SESSION SUMMARY: CONTRIBUTED PAPERS

Stratos Pistikopoulos Centre for Process Systems Engineering Department of Chemical Engineering Imperial College London

Joseph Pekny Department of Chemical Engineering Purdue University

Introduction

The session on contributed papers has enjoyed a great success in attracting over 160 abstracts, out of which 99 papers from 27 countries have been accepted. They represent contributions from academia and research centers, industry and joint collaborations, as listed in Table 1.

The papers have been classified in seven areas: Planning, Scheduling, Control, Identification and Analysis, Design, Information Systems, and Computer Technologies. Each area is further divided in thematic topics. Below, a brief overview of the papers is given.

Planning

There were 20 papers on Planning. Thematic topics are Supply Chain, New Product Development, Operations Optimization and Batch Operations.

Supply Chain

- "Supply Chain Integration at Industrial Zones: Energy Integration" by Turkay, Fujita and Asakura, which discusses the integration of different process systems for improvement of financial and environmental issues.
- "External Supply Chain Management using Real Time Business Management System" by Birewar, which describes how eXternal Supply Chain Management allows multi-company-supply-chain to perform without sharing sensitive data and without exposing critical business knowledge.
- "A Multi-Optimization Approach to Fair Profit Distribution Problem for a Supply Chain Network" by Chen, Wang, Lee and Huang, which explores the fair profit distribution problem of a typical supply chain network involving batch production.
- "Optimizing the Supply Chain of Petrochemical Products under Uncertain Operational and Economical Conditions" by Lababidi, El-Wakeel, Alatiqi and Al-Enzi, which describes an optmization model for the

supply chain of a petrochemical company operating under uncertain operational and economical conditions.

"Supply Chain Planning Optimization in the Fruit Industry" by Masini, Petracci and Bandoni, which presents a midterm tactical planning model (Mixed Integer Lineal Programming) for the supply chain of a typical large company.

New Product Development

- "Risk management in Real Options Based Pharmaceutical Portfolio Planning" by Rogers, Gupta and Maranas, which provides a sensitivity analysis of candidate R&D products valuations and a risk management analysis to balance risks versus reward trade-offs.
- "An Aggregation Approach for Capacity Planning under Uncertainty for the Pharmaceutical Industry" by Gatica, Shah and Papageorgiou, which presents a flexible approach (aggregation vs. disaggregation) for potential products portfolio increases.
- "A Genetic Algorithm-Based Pharmaceutical Portfolio Selection and Scheduling Framework" by Blau, Rajan, Pekny, Varma, and Bunch, which outlines a discrete event simulation for the drug development process combined with a Genetic Algorithm to select the optimal sequence of projects in the presence of uncertainties and dependencies.
- "A New MILP Variable Resource Constrained Scheduling Model for the Testing of Pharmaceuticals and Agrochemicals" by Maravelias and Grossmann, which proposes an innovative scheduling MILP model to minimise the cost of testing and the time to market.
- "A Continuous-Time Formulation for Simultaneous Consideration of Planning and Scheduling Decisions" by Wu and Ierapetritou, which addresses the simultaneous consideration of planning and scheduling problems based on continuous time representation and the idea of periodic scheduling.

