and the steady state offset free behavior is observed.

10:50-11:10 WeMT2.5

NMPC of a Continuous Fermenter Using Wiener-Hammerstein Model Developed from Irregularly Sampled Multi-Rate Data

Dasgupta, Dwaipayan — Indian Inst. of Tech. Bombay
Patwardhan, Sachin — Indian Inst. of Tech. Mumbai

Control of a bio-reactor is a complex task due to inherent non-linearities and unavailability of measurements of the quality variables at regular sampling intervals. In this work, it proposed to identify Wiener-Hammerstein type fast-rate time series models for the quality variables directly from the irregularly sampled multi-rate input-output data. The identified models are further used to develop a multi-rate nonlinear predictive controller. The efficacy of the proposed modelling and control scheme is demonstrated by conducting simulation studies on a continuous fermenter system that exhibits input multiplicity and gain reversal in the desired operating region.

WeMT3 Room B

Systems Biology II (Regular Session) (Joint DYCOPS/CAB Session)

Chair: Bullinger, Eric Univ. of Liege

09:30-09:50 WeMT3.1

Parametric Condition for Multistationarity in Biochemical Reaction Networks

Otero Muras, Irene ETH Zurich
Banga, Julio R. IIM-CSIC (Spanish Council for Scientific Res.
Alonso, Antonio A. IIM-CSIC

Chemical Reaction Network theory allows us to decide whether many classes of networks have the capacity for multiple positive equilibria, based on their structural properties. In this way, the deficiency zero theorem asserts that every weakly reversible network of zero deficiency has a unique equilibrium, in spite of the values of the parameters. We make use and extend CRNT results aiming not only to discriminate whether a (positive deficiency) network can exhibit multiple steady states, but also to characterize the whole space of the parameters regarding to their capability to produce multiplicities. In this work, we provide a condition, on the parameters of biochemical networks, for the appearance of multiple steady states.

09:50-10:10 WeMT3.2

A Robustness Measure for the Stationary Behavior of Gene Regulation Networks

Breindl, Christian Univ. Stuttgart
Waldherr, Steffen Univ. of Stuttgart
Allgower, Frank Univ. of Stuttgart

In this paper the stationary behavior of uncertain and possibly multistable gene regulation networks is considered. We first introduce a modeling framework which is able to represent the qualitative knowledge which is typically available for these systems. Then we turn to the problem of model discrimination: Given several alternative model structures that can all reproduce the experimental observations, is it possible to decide which structure may be the most appropriate description of the real system. To this end, a robustness measure for qualitative multistable gene regulation networks is introduced and also a method for the computation of this measure is presented. The benefit of the developed method is twofold: On the one hand it allows to compare the robustness properties of different model structures, on the other hand also the most fragile interconnections of a network can be detected. Finally, an example network is analyzed with this method.

10:10-10:30 WeMT3.3

Solutions of Weakly Reversible Chemical Reaction Networks Are Bounded and Persistent

August, Elias ETH
Barahona, Mauricio Imperial Coll. London

We present extensions to chemical reaction network theory which are relevant to the analysis of models of biochemical systems. We show that, for positive initial conditions, solutions of a weakly reversible chemical reaction network are bounded and remain in the positive orthant. Thus, weak reversibility implies persistence as conjectured by Martin Feinberg. Our result provides a qualitative criterion to establish that a biochemical network will not diverge or converge to the boundary, where some concentration levels are zero. It relies on checking structural properties of the graph of the reaction network solely. It can also be used to characterise certain bifurcations from stationary to oscillatory behaviour. We illustrate the use of our result through applications.

10:30-10:50 WeMT3.4

Damping Feedback Stabilization for Cyclic Interconnections Systems: Oscillations Suppression and Synchronization

Hudon, Nicolas Queen's Univ.
Guay, Martin Queen's Univ.

This paper considers the problem of stabilizing (bio)chemical reaction networks that can be represented as cyclic interconnections. The objective of the paper is to present a constructive way to compute a dissipative potential function for the system. This potential is then used for constructing a smooth feedback stabilizing controller. We obtain a characteristic one-form for the system by taking the interior product of a non vanishing two-form with respect to the drift vector field. A homotopy operator is then constructed locally around the desired equilibrium, leading to the computation of a dissipative potential for the system. The dynamics of the system is then decomposed into an exact part and an anti-exact one. The exact part is generated by a potential, that is used to construct the smooth stabilizing feedback, under the so-called weak Jurdjevic–Quinn conditions.We consider the problems of oscillations suppression and synchronization of oscillators as illustrations of potential applications of the proposed method.

10:50-11:10 WeMT3.5

Global Sensitivity and Identifiability Implications in Systems Biology

Dobre, Simona Nancy Univ.
Bastogne, Thierry Univ. Henri Poincaré, Nancy 1
Richard, Alain Univ. Henri Poincaré, Nancy 1

In systems biology, a common approach to model biological processes is to use large systems of differential equations. The associated parameter estimation problem requires to prior handle identifiability and sensitivity issues in a practical biological framework. The lack of method to assess global practical identifiability has leaded us

to analyze and establish bridges between global sensitivity and identifiability measures. Specifically, we are interested in deriving conditions of global practical non-identifiability in association with global sensitivity results. Two cases are considered: i) insensitive (or non-observable) parameters; ii) two (or more) correlated sensitivity measures of the model output with respect to model parameters. Propositions of relationships between sensitivity and identifiability, and their proofs are developed herein. Academic examples are also treated in order to illustrate contents of these propositions.

WeMT4 Room C

Modeling and Control of Environmental Processes (Regular Session)
(Joint DYCOPS/CAB Session)

Co-Chair: Baratti, Roberto Univ. degli Studi di Cagliari

09:30-09:50 WeMT4.1

Modeling of the Fouling Probability of an Activated Sludge Dryer

Peeters, Bart Monsanto
Dewil, Raf Campus De Nayer - Katholieke Univ. Leuven
Van Impe, Jan F.M. Katholieke Univ. Leuven
Smets, Ilse BioTeC - Bioprocess Tech. And Control

Better understanding (and so better control) of the stickiness phenomenon of drying sludge is critical for proper operation of a variety of industrial dryers, as is the case for the combined centrifuge-dryer system used on the Monsanto Europe site in Antwerp, Belgium. In this paper a binary logistic regression analysis is performed on a 4-years data base, which resulted in an empirical model for the evaluation of the dryer fouling probability as function of changes in the Sludge Volume Index (SVI) and the dosing of clay additive and tertiary (flotation) sludge to the main secondary (biological) sludge feed to the system. According to the research results, a decreasing SVI increases the probability of obtaining fouling in the dryer. Furthermore, in periods of low SVI, the fouling probability can be reduced significantly by reducing the clay dosing. This extended analysis confirms the hypothesis formulated earlier (Peeters et al., 2009a) that a wetter cake (induced by high SVI and low clay dosing) at the beginning of the drying stage of this system is better to avoid drying sludge fouling the dryer wall.

