Process Systems Engineering

Edited by Efstratios N. Pistikopoulos,
Michael C. Georgiadis, and Vivek Dua

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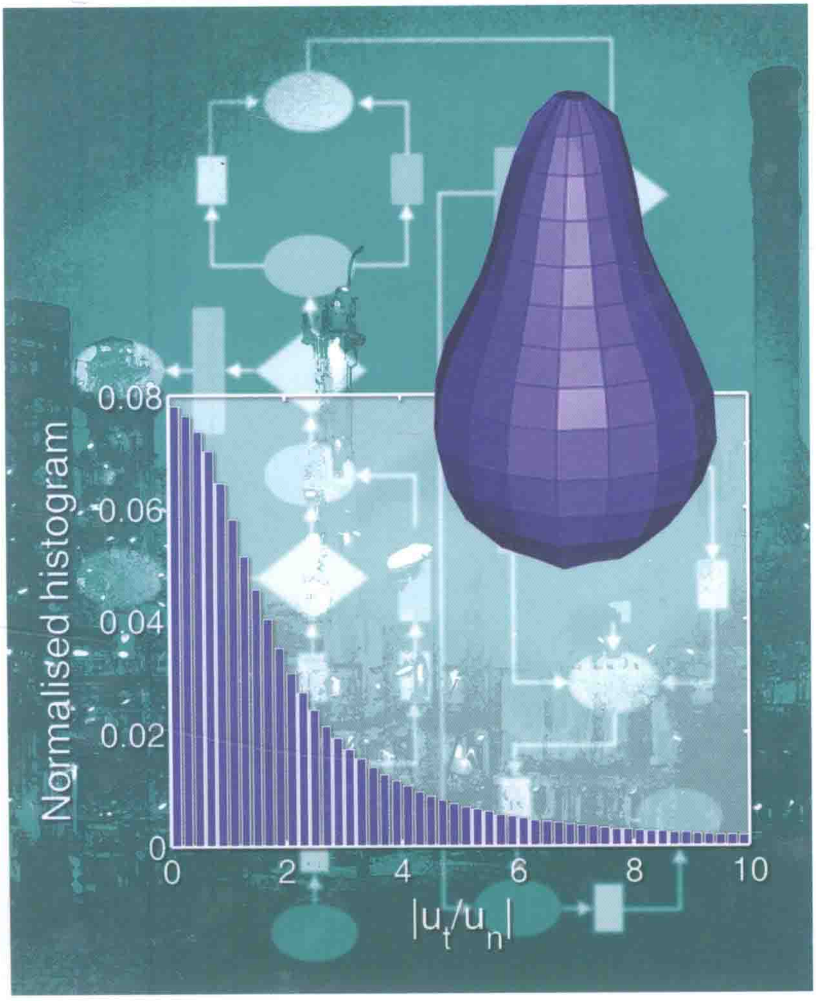
Dynamic Process Modelling



Volume 7

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Centre for
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Volume 7: Dynamic Process Modeling

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Preface

The central role of process modeling in all aspects of process design and operation is now well recognized. Although most early models were steady state, more recently the emphasis has been on dynamic models that can be used for studying transient process behavior. Moreover, there is an increasing trend toward "high-fidelity" models, which can accurately predict the trajectories of the key variables that affect the process performance, safety, and economics. This demand for substantially higher model accuracy can often be traced to the need for extracting further gains in profitability out of processes that have already undergone incremental improvement over several decades. In other cases, it arises from the strict environmental and safety constraints and product specifications under which many processes currently operate [1].

Process modeling has always been an important component of process design, from the conceptual synthesis of the process flowsheet to the detailed design of specialized processing equipment such as advanced reaction and separation devices, and the design of their control systems. Recent years have witnessed the model-based approach being extended to the design of complex products, such as batteries, fuel cells, biomedical, biochemical, drug delivery systems, which can themselves be viewed as miniature plants produced in very large numbers. Inevitably, the modeling technology needed to fulfill the demands posed by such a diverse range of applications is very different from the standard steady-state flowsheeting packages that served the process industries so well in the past [2].