- "Production Planning and Inventory Management under Uncertainty: Stochastic Models and Numerical Solutions with Applications in the Paper Industry" by Yin and Liu, which explores he problem formulation and solution procedures for product planning and inventory management of systems under uncertainties.
- "Financial Risk Management in Planning under Uncertainty" by Barbaro and Bagajewicz, which describes a new two-stage stochastic programming models to manage financial risks.
- "Optimal Waste Reduction and Investment Planning Under Uncertainty" by Linninger, Chakraborty and Colberg, which proposes a systematic methodology for long-range, site-wide management strategies for batch manufacturing sites.
- "Rigorous Simulation Supports LP Models in Accurate Refinery-Wide Decisions" by Oettli and Forrest, which explores the impact of incorporating rigorous model on Linear Program models for decision-taking on plant profitability.
- "A Nonlinear Multiperiod Process Optimization Model for Production Planning in Multi-Plant Facilities" by Jackson, Grossmann, Hofmann and Wassick, which outlines a multi-period nonlinear programming (NLP) formulation that incorporates empirical process models for the optimal planning of a multi-plant production site.
- "A Model Predictive Control Framework for Advanced Planning and Scheduling in Process Industries" by Kaboré, which presents a model predictive control (MPC) formulation for the planning and scheduling problem in process industries.
- "Optimal Operations Planning under Uncertainty by Using Probabilistic Programming" by Li, Wendt and Wozny, which proposes an innovative analysis and optimization framework to address the lack of systematic reliability analysis and intuitive decisions in planning processes under uncertainty.
- "Demand Variations Ask for Cost-Effective Manufacturing Flexibility" by Heijnen, Herder and Grievink, which explores the ways to maximize the flexibility of the plant by varying equipment utilization, while a certain level of profit is guaranteed.
- "A Bilevel Programming Framework for Enterprise-wide Supply Chain Planning Problems under Uncertainty" by Ryu and. Pistikopoulos, which presents a theoretical framework for describing bilevel supply chain planning problems via parametric programming.

Batch Operations

"A Method for Improvement Potential Assessment in Batch Planning and Scheduling Situation" by Roeterink, Verwater-Lukszo and Weijnen, which presents a method for estimating the improvement potential of planning and scheduling in a batch-wise processing company.

Scheduling

There were a total of 18 papers on Scheduling, covering thematic topics on Mixed Integer and Optimization, Uncertainty and Batch Processing

Mixed Integer and Optimization

- "Economic Lot Scheduling Under Performance Decay" by Alle, Pinto and Papageorgiou, which proposes a mathematical programming model for the Economic Lot Scheduling Problem (ELSP) with performance decay.
- "Optimization Model for Production and Scheduling of Catalyst Re-Placement in a Process with Decaying Performance" by Houze, Juhasz and Grossmann, which describes a novel multi-period MINLP optimization model incorporating an empirical model to determine the optimal catalyst replacement policy and meet time varying products demand.
- "A Multi-Week Scheduling Approach for the Steel-Making Process" by Harjunkoski, Grossmann, Friedrich and Holmes, which presents a strategy to obtain optimal casting sequences using an MILP approach.
- "A Comparison of three Different Modelling Approaches for Solving Multi-Product, Multi-Purpose Plant Scheduling Problems" by Jernström and Westerlund, which discusses the scheduling of multi-product, multi-purpose plants with blocking production and move-out times.
- "Crude Oil Scheduling" by Magalhães and Shah, which describes the development of a short-term crude oil scheduling model.
- "Efficient Short-term Scheduling of Refinery Operation Based on Continuous time formulation" by Jia and Ierapetritou, which develops a comprehensive mathematical programming model for the efficient scheduling of oil-refinery operations.
- "Optimal Scheduling of Multistage Polymer Plants" by Yi and Reklaitis, which introduces a new mixed integer linear programming model of the optimal scheduling of multistage polymer plants, considering the extrusion and packaging stages under mild assumptions.
- "An MILP Framework for Reactive Scheduling of Resource-Constrained Multistage Batch Facilities" by Mendez and Cerda, which introduces a MILP framework for reactive scheduling of resource-constrained multistage batch facilities uit parallel units urng at each stage.
- "Plant-wide Scheduling and Marginal Costs Analysis on Refinery" by Wenkai, Hui, Hua and Tong, which presents an integrated refinery scheduling model to improve solution quality and time.

Uncertainty

"A Constraint Programming Approach to the Multi-Stage Batch Scheduling Problem" by Zeballos and Henning, outlines a multi-stage batch scheduling approach handling constrained situations regarding both renewable and non-renewable resources.

"A Two-Stage Stochastic Integer Programming Approach to Real-Time Scheduling" by Engell and Sand, which deals with scheduling problems in flexible batch chemical processes with a special emphasis on their real-time character.

"Robust Optimization for Scheduling under Bounded Uncertainty in Processing Times" by Lin and Floudas, which proposes a novel robust optimization methodology for scheduling under bounded uncertainty in processing times.

Batch Processing

"Environmentally Friendly Scheduling of Primary Steelmaking Processes" by Lee, Moon, Lopes and Park, which presents a multi-objectives short-term scheduling model for the operation in primary steel-making processes.