09:50-10:10 WeMT4.2

Damping Feedback Stabilization of a Wastewater Treatment Plant

Hudon, Nicolas Queen's Univ.
Guay, Martin Queen's Univ.

This paper considers the problem of stabilizing a wastewater plant using damping feedback controller. The nonlinear model used is the AM1 anaerobic digestion model. The proposed approach consists in using a damping state feedback controller that renders a desired equilibrium stable through feedback. We first construct an approximate dissipative potential function centered at the desired equilibrium for the drift system. Then, a damping feedback controller is computed based on the Jurdjevic--Quinn approach. Through numerical simulations, we show that the resulting controller stabilizes the desired equilibrium, and keeps the pollutant at the desired level when input disturbances are applied to the system.

10:10-10:30 WeMT4.3

Improved Economic Operation of MSWC Plants with a New Model Based PID Control Strategy

Leskens, Martijn — Delft Univ. of Tech.
van 't Veen, Peter-Paul — TNO Science and Industry
van Kessel, Robert — KEMA Netherlands B.V.
Bosgra, Okko — Delft Univ. of Tech.
Van den Hof, Paul M.J. — Delft Univ. of Tech.

Municipal solid waste combustion (MSWC) plant operators are currently under an increasing pressure to optimize the economic performance of their plants. A route with high potential for optimizing this performance is by improving the performance of the MSWC plant combustion control system, which typically is of the PID-type. In this paper, motivated by the industrial need to improve the overall economic MSWC plant performance, a model based approach is taken to optimize this control system, using recently derived black and white box MSWC plant models. More specific, from a closer analysis of the dynamics of these models a new PID-type of MSWC plant combustion control strategy is derived. It is shown that this new control strategy has improved setpoint tracking properties compared to PID-type of combustion control strategies typically encountered in the industry. As a result, a significant improvement of the economic performance of an MSWC plant will be obtained when replacing such a control strategy for the new one. However, no improvement of the disturbance rejection properties of existing PID-type of combustion control strategies has been observed with the new control strategy, which would also lead to a significant improvement of the economic performance of an MSWC plant, indicating that other, non-PID, types of combustion control strategies are required for that.

10:30-10:50 WeMT4.4

Optimized Control Structure for a Wastewater Treatment Benchmark

Mulas, Michela — Helsinki Univ. of Tech.
Araujo, Antonio Carlos Brandao de — Federal Univ. of Campina Grande UFCG
Baratti, Roberto — Univ. degli Studi di Cagliari
Skogestad, Sigurd — Norwegian Univ. of Science & Tech.

In this paper, we define and implement the design of an optimized control structure for the activated sludge process given as COST/IWA benchmark simulation model No.1. Emphasis is given to the identification of controlled variables that contribute to minimize economic costs while the effluent requirements are met. This is achieved considering the self-optimizing procedure as reference method for the controlled variables selection. The proposed optimal control strategy consist of multivariable PID loops which manipulate the airflow rate in the aerobic basins, the nitrate and sludge recirculation flows and the waste sludge flow proportionally to the influent flow such that the overall cost function is minimized. Dynamic simulations validate the resulting optimized controller structure, showing that minimal costs can be achieved.

10:50-11:10 WeMT4.5

Model Reduction of the ASM3 Extended for Two-Step Nitrification

Cruz Bournazou, Mariano Nicolas TU-Berlin
Arellano-Garcia, Harvey TU Berlin
Wozny, Günter TU-Berlin
Lyberatos, Gerasimos Univ. of Patras
Kravaris, Costas Univ. of Patras

The Activated Sludge Model No. 3 (ASM3) extended for two-step nitrification is analyzed and reduced to enable fast and accurate simulations under typical process conditions. Due to the addition of a storage equation, ASM3 enables the description of the substrate consumption as well as the Oxygen uptake with a higher precision than the older versions of the family of ASM. In addition the extension of the model to describe the two step nitrification enables the calculation of NO2- and NO3- concentrations during the process. An exhaustive analysis of the model results in a number of modifications, which reduced the model drastically, while keeping its description accuracy.

WePlenaryT5 Room ZVH
Plenary Session 4 (Plenary Session) (Joint DYCOPS/CAB Session)
Chair: Vande Wouwer, Alain Univ. de Mons

11:30-12:30 WePlenaryT5.1

Hurdles and Challenges for Modelling and Control of Microalgae for CO2 Mitigation and Biofuel Production

Bernard, Olivier Inria

Oleaginous microalgae are seen as a potential major biofuel producer in the future since, under conditions of nitrogen deprivation, they can contain high amounts of lipids, while they consume CO2 from power plants. These photosynthetic microorganisms are however rather different from the microorganisms usually used in biotechnology. In particular, predicting the behaviour of microalgal based processes is delicate because of the strong interaction between biology (microalgal development and respiration), and physics (light attenuation and hydrodynamics). This paper reviews existing models, and in particular Droop Model which has been widely used to predict microalgal behaviour under nutrient limitation. It details a model for photobioreactors or raceways, when both light and nutrients are limiting. The challenges and hurdles to improve photobioreactor modelling and control in order to optimise biomass or biofuel production are then discussed.

WeAT1 Room ZVH

Process and Performance Monitoring I (Regular Session)

Chair: Kano, Manabu Kyoto Univ.

Co-Chair: Scali, Claudio Univ. of Pisa

14:00-14:20 WeAT1.1

Control Performance Assessment for Hammerstein-Wiener Models

Yu, Wei The Univ. of Auckland

Wilson, David I. Auckland Univ. of Tech.

Harris, Tom Queen's Univ.

Young, Brent Univ. of Auckland

Control performance assessment, or CPA, is an increasingly vital tool to quantify the performance of industrial control loops. While most of the research and commercial activity in CPA has been applied to linear systems to date, those researchers investigating nonlinear systems fall into one of two groups.

The first group focused on the diagnosis of a common specific nonlinearity, namely valve stiction, while the second group tried to establish the minimum variance performance lower bound (MVPLB).

In this paper we will continue to investigate CPA for a popular and versatile class of nonlinear model; the Hammerstein-Wiener (HW) model. Since the minimum performance lower bound is hard to establish for nonlinear systems, we propose two new performance indices which can be reliably estimated from the routine closed loop data.

These indices can be used in a manner similar to the standard linear CPA performance index. The estimates are obtained by fitting the output data to a nonlinear autoregressive and moving average (NARMA) model. The results of two simulation examples illustrate that the proposed methodology is efficient and accurate for the class of HW models.

14:20-14:40 WeAT1.2

A Simple Harmonics Based Stiction Detection Method

Ahammad, Monir Bangladesh Univ. of Engineering and Tech.

Choudhury, M.A.A. Shoukat Bangladesh Univ. of Engineering Tech.

Oscillation or large variability of the control loops results decreased economical advantage to process industries due to inferior quality products, larger rate of rejections, reduced average throughput and overall increased energy requirements. Stiction is one of the root cause of oscillation. Many studies suggest that 30% of the control loops are oscillatory because of control valve problems such as stiction, deadband and hysteresis. In this study, a simple method has been developed to detect stiction. It has been shown that stiction in control valves produces signals containing odd harmonics. The proposed method estimates frequencies and amplitudes of control error signal using least square method. Then, harmonic

relations among the frequencies are examined. The presence of odd harmonics indicates valve stiction. The method has been evaluated successfully using simulated, experimental and industrial data sets.

