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Preface

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Preface

This special issue contains selected papers from the 18th European Symposium of Computer Aided Process Engineering (ESCAPE-18) which took place in Lyon, France, 1–4 June 2008. ESCAPE-18 was the 667th event of the European Federation of Chemical Engineering (EFCE) under responsibility of its CAPE Working Party. CAPE refers to computer aided methods, algorithms and techniques related to process and product engineering. The ESCAPE series brings the latest innovations and achievements by leading professionals from the industrial and academic communities. It serves as a forum for engineers, scientists, researchers, managers and students from academia and industry to present and discuss progress being made in the area of CAPE.

The special theme for ESCAPE-18 was "CAPE for the Users!". CAPE systems are to be put in the hands of end users who need functionality and assistance beyond the core scientific and technological capacities of the systems. User-friendliness, on-line or web-based advice, decision support, knowledge management and organisational issues are important points that must be taken into account when deploying a CAPE system. These issues were addressed in a special track including industrial case studies illustrating CAPE methods and tools. The other six main topics covered the usual scope of ESCAPE conferences, from off-line synthesis and design to on-line systems, including numerical and computational methods, integrated and multiscale modeling, societal aspects and CAPE education.

ESCAPE-18 included a rich programme of five plenary lectures and six keynote talks from leaders in science and industry, 101 contributions presented in 26 oral sessions and two poster sessions for other 247 contributions. After the symposium 32 corresponding authors were invited to submit an extended version of their contribution. All submitted papers were reviewed according to the standards of *Computers and Chemical Engineering*. Finally 22 papers have been accepted for publication in this special issue.

The content of this issue is organised along the main topics of ESCAPE-18, starting with two papers from the special theme "CAPE for the Users!": the opening plenary talk by Bañares-Alcantara on policy design and a technical paper by Morbach et al. on the design of OntoCAPE, an ontology for the domain of CAPE.

The next six papers relate to optimization, control and diagnosis of processes, starting with a plenary talk by Bonvin and Chachuat on real time optimisation strategies. The next paper on chance constrained optimization under uncertainty, by Arellano-Garcia and Wozny, covers work conducted during Arellano-Garcia's PhD Thesis. He was the winner of the EFCE Excellence Award 2008 in Recognition of an Outstanding PhD Thesis on CAPE. His PhD Thesis, completed at Technical University Berlin under the supervision of Pr. Wozny, received the best evaluation results in terms of innovativeness, breadth and depth of the study, quality of publications, industrial relevance, and international dimension. The next two papers, Collazos et al. and Ferreira and Zhang, deal with optimal control approaches. The section continues with a paper from Chao and Wang on genetic programming as a tool to extract knowledge from process historical data. Then follows a paper by Olivier-Maget et al. on model-based fault diagnosis in the case of hybrid systems.

The next series of six articles deals with various issues in process design and scheduling with a strong focus on batch processes. The first one by Denes et al. presents feasibility studies of a new double column system for batch distillation. Then, two papers on batch scheduling are given: Gimenez et al. give the second part of a series of two articles on a network based continuous representation which can be applied to maintenance and a few other activities, and to rescheduling when some of the schedule is already fixed; Subbiah et al. also extend previous work done with timed automata for the problem of tardiness minimization. The next paper is of industrial origin, with two authors from the Akzo-Nobel company, and deals with optimal choice of solvents and operating conditions in the production of free radical solution copolymers. The last two papers in this section address crystallization processes: the paper by Nagy, who won the best oral presentation award, presents a robust optimal control scheme, which takes parametric uncertainties into account to provide decreased variability of the shape of crystal size distribution; the paper by Lakerveld et al. shows a conceptual design approach using functional tasks – which represent fundamental physical events – in order to get a better control over crystalline product quality.

The theme integrated and multiscale modeling and simulation is represented by two papers. In his contribution, Fermeglia presents a hierarchical procedure for bridging the gap between atomistic and macroscopic modeling passing through mesoscopic. The concept of multiscale modeling is perfectly illustrated through applications of industrial interest. Van Dam et al. assess different modeling paradigms – equation-based models and agent-based models – and give recommendations for their use for supply chain management.

How to push away the limits of numerical solving strategies? Manca et al. discuss the feasibility and the methods for solving very large and sparse systems of nonlinear algebraic equations. Zavala and Biegler demonstrate that a full-discretization approach coupled to a sparsity-exploiting interior point solver result in a fast strategy to solve both the NMPC (Nonlinear Model Predictive Control) and MHE (Moving Horizon Estimator) problems. They apply their strategy on low-density polyethylene tubular reactors.

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The last papers concern societal and educational issues. Bojarski et al. address the optimization of Supply Chain (SC) planning and design considering economical and environmental issues. A Life Cycle Assessment (LCA) approach is envisaged to incorporate the environmental aspects of the model. Professor Luis Puigjaner, co-author of this paper, received the long term achievements (LTA) award from the CAPE Working Party during ESCAPE-18. This CAPE award for long term achievements is given in recognition of a collection of outstanding achievements over an extended period of time to CAPE methods, tools and/or applications for the advancement of science, engineering and technology. The best poster presentation award was won by Estrada et al. for the poster entitled: "Developing a Lake Eutrophication Model and Determining Biogeochemical Parameters: a Large Scale Parameter Estimation Problem". The extended version of their paper is published in this special issue. Ayoub et al. propose a design and evaluation methodology for Biomass Utilization Networks (B-NETs) planning in local areas. Finally the last paper deals with the most important challenge for the future of CAPE community: Education. We thank professors Cameron and Lewin to share their vision of important issues in the area of CAPE education in the face of contemporary changes in knowledge development, information and communication technology advances and the practice of professional engineering.

As Guest Editors of this Special Issue, we are grateful to the numerous reviewers for their efficient and fruitful collaboration and their insightful comments and recommendations which have contributed a lot to the improvement of the overall quality of the papers. We also wish to thank Elsevier and professor Rafiqul Gani for enabling the publication of this special issue in due time.

We hope that this special issue will serve as a reference to the scientific and industrial community and will contribute to the progress in computer aided process and product engineering.

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