"Reactive Scheduling in Real-Time Operation of Batch Chemical Plants" by Cantón, Nougués, Rabiza, Gonzalez, Espuña and Puigjaner, which describes the interaction between the information levels of the CIM architecture.

"Industrial Application of Process Systems to Improve Specialty Batch Polymerisation Process" by Romero, Puigjaner, Malikand and Sievert, which aims at finding the optimal values for initial variables and controller settings to maximise process profitability in batch process industry.

"Improved Integration of Enterprise and the Control Level with Combining ISA Batch Standards and Process Models" by Verwater-Lukszo, Verhofstad and van Wissen, which discusses the industrial need for extension of the existing MES approaches with a model-based operation improvement module, that easily communicate with other modules.

"Batch Plant Integration in Need of More Support" by Heijnen and Verwater-Lukszo, which investigates multipurpose multi-product character of batch manufacturing plants and their need to integrate information form operational activities in the plant.

"Overcoming the Barriers to Batch Process Scheduling" by Siletti and Petrides, which envisages a solution for gap in the tools for batch process scheduling in the fully automated batch plant.

Control

There were 12 papers on control, divided into thematic topics on Six Sigma, Safety Analysis, Hybrid Systems, Control Optimization.

Six Sigma

"E-Process - A New Way to Benchmark and Improve our Production Process" by Joshi, Su, Potaraju, Daszkowski and Felde, which aims to digitalize process information and then maintain the gap between designed and actual performances at optimum.

"Evolution of Multivariate Statistical Process Control: Application of Independent Component Analysis and External Analysis" by Kano, Hasebe, Hashimoto and Ohno, which proposes a new MSPC method based on independent component analysis, that by extracting and monitoring essential variables, improve the process performance.

Safety Analysis

"Quantitative Analysis of the Safety and Flexibility of Nonlinear Dynamic Systems" by Huang, Adjiman and Shah, which presents a methodology for the identification of safe or feasible operating regions in the space of key operational variables and unknown parameters for processes by non-linear dynamic or algebraic equations.

"Dynamic Simulation of the Cleavage Section in a Phenol Plant for Safety Analysis" by Pellegrini, Bonomi and Biardi, which develops a dynamic model of the cumene hydroperoxide cleavage reactor in a phenolfrom-cumene plant in oredr to simulate its transient behaviour.

"Advanced Feedback-Feedforward Control of a Tubular Reactor for a High Productivity Ethanol Process: Application of an Alternative Structured Model" by Stremel, Vasco de Toledo, Maciel Filho and Pontarolo, which presents an alternative dynamic structured model, adapted from a structured growth model and modified with the objective to simulate and to control a high productivity tower bioreactor.

"Quantitative Decision-Making Based on Safety Information Management System in Chemical Plants" by Yoon and Moon, which develops a Safety Information Management System for human knowledge, safety history, process and business information.

Hybrid Systems

"Discrete Event Modeling and Dynamic Optimization of a Sugar Plant" by van Wissen, Smeets, Muller and Verheijen, which describes the modelling and optimization of a sugar plant in a Model predictive Control framework.

"Model-based Control of the Operation Procedure of an Emulsification Process" by Stork, Tousain, Krijgsman, de Krijger and Bosgra, which illustrates the benefits of using model-based optimization for improving the operation procedure of emulsification.

"A Multi-Level, Control-Theoretic Approach to Reactive Scheduling in Continuous Plants" by Munawar, Bhushan, Gudi and Belliappa, which presents a receding horizon based approach to reactive scheduling of continuous plants.

Control Optimization

"Controllability Analysis of Industrial Five Effects Evaporator System" by Ekawati, Bahri, LePage and Nooraii, which examines various operational modes and control loops in the process superstructure, involving solution of the Mixed Integer NonLinear Problem, and geometric representation of feasible operating space and process dynamic responses within the Dynamic Operability Framework.

"Dynamics and Advanced Control of a Fluid Catalytic Cracking Plant" by Vasconcelos, Wolf-Maciel, Maciel Filho and Spandri, which reports on simulation, optimization and control of an FCC plant.