Volume 7 of this book series has attempted a review of some of the current trends in process modeling and its practical application during the past few years. It focuses on modeling frameworks for complex systems including chemical, biochemical, bio-processing, biological, and energy systems.

In Chapter 1, Mark Matzopoulos from Process Systems Enterprise Ltd summarizes his long experience in the area of process modeling. He presents a model-based engineering approach to the construction and application of detailed dynamic process models. He first summarizes the key concepts and consideration to be taken into account when building first principle of the dynamic modeling. Then he introduces a *model-based engineering* (MBE) approach, which involves engineering activities with the assistance of a mathematical model of the process under investigation. A step-by-step approach is nicely described for the construction

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of high-fidelity predictive models including estimation of model parameters from data, analysis of the experimental data, and design of experiments, if necessary. The applicability of the overall modeling approach is illustrated in a multitubular reactor design problem. A number of benefits using a high-fidelity predictive modeling approach are revealed.

In Chapter 2, Ingram and Cameron discuss a multiscale modeling approach for granulation processes. The industrial significance of granulation processes is first introduced and the multiscale nature of process systems, general characteristics of multiscale models, and the emerging practice of multiscale modeling are then presented in details. The relevant scales of observation for granulation processes are outlined and several examples of the modeling techniques used at each scale are provided. Key multiscale granulation models appearing in the literature are discussed and then a handful of them are reviewed in more detail.

In Chapter 3, Amaro and Pistikopoulos discuss a number of theoretical principals behind polymerization process modeling, applied to free-radical polymer reactions. Comprehensive kinetic schemes encompassing a large number of reactions that might occur during these processes were discussed in details. The specific modeling of polymer molecular properties was highlighted and exemplified for molecular weight distribution with different approaches regarding its representation. In conclusion, it was emphasized that modeling of polymerization processes is a powerful tool allowing researchers and companies to perform a broad variety of simulations, allowing for a number of model-based activities such as optimization and control.

Panos and coworkers in Chapter 4 present a detailed dynamic model for PEM fuel cell stack. The model has the great advantage of less computation time consuming while providing results consistent with the literature, and well oriented toward control. Then a reduced order state space model is designed for optimal control studies. Finally an explicit/multiparametric MPC controller has been developed to keep the controlled variables close to the set points while taking care of the physical constraints on the manipulated variables, namely the reactant and coolant mass flows. The controller finally selected shows good performance to resist the disturbances in the load.

In Chapter 5, Kikkinides and coworkers present a detailed modeling framework for pressure swing adsorption flowsheets. Several research challenges are identified and a generic modeling framework for the separation of gas mixtures using multibed PSA flowsheets is presented. The core of the framework represents a detailed adsorbent bed model relying on a coupled set of mixed algebraic and partial differential equations for mass, heat, and momentum balance at both bulk gas and particle level, equilibrium isotherm equations, and boundary conditions according to the operating steps. The adsorbent bed model provides the basis for building PSA flowsheets with all feasible interbed connectivities. Operating procedures are automatically generated, thus facilitating the development of complex PSA flowsheet for an arbitrary number of beds. Finally, a case study concerning the separation of hydrogen from steam-methane reforming of gas is used to illustrate the application and efficiency of the developed framework.

In Chapter 6, Kenig introduces a complementary modeling approach for the reactive separation process based on a reasonable and efficient combination of different approaches. He presented a classification of kinetics-based models based on the complexity of the process fluid dynamics. He concluded that for geometrically simple flows, the fluid dynamic approach (FDA) should be applied as it gives full information about the process in a purely theoretical manner. For very complex flow patterns, the rate-based approach (RBA) represents a good choice provided that the model parameters are determined properly. The hydrodynamic analogy approach serves as an intermediate between the FDA and RBA and is suitable for those processes in which a certain structure or order exists. Several case studies were used to highlight the use of all approaches.