14:40-15:00 WeAT1.3

Detection of Significant Model-Plant Mismatch from Routine Operation Data of Model Predictive Control System

Kano, Manabu — Kyoto Univ.
Shigi, Yohei — Kyoto Univ.
Hasebe, Shinji — Kyoto Univ.
Ooyama, Satoshi — Mitsubishi Chemical Corp.

The maintenance of model predictive control (MPC) systems is one of the major problems identified by industrial process control engineers. Since performance deterioration is usually caused by changes in process characteristics, effective re-modeling is the key to success. Obviously, not all sub-models have to be reconstructed; thus, it is crucial to identify sub-models that have significant model-plant mismatch. In the present work, a novel method is proposed for significant model-plant mismatch detection from routine closed-loop operation data on the basis of the statistical test concept. The effectiveness of the proposed method is demonstrated through case studies. The results clearly show not only that the proposed method can detect sub-models that have significant mismatch but it is superior to the other methods based on multivariate analysis.

15:00-15:20 WeAT1.4

Key Parameters Calibration and Benefits Evaluation of a Closed Loop Performance Monitoring System

Scali, Claudio — Univ. of Pisa
Marraccini, Stella — Univ. of Pisa (italy)
Farnesi, Marco — ENI, Refining & Marketing, Raffineria di Livorno (Italy)

The paper presents results from field validation of a closed loop performance monitoring system installed on several units of a refinery plant. The system supervises more than 1200 base control loops and evaluates performance periodically, after scheduled data acquisitions followed by off-line analysis. The first point taken into account is a comparison between verdicts issued by the system and indications by control operators: the large number of issued verdicts indicating scarce performance, but considered still acceptable by operators, results practically in False Alarm and forced to revisit the criterion adopted to classify a response as excessively oscillatory. New threshold values for the widely used Hägglund criterion (1995) were found and similar criteria were proposed and compared in order to match operators practical indications. The efficiency of criteria and threshold values depend on the type of loop (i.e. flow, pressure, level or temperature). The second point examined concerns validation of valve stiction diagnosis: indications from the monitoring systems are compared with evidence before and after plant shut down. Results confirm that oscillations in valves indicated as sticky disappeared after the

operation, while many valves which underwent the maintenance procedure on the basis of a time schedule did not require it. Therefore, a systematic application of diagnostics tools for maintenance scheduling would be beneficial in order to focus on real needs and avoid unnecessary revision costs.

15:20-15:40 WeAT1.5

Identification of Noise Covariances for State Estimation of a Continuous Fermenter Using Extended EM Algorithm

Bavdekar, Vinay Indian Inst. of Tech. Bombay
Patwardhan, Sachin Indian Inst. of Tech. Mumbai

Despite developments in sensor technology, monitoring a biological process using regular sensor measurements is often difficult. Development of Bayesian state observers, such as extended Kalman filter(EKF), is an attractive alternative for soft-sensing of such complex systems. The performance of EKF is dependent on the accurate characterisation of the uncertainties in the state dynamics and in the measurements. In this work, an extended expectation maximisation (EM) algorithm is developed for estimation of the state and measurement noise covariances for the EKF using irregularly sampled multi-rate measurements. The efficacy of the proposed approach is demonstrated on a benchmark continuous fermenter system. The simulation results reveal that the proposed approach generates fairly accurate estimates of the noise covariances.

15:40-16:00 WeAT1.6

Correlation-Based Spectral Clustering for Flexible Soft-Sensor Design

Fujiwara, Koichi Kyoto Univ.
Kano, Manabu Kyoto Univ.
Hasebe, Shinji Kyoto Univ.

The current issues concerning soft-sensors are how to cope with changes in process characteristics and how to cope with parallelized, slightly different, multiple processes. To make soft-sensors adaptive and flexible, the development of practical design techniques, instead of impracticable ideas, is crucial; this is the motivation of the present research. In practice, it is difficult to successfully apply a single soft-sensor to parallelized production devices due to their individual difference. Since the individual difference is expressed as difference of the correlation among variables, it is useful to classify samples into multiple clusters according to the correlation in order to adopt a multi-model approach. In the present work, a new correlation-based clustering method, referred to as NC-spectral clustering, is proposed by integrating the nearest correlation (NC) method and spectral clustering. The NC method can detect samples that are similar to the query from the viewpoint of the correlation. In the proposed method, the NC method is used for constructing the weighted graph that expresses the correlation-based similarities between samples and the constructed graph is partitioned by using spectral clustering. In addition, a new soft-sensor design method is proposed on the basis of the proposed NC-spectral clustering. The superiority of the proposed method over conventional methods is demonstrated through a numerical example and a case study of parallelized batch processes.

WeAT2 Room A

Optimization and Control of Continuous Chemical Reactors (Regular Session)

Chair: Romagnoli, Jose — Louisianna State Univ.

Co-Chair: Dochain, Denis — Univ. Catholique de Louvain

14:00-14:20 WeAT2.1

Power-Shaping Control of the CSTR: From Thermodynamics to the Brayton-Moser Formulation of the Dynamics

Favache, Audrey — Univ. catholique de Louvain

Dochain, Denis — Univ. Catholique de Louvain

The non-isothermal continuous stirred tank reactor (CSTR) is a classical yet complex case study of nonlinear dynamical systems. Power-shaping control is a recent approach for the control of nonlinear systems based on the physics of the dynamical system and it rests on the formulation of the dynamics in the Brayton-Moser form. The Brayton-Moser formulation of the non-isothermal continuous stirred tank reactor is investigated based on physical considerations on the system.

14:20-14:40 WeAT2.2

Hamiltonian Formulation and IDA-PBC Control of Non Isothermal Continuous Stirred Tank Reactors

Hoang, Ngoc Ha — Univ. Claude Bernard Lyon 1

Couenne, Francoise — Univ. of Lyon 1

Jallut, Christian — Univ. Claude Bernard Lyon 1

Le Gorrec, Yann — FEMTO-ST

This paper proposes a pseudo port Hamiltonian formulation of non isothermal Continuous Stirred Tank Reactor (CSTR) model. This structured modeling shows how the opposite of the entropy can be used as Hamiltonian function and how the associated dissipation can be related to the irreversible entropy production due to chemical reaction. The IDA-PBC approach based control is then applied to stabilize the continuous system about an unstable equilibrium point. The chosen control variables are the jacket temperature and the inlet molar flow rate. The chosen hamiltonian storage function of the closed loop system is the thermodynamic availability function. Theoretical developments are illustrated on a first order chemical equilibrated reaction. Some stability properties and analysis of the admissibility of the control variables are given.