"Strategies for the Operation and Control of Heat Exchanger Networks" by Westphalen, Young, Svrcek and Broussard, which shows the importance of dynamic simulations in the synthesis of workable control structure.

Identification and Analysis

There were 10 papers on Identification and Analysis. Thematic topics are Error Analysis, Sensor Location and Design of Experiments.

Error Analysis

- "A Real-Time Optimization Strategy for Petroleum Processes with Successive Adaptive Model Refinement" by Briesen and Marquardt, which shows that by reducing dead time in which the process runs off the optimum operating points, yield a large economical potential.
- "A Mixed Integer Nonlinear Optimization Based Approach to Simultaneous Data Reconciliation and Bias Identification" by Soderstrom, Himmelblau and Edgar, which outlines an extension of the technique that combines data reconciliation with identification of gross errors within a mixed integer optimization framework to situations where the model contains only bilinear terms as well as general nonlinear ones.
- "Approach to Dynamic Data Reconciliation Based on Extended Warm-Start Technique" by Mingfang, Bingzhen, Xiaorong and Shanying, which applies the warm-start technique to dynamic data reconciliation.

Sensor Location

"Sensor Network Reallocation and Upgradation for Efficient Fault Diagnosis" by Bhushan, Narasimhan and Rengaswamy, which presents formulations based on minimizing costs requirements to achieve the desired reliability, and maximising reliability for a given cost.

"Analysis and Detection of Outliers and Systematic Errors from an Industrial Data Plant" by Alves, Nascimento and Carneiro, which describes the approach based on either statistics or first principle equations or a composition of both, beside the knowledge of the process.

"Instrumentation Design and Upgrade Using Unconstrained Method with Pure Economical Objectives" by Bagajewicz and Markowski, which links the accuracy of key variables to a value function originating a net present value function, to be minimized over all possible configurations of sensors.

Design of Experiments

"On the Design of Optimally Informative Experiments for Model Discrimination Among Dynamic Crystallization Process Model" by Chen, Bermingham, Neumann, Kramer and Asprey, which presents methods to address the optimal design of dynamic experiments for model discrimination among several crystallization kinetics models.

"Statistical Analysis of Large Pilot Plant Datasets" by Schnelle and Armstrong, which describes an improvement project using recently developed mining techniques and Six Sigma methodology to resolve the operating differences between two plants.

"Experimental Designs that Maximize Information for Nonlinear Dynamic Process" by Rollins, Bhandari and Pacheco, which presents an index to measure the information content in a design of experiments.

"Strategy for Improving Data Quality for a Kraft Pulp Mill Recausticizing Plant" by Jiang, Stuart, Chen and Jasim, which describes a steady state simulation of a kraft pulp mill recausticizing plant for the purpose of area upgrade.

Design

There were 11 papers on Design, with topics on Synthesis and Models.

Synthesis

"A Conceptual Design Based Method for Generation of Batch Recipes" by Papaeconomou, Jørgensen, Gani and Cordiner, which describes a simple methodology of batch operational sequences for a reaction and distillation operations.

"Pinch Analysis of Supply Chains" by Singhvi, Madhavan and Shenoy, which introduces a novel approach for aggregate planning in supply chains.

"A General Disjunctive Model for the Retrofit of Multiproduct Batch Plants" by Montagna and Vecchietti, which presents a study on the solutions offered by a disjunctive model in a retrofit of multiproduct batch plants.

"A New Strategy and Algorithm of Modular Based MINLP for Synthesis of Chemical Processes" by Hehua, Yu, Shiqing and. Huanong, which presents the solution of a class of Mixed-Integer NonLinear Programming problems, applied to optimal synthesis of process systems in a modular simulator environment.

"Steady State Optimization of the Cyclohexanol Production Unit" by dos Santos and Maciel Filho, which covers the first stage of a real-time optimization project for a cyclohexanol production multiphase reactor.

"Strategies for Solving the Synthesis Problem in Multiproduct Batch Protein Production Processes" by Vecchietti, Montagna and Iribarren, which deal with synthesis and design of a multi-product batch protein production processes.

Models

"Phenomenon of the Existence of Continuum of Steady States in the Recycle System: Reactor Separating Unit" by Boyarinov and Duev, which studies a reactorseparator recycle system.

"A Formal Enterprise Model for Project-Oriented Management of Batch Plants" by Canavesio and Martinez, which proposes a formal modelling framework for batch plants using projects and situation calculus.

"Green Production and Logistics Simulation for Product Lifecycle Assessment" by Aoyama, Naka and Shimizu, which analyses PET recycling technologies and their environment impacts.

"Modeling Pyrolysis and Carbonization of Petroleum Distillation Residues in Delayed Coking Operations" by Rajagopal, Ahon and Sugaya, which compares Group Contributions Methods and Molecular Simulation Methods for estimation of properties.

"Simulation of the Pervaporation Process for Separating Organic Mixtures Using Solution-Diffusion Model" by Torres-Alvarez and Wolf-Maciel, which presents simulation of the pervaporation process for separating water-methyl acetate.

Information Systems

There were a total of 12 papers on Information Systems. The sub thematic topics are Systems Integration and Fault Diagnosis.

Systems Integration

"The "Smart" Plant: Economics and Technology" by D.C. White, which discusses recent developments in high performance computing and high speed communication technologies applied to process plants, and analyses the interplay of "technology push" and "economics pull".

"Missions of the CAPE-OPEN Laboratories Network" by Banks, Irons, Merk, Pons and Belaud, which gives an overview of the features of the CAPE_OPEN laboratories Network (CO-LaN).

"Modeller - An Interactive Model Editor for Physical, Chemical and Biological Processes" by Preisig and Westerweele, which describes the key features of Modeller – a modelling environment.

"Grid-Enabled Distributed Computations in the Chemical Process Industries" by Karakostas and Kokossis, which presents a computing architecture suitable for the information management and the demanding calculations of the supply chain.

"Optimization Opportunities in Process Control for Industry/University Research" by High, Ren, Alam, Rhinehartand Gemperline, which explores opportunities for optimization in process control.

"Real-time Enterprise Optimization in the Polymer Manufacturing Industry" by Schweiger, which outlines the need for flexibility in the plant operation, considering in the decision-making process all the available options and trade-offs for the process operation.

"Dynamic Information Management for Web-Enabled Environments in the Chemical Process Industries" by Kokossis, and Banares-Alcantara, which describes the development of a knowledge management platform for web-enabled environments featuring intelligence and insight capabilities.

"Survey of Data Management Systems Used in the Pulp and Paper Industry" by Janssen, Laflamme-Mayer, and. Stuart, which reports the implementation of process information systems in pulp and paper mills to better track troubleshoot and optimize their process.

Fault Diagnosis

"Computer-Aided Hazard Life Cycle-Oriented Safety Engineering: Concept and Functional Requirements" by Kirillov, Panasenko, Lukashevich and Lobanov, which describes a hazard life cycle-oriented approach to safety engineering of the chemistry- or energy-loaded industrial processes and units.

"Virtual Reality and Scientific Content for Environments Safety and Accident Consequences Analyses Applications" by Lukashevich and Kirillov, which presents a set of innovative, high-end capabilities, provided by Virtual Reality Systems for the research and engineering communities in the industrial safety and loss prevention domain.

"Adaptive Root Cause Analysis under Uncertainties in Industrial Process Operation" by Weidl, Vollmar and Dahlquist, which discusses a Root cause Analysis system implementing a probabilistic approach based on Bayesian inference for adaptive reasoning under uncertainties in industrial process operation.

"Establishment of Integrated Risk Management System (IRMS) by Kwon, Seong, Chung and Moon, which explains the methodologies of an Integrated Risk Management System for the estimation of the environmental, health and safety risks.

Computer Technologies

There were 16 papers on Computer Technologies, with thematic topics on Optimization Technologies, Control Technologies and Models.