14:40-15:00 WeAT2.3

LQ Control of Coupled Hyperbolic PDEs and ODEs: Application to a CSTR-PFR System

Alizadeh Moghadam, Amir — Univ. of Alberta

Aksikas, Ilyasse — Univ. of Alberta

Dubljevic, Stevan — UCLA

Forbes, J. Fraser — Univ. of Alberta

In this paper an infinite-dimensional LQR control-based design for a system containing linear hyperbolic partial differential equations coupled with linear ordinary differential equations is presented. The design is based on an infinite-dimensional Hilbert state-space representation of the coupled system. The feedback control gain is obtained by solving algebraic and differential matrix Riccati equations that result from an operator Riccati equation solution. The designed LQR control is applied to a system containing a continuous stirred tank reactor (CSTR) and a plug flow reactor (PFR) in series with the recycle-rate from PFR to CSTR as controlled variable. The LQR controller's performance is evaluated by numerical simulation of the original nonlinear system.

15:00-15:20 WeAT2.4

Super-Twisting Observer-Based Output Feedback Control of a Class of Continuous Exothermic Chemical Reactors

Moreno, Jaime A. — Univ. Nacional Autonoma de Mexico-UNAM
Alvarez, Jesus — Univ. Autonoma Metropolitana
Rocha-cozatl, Edmundo — Facultad de Ingeniería. Univ. Nacional Autonoma De Mexico
Diaz-Salgado, Jorge — Univ. nacional Autonoma de Mexico

In this paper, the problem of designing an output feedback (OF) stabilizing control scheme for (possibly open-loop unstable) exothermic reactors with temperature measurements is addressed. The proposed OF controller consists of the combination of a nonlinear state-feedback (SF) passive controller (built by passivation by backstepping) with a finite-time robustly convergent Supertwisting Observer (STO). The approach is tested with a representative example through simulations finding that the proposed controller behavior outperforms the one of its couterpart implemented with an asymptotic (infinite-time convergent) Extenden Kalman Filter (EKF).

15:20-15:40 WeAT2.5

Optimal Startup Operation of Simulated Moving Bed Chromatographic Processes

Li, Suzhou — Max-Planck-Inst. for Dynamics of Complex Tech. Systems
Kawajiri, Yoshiaki — Georgia Inst. of Tech.
Raisch, Joerg — Tech. Univ. Berlin
Seidel-Morgenstern, Andreas — Otto-von-Guericke Univ.

SMB represents one of the widely established periodic adsorption processes and its periodic and nonlinear dynamics presents a significant challenge to the formulation and solution of the optimal startup issue. A multistage startup concept allowing to adjust operating conditions stage-wise is proposed. The startup problem is then formulated aiming at driving the system towards the reference cyclic steady state (CSS) in an optimum manner. A tailored decomposition algorithm is developed to

tackle the resulting optimization problem and guarantee numerical tractability. The feasibility of the solution approach is demonstrated on a binary separation with nonlinear competitive isotherms. It is found that the new startup policy dramatically reduces transient time and desorbent consumption. The startup performance in terms of product concentration and purity is also evaluated quantitatively.

15:40-16:00 WeAT2.6

A Performance Study of a Novel Dynamic Real-Time Optimisation Engine Applied to an Industrial Continuous Pulping System

Rolandi, Pablo Adrian — Process Systems Enterprise ltd
Romagnoli, Jose — Louisianna State Univ.

In this work we present a flexible real-time dynamic optimisation engine that successfully decouples the controller design and innovation space into three orthogonal axes given by the model formulation, the problem formulation and the solution methods. A simulation of an industrial continuous pulping system is used to run several performance studies with an emphasis on the effect of different model formulations in various production transition scenarios.

WeAT3 Room B

Dynamic Process Optimization (Regular Session)

Chair: Perrier, Michel Ec. Pol.

Co-Chair: Gopaluni, Ratna Bhushan Univ. of British Columbia

14:00-14:20 WeAT3.1

Hybrid Shooting - a New Optimization Method for Unstable Dynamical Systems

Hartwich, Arndt RWTH Aachen Univ.

Assassa, Fady RWTH Aachen Univ.

Marquardt, Wolfgang RWTH Aachen Univ.

Chemical processes are modeled by large-scale, highly-nonlinear process models often governed by unstable dynamics. Dynamic optimization is required to exploit economical performance of these processes in their unstable regions. On the one hand, direct single shooting is able to solve large-scale dynamic optimization problems, but lacks the ability to cope properly with unstable dynamical systems. On the other hand, the multiple shooting method is capable of dealing with instabilities but results in larger optimization problems. This work deals with a novel parameterization approach, termed *hybrid shooting*, which combines the advantages of single and multiple shooting into one approach. Similar to multiple shooting, stages are introduced and states with unstable properties are parameterized by free initial values at the beginning of each stage. This approach signi_cantly enhances the behavior of the optimization problem by improving the condition of the underlying initial value problem (IVP).

14:20-14:40 WeAT3.2

Global Optimization of Two-Input Systems Using Multi-Unit Adaptation

Esmaeilzadeh Azar, Farhad Ec. Pol. Montreal

Perrier, Michel Ec. Pol.

Srinivasan, B. Ec. Pol. Montreal

Model-free unconstrained real-time optimization can be realized by controlling the gradient to zero. In this paper, the multiunit optimization framework is used where the gradient is estimated using finite difference between two identical units operating with an offset. It has been recently shown that the global optimization is achieved by reducing this offset to zero for scalar nonlinear maps. In this paper, this scheme is extended to the case of two-input systems, by repeating mono-variable global optimization on the circumference of a circle of reducing radius. The theoretical concepts are illustrated on the global optimization of two examples.

14:40-15:00 WeAT3.3

A Simultaneous Approach for Correcting Differences between Units in Multi-Unit Optimization

Woodward, Lyne — École Pol. de Montréal
Perrier, Michel — Ec. Pol.
Srinivasan, B. — Ec. Pol. Montreal

Multi-unit optimization is a recently proposed extremum-seeking technique where the gradient, estimated by finite difference between two identical units, is controlled to zero. The main assumption of having two identical units is rarely verified in practice and it has been noted that differences in the static characteristics can affect the stability and the equilibrium point. So, correctors have been proposed, where optimization and correction for differences are performed alternatively. This, in turn, causes a discontinuous operation leading to a hybrid dynamics. To avoid such a scenario, an approach where optimization and correction take place simultaneously, is presented. A proof of stability of the simultaneous scheme is also provided.

15:00-15:20 WeAT3.4

Solving Infeasibilities in Dynamic Optimization Problems

Almeida, Euclides — Petrobras
Secchi, Argimiro R. — PEQ - COPPE/UFRJ

DRTO Systems sometimes present failures when solving dynamic optimization problems. There are situations where the infeasibilities are due to the initial conditions, changing of constraints during the operation, or even in presence of conflicts between some specifications. The proposed method consists in solving these infeasibilities by reformulating the DAOP as a multi-objective optimization problem by relaxing the constraints. The goal programming approach was used to solve the dynamic optimization problem. Two examples, exploring different characteristic of these kinds of problems, were used to illustrate the methodology. The results show the ability of the proposed approach in locating and solving the infeasibilities, increasing the robustness of DRTO systems.

15:20-15:40 WeAT3.5

Economic Performance Assessment with Optimized LQG Benchmarking in MIMO Systems

Marshman, Devin James — Univ. of British Columbia
Chmelyk, Terrance — NORPAC Controls
Sidhu, Manny — NORPAC Controls
Gopaluni, Ratna Bhushan — Univ. of British Columbia
Dumont, Guy — Univ. of British Columbia

The objective of an economic performance assessment strategy is to quantitatively measure the effectiveness of a process in an economic framework. Such procedures typically involve the comparison of current operation with an appropriate benchmark to determine potential improvement through improved process control. In this work, a linear quadratic Gaussian (LQG) controller is used as a benchmark under conditions

of uncertainty. By relating key process variables to a function describing the profitability of a process, the current and potential (with LQG control) modes of operation can be assessed in an economic framework. This work provides an approach to such an assessment for a MIMO system through economic optimization of an LQG controller weighting matrix, and illustrates results in the form of a case studies.

15:40-16:00 WeAT3.6

Combining Direct and Indirect Methods for Optimal Control - a Case Study

Hannemann, Ralf RWTH Aachen Univ.
Marquardt, Wolfgang RWTH Aachen Univ.

Adaptive control vector parameterization for the solution of optimal control problems approximates the original infinite-dimensional optimal control problem by a set of finite-dimensional nonlinear programs (NLPs) whose control grids are iteratively refined. The refinement is stopped by a heuristic stopping criterion. The Hessians of the Lagrangian of these NLPs can be efficiently computed by the technique of composite adjoints as recently proposed by the authors. By means of a case study, namely the optimal control of the Williams-Otto semi-batch reactor, we show how to interpret composite adjoints as estimates for the continuous adjoints referred to by Pontryagin's Minimum Principle. Thus, these composite adjoints can be used to (i) construct a novel and mathematical sound stopping criterion for the iterative refinement of the control grid and to (ii) setup an indirect multiple shooting method the solution of which verifies and improves the approximate solution to the exact one.

WeAT4 Room C

Control of Biological Processes (Regular Session)
(Joint DYCOPS/CAB session)

Chair: Dochain, Denis Univ. Catholique de Louvain

14:00-14:20 WeAT4.1

Batch-To-Batch Iterative Learning Control of a Fed-Batch Fermentation Process Using Incrementally Updated Models

Jewaratnam, Jegalakshimi Newcastle Univ.
Zhang, Jie Univ. of Newcastle Upon Tyne
Azlan Hussain, Mohd Univ. of Malaya
Morris, Julian Newcastle Univ.

Batch-to-batch iterative learning control of a fed-batch fermentation process using batchwise linearised models identified from process operation data is presented in this paper. Due to model-plant mismatches and the present of unknown disturbances, off-line calculated control policy may not be optimal when implemented to the real process. The repetitive nature of batch process allows information from the previous batches being used in modifying the control policy of the next batch in the framework of iterative learning control. In order to cope with nonlinear behaviour of batch fermentation processes, the model is linearised using the immediate previous batch as a reference batch and the model is updated from batch to batch. The control policy (feed rates) at different batch stages are generally correlated as the overall control policy is obtained to maximize the amount of product at the end of a batch. To address the colinearity issue of the control variable, principal component regression and partial least squares regression are used in estimating the linearised model parameters. Application results on a simulated industrial scale fed-batch fermentation process demonstrate that the proposed strategy is effective.

14:20-14:40 WeAT4.2

***Neurofuzzy Control Strategy for an Abattoir Wastewater Treatment Process*,**

Carlos-Hernandez, Salvador Cinvestav, Unidad Saltillo
Sanchez, Edgar N. CINVESTAV
Bueno, J. Andres Cinvestav Guadalajara

In this paper a neurofuzzy control strategy, composed by a neural observer and a fuzzy supervisor, for an anaerobic wastewater treatment process is proposed. The neural observer is based on a recurrent high order neural network (RHONN) which is trained by an extended Kalman filter. The main objective of the observer is to estimate methanogenic biomass, which is employed by a fuzzy supervisor. The tasks of this supervisor are: to detect the biological activity inside the bioreactor, to select and to apply an adequate control action depending on the operating conditions in order to avoid washout. The applicability of the proposed scheme is illustrated via simulations considering the model of a prototype bioreactor which is used to treat effluents collected from an abattoir.

14:40-15:00 WeAT4.3

Integration of Model-Predictive Scheduling, Dynamic Real-Time Optimization and Output Tracking for a Wastewater Treatment Process

Elixmann, David RWTH Aachen Univ.
Busch, Jan RWTH Aachen Univ.
Marquardt, Wolfgang RWTH Aachen Univ.

A hierarchical control architecture for the integration of scheduling decisions, dynamic real-time optimization and tracking control is proposed. It is shown how the discrete-continuous problem of simultaneous scheduling and trajectory optimization on a receding horizon can be integrated within the upper control layer of a two-layer architecture. On the upper layer, the optimal plant strategy defined by a sequence of control objectives and optimal control moves is computed on a long time horizon. The lower control layer consists of a state observer and a fast-acting tracking controller which operates on a short time horizon. The properties of this architecture are illustrated by a case study in which a wastewater treatment plant is operated under the influence of external disturbances. Conflicting operational objectives may be valid, depending on the state of the plant and the expected disturbances. By calculating an optimal sequence of operational strategies and control moves on the receding horizon, economically optimal operation of the plant can be achieved.

15:00-15:20 WeAT4.4

Minimal Time Control of Fed-Batch Processes with Growth Functions Having Several Maxima

Rapaport, Alain INRA
Dochain, Denis Univ. Catholique de Louvain

In this paper we address the issue of minimal time optimal control of fedbatch reactor in presence of complex non monotonic kinetics, that can be can be typically characterized by the combination of two Haldane models. Global optimal trajectory results are provided on the basis of a numerical approach that considers smooth control inputs.

15:20-15:40 WeAT4.5

Observer-Based Output Feedback Linearizing Control Applied to a Denitrification Reactor

Torres, Ixbalank LAAS-CNRS
Queinnec, Isabelle LAAS-CNRS
Vande Wouwer, Alain Univ. de Mons

In this work a late lumping approach is used in order to design a state feedback linearizing controller for influent disturbance attenuation and regulating the nitrogen concentration at the output of a denitrification biofilter. This controller is associated to a distributed parameter observer to estimate all the states needed to compute the controlled input. It results in an output feedback nonlinear controller with stable closed-loop dynamics.

15:40-16:00 WeAT4.6

Adaptive Extremum Seeking Control of Fedbatch Bioreactors : The Single Measurement Case

Cougnon, Pascal — Univ. catholique de Louvain
Dochain, Denis — Univ. Catholique de Louvain
Guay, Martin — Queen's Univ.
Perrier, Michel — Ec. Pol.