Optimization Technologies

- "Dynamic Optimization for Switching Between Operating Modes in Cryogenic Plants" by Diaz,. Tonelli, Bandoni, Biegler, which addresses dynamic optimization of the cryogenic sector of a large-scale natural gas processing plant through the formulation of rigorous unit dynamic models.
- "Nonlinear Programming Algorithms for Large Nonlinear Gasoline Blending Problems" by Poku, Biegler, Kelly, Coxhead and Gopal, which compares and analyses numerical results of several large-scale gasoline blending models using NonLinear Programming solvers.
- "Chance Constrained Batch Distillation Process Optimization under Uncertainty" by Arellano-Garcia, Martini, Wendt, Li and Wozny, proposes a new approach for nonlinear chance constrained process optmization, realized for a steady state process.
- "A Strategy for MINLP Synthesis of Flexible and Operable Processes" by Novak Pintaric and Kravanja, which presents a sequential two-stage strategy for the stochastic synthesis of chemical processes.
- "An Algorithmic Framework for Improving Heuristic Solutions Applied to New Versions of the Traveling Salesman Problem" by Choi, Lee and Realff, which proposes a novel method to improve upon a solution, obtained from heuristics by applying dynamic programming to the subset of states visited by the heuristics.
- "Multiobjective Process Optimization by Applying Conflict-based Approach" by Li, Rong and Kraslawski, which proposed a two-stage strategy to deal with multi-objective conflicts in the process synthesis and operation.
- "Application of Genetic Algorithms to the Optimization of an Industrial Reactor of Production of Cyclohexanol" by Victorino, Maciel-Filho, Martini and Wolf Maciel, which describes the successful application of a Generic Algorithm in an industrial reactor of cyclohexanol production for the optimization of operational parameters.
- "Optimization of Nonlinear Manufacturing Systems under Uncertainty" by Salgueiro, Moncada and Acevedo, which presents a new algorithm for the optimization of nonlinear systems under uncertainty.

"Parallel Optimization of Operation for Ethylene Cracking Furnace" by Wang, Xu, Chen and He, which presents how to reduce the time-consuming optimization through an effective parallel strategy.

Control Technologies

- "On-line Optimization of a Paraffins Separation Plant" by Eloy Sequeira, Graells and Puigjaner, which investigates the on-line optimization of a petro-chemical plant.
- "Towards Integrated Dynamic Real-Time Optimization and Control of Industrial Processes" by Marquardt, Schlegel, Backx, Bosgra, Brouwer and Kadam, which presents a two-level approach for integrating model based dynamic real-time optimization and control of industrial processes.
- "Computer-Aided Hazard Identification in Sequential Operations Using Petri Nets" by Wang and Chang, which reports on the performances of Petri Nets for modelling the fault propagation behaviours in sequential operations.

Models

- "LP-Based Strategies for Modeling and Optimization Using Interval Methods" by Lin and Stadtherr, which presents how LP programming techniques provide the power to solve nonlinear equation solving and global optimization problems with complete mathematical and computational certainty.
- "Direct Computer Mapping of Process Models" by Csukas and Bankuti, which proposes direct computer mapping for process modelling, which combines the rule based information model and the balance based model.
- "A Multiscale Model for Conceptual Design and Simulation of Carbothermic Reduction Process for Aluminium Production" by Gerogiorgis and Ydstie, which discusses the fundamental considerations required for the development of a multiscale model, in the context of a conceptual high-temperature multiphase reactor.
- "Site-Modeling and its Applications" by Cheung, Hui, Sakamoto and Hirata, which presents some experiences in constructing a site-model based upon linear plant data.

Summarv

This has been a very exciting session with excellent contributions, covering most contemporary issues of process operations. It will certainly serve as an excellent starting point of the current state-of-the-art and to set the research directions for the years to come.

Table 1: Paper Contributions by Country and Sector

Country	Academia/Research Centres	Industry	Collaboration	Total by country
US	16	7	9	32
Germany	4	2	5	11
UK	8		3	11
Brazil	5		4	9
Netherlands	5		4	9
Argentina	7			7
Canada	1	1	3	5
China	3		2	5
Japan	2		2	4
Korea	4			4
Spain	3		1	4
Russia	3			3
Finland	2			2
India	1		1	2
Australia			1	1
Denmark			1	1
France			1	1
Hong Kong			1	1
Hungary	1			1
Italy	1			1
Kuwait			1	1
Mexico	1			1
Poland	1			1
Slovenia	1			1
Sweden			1	1
Taiwan	1			1
Turkey			1	1
Total by sector	70	10	40	