In this paper, we present an adaptive extremum seeking control scheme for fed-batch bioreactors with Haldane kinetics. The proposed adaptive extremum seeking approach utilizes the structure information of the process kinetics to derive a seeking algorithm that drives the system states to the desired set-points that maximize the value of the biomass production. Unlike in previous works, it assumes that only the substrate concentration is available for on-line measurement. Lyapunov's stability theorem is used in the design of the extremum seeking controller structure and the development of the parameter learning laws. The performance of the approach is illustrated via numerical simulations.

WeET1 Room ZVH

Process and Performance Monitoring II (Regular Session)

Chair: Huang, Biao Univ. of Alberta

Co-Chair: Morris, Julian Newcastle Univ.

16:30-16:50 WeET1.1

Multiple Model Approach for Inferential Instruments Design

Domlan, Elom Ayih Department of Chemical and Materials Engineering, Univ. of

Huang, Biao Univ. of Alberta

Xu, Fangwei Syncrude Canada Ltd.

Espejo, Aris Syncrude Canada Ltd.

In this paper, an application of a multiple model approach for the design of inferential instruments is reported. The multiple model of interest presents a decoupled structure in the sense that the sub-models do not share the same state variable. A two-stage identification procedure is developed for the model identification and a soft sensor application is later conducted with the decoupled multiple model structure. The soft sensor aims at predicting a quality variable for an industrial separation unit. The decoupled multiple model structure allows obtaining a dynamical model for the soft sensor despite the presence of practical constraints related to multi-rate sampling problem. Real-time implementation results are presented.

16:50-17:10 WeET1.2

Measurement Structure Design for Multicomponent Distillation Column with Specific Estimation Objective

Frau, Andrea Univ. degli Studi di Cagliari

Baratti, Roberto Univ. degli Studi di Cagliari

Alvarez, Jesus Univ. Autonoma Metropolitana

In this work, the problem of designing the estimation structure to infer some of the effluent compositions in a multicomponent distillation column is addressed, with the aim being the determination of the structure that yields the best estimator functioning in the sense of a suitable compromise between performance versus complexity, regardless of the particular estimation algorithm employed. The structure design involves the selection of (i) the number of modeled components, (ii) the innovated components, and (iii) the number and locations of sensors. The consideration of the problem within the adjustable-structure geometric estimation framework in the light of the column characteristics leads to a methodology with an analysis stage, where structures are screened and candidate ones are produced, followed by a synthesis stage which yields the structure with the best estimator functioning. The proposed approach is applied through simulations to an industrial-type hexacomponent distillation column, finding that the estimation task can be adequately performed with a algorithm whose number of ODEs (77) is considerably smaller than the one (17390) that results from the direct application of the standard EKF technique.

17:10-17:30 WeET1.3

Global-Nonlinear Stochastic Estimation of Exothermic Reactors with Temperature Measurement

Tronci, Stefania — Univ. degli Studi di Cagliari
Balzano, Andrea — Univ. of Cagliari
Baratti, Roberto — Univ. degli Studi di Cagliari
Alvarez, Jesus — Univ. Autonoma Metropolitana

In this work, the problem of estimating the concentration of exothermic rectors with temperature measurement is addressed. The problem is treated within a global nonlinear stochastic framework, according to the Fokker Plank-based Kushner filtering theory. The on-line solution of the associated two-dimensional partial differential equation driven by the temperature measurements yields the evolution of the conditioned concentration-temperature probability density function (PDF), with considerable more information than the one provided by standard EKF based on a local-nonlinear approach. A catalytic reactor with deterministic multistability, experimental data, and previously addressed with EKF is addressed as case example, yielding: (i) the on-line evolution of the (possibly bimodal) conditioned concentration probability density function, and (ii) mean uncertainty values which are better than the ones drawn with EKF.

17:30-17:50 WeET1.4

Modified PI Controller for Stiction Compensation

Farenzena, Marcelo — Federal Univ. of Rio Grande do Sul
Trierweiler, Jorge Otávio — Federal Univ. of Rio Grande do Sul

Stiction is a well known problem of the process performance. Compensate its effect is essential, because most of sticky valves cannot be replaced and they remain working for months or years. The scope of this work is to propose a novel methodology to compensate stiction effects, through the modification of the controller (PI) block in the control loop. The proposed approach is based on the two moves method, however it allows to specify closed loop performances faster than open loop and reject load disturbances efficiently. We assume here that a small offset between process variable and setpoint is accepted, what decreases significantly the valve traveling, comparing with available approaches. The method is described for both setpoint tracking and disturbance rejection. The efficacy is corroborated by a case study, considering setpoint changes and disturbance rejection.

17:50-18:10 WeET1.5

A Novel State Space Stochastic Estimation Algorithm and Improved Fault Detection Using Combined Index Monitoring for Dynamic Processes

Stubbs, Shallon — Newcastle Univ.
Zhang, Jie — Newcastle Univ.
Morris, Julian — Newcastle Univ.

Larimore's state space model derivation and stochastic estimation algorithm, first published in 1983, have been the adopted standard for deriving the state variables and parameters of the five (5) matrices state space model representation which continues to be applied extensively in the literature for applications ranging from controls, system identification and process monitoring. This paper presents an alternate derivation and stochastic estimation algorithm. The paper also discusses how strategic classification of the process inputs may, for some applications, facilitate the use of a simplified stochastic estimation algorithm. The alternative state space modeling approaches demonstrated better fault monitoring statistic performance for specific types of faults simulated. The canonical variate based state space modeling approaches were evaluated on a simulate CSTR process – with recycle through a heat exchanger. The results demonstrates the potential benefits to be derived from using a combined monitoring index based upon monitoring statistics derived from independent state space models for improved overall fault detecting capabilities and reliability of the fault monitoring scheme.

18:10-18:30 WeET1.6

Lattice-Size Dependence and Dynamics of Surface Mean Slope in a Thin Film Deposition Process

Huang, Jianqiao Univ. of California at Los Angeles
Hu, Gangshi Univ. of California at Los Angeles
Christofides, Panagiotis D. Univ. of California at Los Angeles

This work focuses on the study of the dynamic behavior and lattice size dependence of the surface root-mean-square slope in a porous thin film deposition process taking place on a triangular lattice. The simulation results indicate that the expected mean slope square reaches quickly a steady-state value and exhibits a very weak dependence with respect to lattice size variation. The simulation findings are corroborated by an analysis of appropriate finite-difference discretizations of surface height profiles computed by an Edwards-Wilkinson-type partial differential equation that can be used to describe the dynamics of surface height profile in the thin film deposition process under consideration.

WeET2 Room A

Modelling, Control and Optimization of Energy Systems - II (Invited Session)

Chair: Budman, Hector M. Univ. of Waterloo
Co-Chair: Christofides, Panagiotis D. Univ. of California at Los Angeles
Organizer: Budman, Hector M. Univ. of Waterloo

16:30-16:50 WeET2.1

Control of Solar Power Systems: A Survey

Camacho, Eduardo F. Univ. of Seville
Berenguel, Manuel Univ. of Almeria
Limon, Daniel Univ. de Sevilla
Alvarado, Ignacio Univ. of Seville

This paper deals with the main control problems found in solar power systems and the solutions proposed in literature. The paper fi_rst describes the main solar power technologies, its development status and then describes the main challenges encountered when controlling solar power systems.

16:50-17:10 WeET2.2

Robust Control of Solar Plants with Distributed Collectors

Cirre, Cristina M. Univ. de Almeria
Moreno, Jose Carlos Univ. OF ALMERIA
Berenguel, Manuel Univ. of Almeria
Guzman, Jose Luis Univ. of Almeria

This paper presents a robust control scheme for a distributed solar collector (DSC) field. As DSC are systems subjected to strong disturbances (mainly in solar radiation and inlet oil temperature), a series feedforward is used as a part of the plant, so that the system to be controlled has one input (fluid flow) and one output (outlet temperature) as the disturbances are partially compensated by the series feedforward term, so that the nonlinear plant is transformed into an uncertain linear system. The Quantitative Feedback Theory technique (QFT) has been used to design a control structure that guarantee desired control specifications, as settling time and maximum overshoot, under different operating conditions despite system uncertainties and disturbances. To account for input and output constraints, both an antireset-windup mechanism and a reference governor have been used. Experimental tests are presented.

17:10-17:30 WeET2.3

Supervisory Predictive Control of an Integrated Wind/Solar Energy Generation and Water Desalination System

Christofides, Panagiotis D. Univ. of California at Los Angeles
Qi, Wei Univ. of California, Los Angeles
Liu, Jinfeng Univ. of California, Los Angeles

This work focuses on the design of a supervisory predictive control system for the optimal management and operation of a stand-alone wind-solar energy generation system which provides power to a reverse-osmosis (RO) water desalination system. We design the supervisory control system via model predictive control which coordinates the wind and solar subsystems as well as a battery bank to best satisfy the power demand of the RO system. Simulations are carried out to illustrate the applicability and effectiveness of the proposed supervisory predictive control design.

17:30-17:50 WeET2.4

Optimization of a Membrane Filtration Process for Drinking Water Treatment Using Fluorescence-Based Measurements

Peiris, Ramila Hishantha Univ. of Waterloo
Budman, Hector M. Univ. of Waterloo
Moresoli, Christine Univ. of Waterloo
Legge, Raymond Louis Univ. of Waterloo

Membrane fouling control is of paramount importance for sustainable operation of membrane-based drinking water treatment processes. Natural organic matter (NOM) is considered as the major membrane foulant and therefore its characterization is important for implementing fouling control strategies. This study proposes a fluorescence-based modelling approach for estimating and predicting the fouling dynamics in a bench-scale ultrafiltration (UF) membrane cross flow set-up for drinking water treatment. Principal component analysis (PCA) was used to extract the information that is relevant for membrane fouling from fluorescence excitation-emission matrix measurements captured during UF operation. PCA extracted principal components (PCs) that were related to major NOM membrane foulants. The model predictions were based on PC scores of retentate and permeate captured at time = 15 min of the UF experiments. The proposed fluorescence-based modelling approach is able to forecast different fouling behaviours with good accuracy. This proposed approach was then used for optimization of the UF process in which membrane back-washing times were estimated in order to achieve minimum energy consumption while ensuring maximum production of drinking water.

17:50-18:10 WeET2.5

Operation of Reverse Osmosis Plants with Optimal Energy Consumption

Gomez Palacin, Luis Univ. of Valladolid
de Prada, Cesar Univ. of Valladolid
Tadeo, Fernando Univ. of Valladolid Q4718001C
Salazar, Johanna Univ. of Valladolid

This paper deals with the optimal operational strategy of a reverse osmosis (RO) plant for remote sites. The electricity supply to these plants comes usually from renewable energies (wind and solar) helped by a diesel generator and batteries when they are not available. The water demand of small settlements in arid regions suffers strong variations along a day. Because the higher values of water demand

occur when more solar energy usually is available, the operational expenses can be minimized by considering the RO plant as an active load. A good control strategy, will implement a variable operation point, taking into account the predictions of water demand, the expected variation of the available energy sources and the scheduling of cleaning operations in the RO plant in order to optimize the energy consumption. In this paper a hybrid predictive control has been used to implement this task. Simulations of a specific plant show that an optimal operation reduces the diesel energy consumption, while satisfying the daily variable water demand.

18:10-18:30 WeET2.6

Two-Layered Real-Time Optimization of a Solid Oxide Fuel Cell Stack

Bunin, Gene — Ec. Pol. Fédérale de Lausanne
Francois, Gregory — Ec. Pol. Federale de Lausanne
Bonvin, Dominique — EPFL

The optimal operation of a solid oxide fuel cell stack is addressed in this paper. Real-time optimization, performed at a slow time scale via constraint adaptation, is used to account for uncertainty and degradation effects, while model-predictive control is performed at a faster time scale to reject process disturbances and to safely adapt the system to the specified output constraints following changes in cell power demand. To ensure that these constraints are strictly honored, an adaptation algorithm that uses the built-in constraint handling of quadratic programming is implemented within the model-predictive controller, allowing for the on-line adaptation of the feasibility region as a means to reject uncertainty. Simulation results illustrate the efficacy of this approach in the solid oxide fuel cell system.

WeET3 Room B

Systems Biology III (Regular Session) (Joint DYCOPS/CAB Session)

Chair: Ferreira, Eugenio Univ. of Minho

16:30-16:50 WeET3.1

Evaluating the Integration of Proteomic Data for the Prediction of Intracellular Fluxes after Knockout Experiments

Costa, Rafael Univ. of Minho
Moutinho Machado, Carlos Daniel Univ. do Minho
Rocha, Isabel Univ. of Minho
Ferreira, Eugenio Univ. of Minho

So far, few large scale kinetic models of metabolic networks have been successfully constructed. The main reasons for this are not only the associated mathematical complexity, but also the large number of unknown kinetic parameters required in the rate equations to define the system. In contrast to kinetic models, the constraint-based modelling approach bypasses these difficulties by using basically only stoichiometric information with certain physicochemical constraints to delimit the solution space without large fitted parameter sets. Although these constraint-based models are highly relevant to predict feasible steady-state fluxes under a diverse range of genetic and environmental conditions, the steady-state assumption may oversimplify cellular behaviour and cannot predict time-course profiles. To overcome these problems, combining these two approaches appears as a reasonable alternative to modelling large-scale metabolic networks. On the other hand, several of the experimental data required for model construction are often rare and in this way it is usually assumed that the enzyme concentrations are constant. In this work, we used a central carbon metabolic network of E. coli to investigate whether including high throughput enzyme concentration data into a kinetic model allows improved predictions of metabolic flux distributions in response to single knockouts perturbations. For this purpose, an E. coli model, based on results obtained from flux balance analysis (FBA) and approximate lin-log kinetics was constructed. The intracellular fluxes distributions, obtained using this model, were compared with published in vivo measurements.

16:50-17:10 WeET3.2

Merlin: Metabolic Models Reconstruction Using Genome-Scale Information

Dias, Oscar Univ. of Minho
Rocha, Miguel Univ. of Minho
Ferreira, Eugenio Univ. of Minho
Rocha, Isabel Univ. of Minho

This article describes Merlin, a user-friendly program that performs functional genomic annotations of lists of genes. Merlin retrieves information of each homologue and automatically scores the results, allowing the user to change the score selection, and dynamically (re-)annotate the genome. Merlin expedites the transition from genome-scale data to SBML metabolic models, allowing the user to have a preliminary view of the biochemical network.

17:10-17:30 WeET3.3

Understanding Clostridium Acetobutylicum ATCC 824 Metabolism Using Genome-Scale Thermodynamics and Metabolomics-Based Modeling

Salimi, Fahimeh — Univ. of Toronto
Mandal, Rupasri — Univ. of Alberta
Wishart, David — Univ. of Alberta
Mahadevan, Radhakrishnan — Genomatica Inc.

Biobutanol has a potential application as a biofuel and can replace gasoline as an alternative fuel. However, the productivity of the biobutanol process has to be increased significantly, before it can be commercialized. *Clostridium acetobutylicum* has been the primary microbial host used for biobutanol production. Consequently, systems biology based genome-scale metabolic model of *C. acetobutylicum* metabolism is essential to optimize the biobutanol production rate via genetic and process optimization and metabolic engineering. An updated genome-scale metabolic model of *C. acetobutylicum* ATCC824 consists of 700 genes, 709 reactions, 29 exchange reactions, and 679 metabolites, which covers 16.3% of ORFs and is more comprehensive compared to two other existing models. This metabolic network was used as a platform for simulating phenotypes using the constraint-based modeling approach. Flux variability analysis shows the presence of alternate carbon and electron sinks that allows for different carbon assimilation patterns and ranges of product formation rates. Incorporation of metabolomics and thermodynamics data into this model results in thermodynamically feasible flux distributions. We apply an NMR based approach to quantify 31 intracellular metabolites in both metabolic phases. The total molar concentration of metabolites was approximately 245mM, where asparagine was the most dominant metabolite.

WeET4 Room C

Multi(scale) Modeling of Chemical Processes (Regular Session)

Chair: Adomaitis, Raymond Univ. of Maryland

Co-Chair: Zhu, Yucai Eindhoven Univ. of Tech.

16:30-16:50 WeET4.1

Identification and MPC Control of a Circulation Fluidized Bed Boiler Using an LPV Model

Huang, JiangYin Xiamen Univ.

Ji, Guoli Xiamen Univ.

Zhu, Yucai Eindhoven Univ. of Tech.

Lin, Wei Xiamen Univ.

This work studies the identification and control of circulation fluidized bed (CFB) boilers. The CFB boiler under investigation shows strong nonlinearity due to big changes of steam load. A linear parameter varying (LPV) model is used to represent the process dynamics and used in control. The steam flow is used as the working-point variable (scheduling variable) of LPV model. Multivariable plant tests were carried out and a LPV model and a linear model were identified. The identification results of the industrial CFB boiler show that the LPV model has much higher accuracy than the linear model. The simulation studies for the MPC control of the CFB boiler have been performed using both the LPV model and the linear model. The simulation results show that the MPC using the LPV model performs better than the MPC using the linear model.

16:50-17:10 WeET4.2

Multiscale Modeling and Optimization of an Atomic Layer Deposition Process for Nanomanufacturing Applications

Adomaitis, Raymond Univ. of Maryland

A multiscale model of atomic layer deposition (ALD) inside a nanoporous material is developed. The overall model couples a lattice Monte Carlo simulator describing molecular-scale growth of the ALD film to a continuum description of the precursor transport within the nanopore. The multiscale simulation approach is used to study how intra-pore precursor depletion leads to nonuniform ALD films and can be used to examine whether film properties, such as composition and surface roughness, are functions of position within the pore. The simulator developed in this study is used to optimize the film growth process by manipulating the level of exposure to the precursor species to produce nearly perfectly uniform films within the nanopores.

17:10-17:30 WeET4.3

Modeling of Gate Control Neuronal Circuitry Including Morphologies and Physiologies of Component Neurons and Fibres

Agi, Egemen Middle East Tech. Univ.
Ozgen, Canan Middle East Tech. Univ.
Purali, Nuhan Hacettepe Univ.

In this work mathematical model of gate control theory, which explains the modulation of pain signals with tactile signals, is done. The difference of the current developed model from the previous modeling trials is that electrophysiological and morphological properties of component neurons and fibers that constitute the gate control structure are included to observe the structure-function relationship. Model of a single excitable cell is used as the main building block of the models of one unmyelinated fiber, one myelinated fiber, one interneuron and one projection neuron. The conduction velocities in the unmyelinated and myelinated fibers are found as 0.43m/s and 64.35 m/s, respectively. For both fibers input current intensity-frequency relationships are constructed. In addition, synapses between neurons are developed as two independent tanks and developed synapse model exhibits the summation and tetanization properties of real synapses while simulating the time dependency of neurotransmitter concentration in the synaptic cleft. All of the individual parts of the gate control system are connected and the whole system is simulated for different connection configurations.

17:30-17:50 WeET4.4

Multimodel Decomposition of Nonlinear Dynamics Using Fuzzy Classification and Gap Metric Analysis

Gugaliya, Jinendra Honeywell
Gudi, Ravindra IIT Bombay

Identification of accurate nonlinear models is central to the success of the nonlinear model based schemes. Approximation of the nonlinear system dynamics in a multiple linear model framework has been well addressed in the literature. However, such multimodel decomposition can result in unstable local models. Additionally, the number of local models to be selected for the nonlinear identification is critically dependant on the partitioning approach. This paper proposes a novel gap metric based fuzzy decomposition of nonlinear dynamics using multiple, locally linear models. Such a decomposition is shown to result in a stable and parsimonious model set which can be deployed for online control. A simulation case study involving nonlinear polystyrene reactor, is presented to illustrate the proposed approach.

17:50-18:10 WeET4.5

Identification of Nonlinear Process Models in an LPV Framework

Tóth, Roland Delft Univ. of Tech.
Van den Hof, Paul M.J. Delft Univ. of Tech.
Ludlage, Jobert IPCOS B.V.
Heuberger, Peter Delft Univ. of Tech.

Driven by the current economical needs, developments in process design and control point out that deliberate operation of chemical process requires better models and control designs than what is offered by the traditional Linear Time-Invariant (LTI) framework. In this paper an identification approach based on Linear Parameter-Varying (LPV) models is introduced for process systems which enables the use of powerful LPV control synthesis tools. LPV systems represent an intermediate step between LTI and nonlinear descriptions as they are capable of describing the system over its whole operating range but preserve many advantages of LTI descriptions. Estimation of LPV models is efficiently solvable by using series expansion type of model structures, like orthonormal basis function models. Advantageous properties of this approach and modeling paradigm are investigated with respect to process models and the added value over LTI models is demonstrated via an example of a continuous stirred tank reactor.