Seferlis and coworkers in Chapter 7 discuss efficient *reduced order dynamic modeling* techniques of *complex reactive and multiphase separation processes.* They illustrated that combined *nonequilibrium* and *orthogonal collocation on finite elements* (NEQ/OCFE) models become quite attractive for real-time control applications of these processes. A novel optimization-based finite element partition algorithm is then presented to enhance the ability of the proposed models to control the approximation error along the column within reasonable levels despite the influence of exogenous disturbances responsible for the formation of steep fronts in the composition and temperature profiles. Case studies that involve reactive absorption, reactive distillation, and multiphase reactive distillation illustrated the strengths of the NEQ/OCFE techniques.

In Chapter 8, Abbas and coworkers discuss the modeling of crystallization processes. An overview of industrial crystallization, crystallization fundamentals, and mechanisms is first presented followed by detailed discussions on crystallization modeling, model solution techniques, and model analysis. Various model application areas are illustrated before finishing with two examples, namely, antisolvent crystallization and seeded cooling crystallization.

In Chapter 9, Mujtaba highlights the state-of-the-art and future challenges in modeling of multistage flash (MSF) desalination process. He presents how *computer-aided process engineering* modeling techniques and the practitioners of desalination can address sustainable freshwater issue of tomorrow's world via desalination. He also emphasizes that the exploitation of full economic benefit of replacing time-consuming and expensive experimental studies of MSF processes requires development of accurate mathematical models and model-based applications such as optimization and control. Several research challenges in this area are also introduced.

Recognizing the importance of a mechanistic systems approach to biological sciences, Androulakis in Chapter 10 discusses the potential role of systems-based approaches in the quest to better understand critical physiological responses. He demonstrated how quantitative models of inflammation can be used as minimal representations of biological reality to formulate and test hypotheses, reconcile observations, and guide future experimental design. He also demonstrated the possibility of the generalization of this framework in a wide range of disease progression models. It was emphasized that it is important to realize that *in silico* models will never replace either biological or clinical research. They could, however, rationalize the decision-making process by establishing the range of validity and predictability of intervention strategies, thus enabling the use of systems biology in translational research.

In Chapter 11, Alonso and coworkers consider the dynamic modeling of distributed (bio)processes, that is, those described by partial differential equations. Their contribution considers aspects that are particularly relevant for robust control, with emphasis on model reduction techniques for convection–diffusion–reaction processes. These techniques are illustrated with examples, including a bioreactor for the production of gluconic acid and the control of a tubular reactor.

Paving the way toward a "closed-loop" holistic framework for bioprocess automation, Kiparissides and coworkers in Chapter 12 cover the development of dynamical models of biological systems. They introduced and explained in a step-by-step fashion a biological model development framework. The scientific concerns, challenges, and "real-life" problems associated with each step of the framework were clearly highlighted. Adapting a "real-life" example from their previous work, the logical and systematic evolution of a model were presented from the conception to validation as it flows through the various steps of the model development framework. The key conclusion of this contribution is that by utilizing a systematic way of organizing available information, one can avoid conducting experiments for the sake of experimentation and develop models with an *a priori* set aim.

Balsa-Canto and coworkers in Chapter 13 consider optimal identification strategies and their application in bioprocess engineering. Dynamic model building is presented as an iterative loop with three key topics: parameter estimation (model calibration), identifiability analysis, and optimal experimental design. These authors highlight the need of checking identifiability and using global optimization techniques for proper parameter estimation in nonlinear dynamic models. Further, the use optimal experimental design to increase the identifiability is motivated. These techniques are illustrated with two examples – one related with dynamic modeling of microbial growth, and another with dynamic modeling of the production of gluconic acid in a fed-batch bioreactor.

In Chapter 14, Nicolaï and coworkers consider the multiscale dynamic modeling of transport phenomena in foods, with emphasis in plant-based foods. These authors show how the multiscale paradigm combines micro- and macro-scale models through homogenization and localization, and which numerical methods should be used to solve the resulting model. The use of this approach is exemplified with a case study considering application of multiscale gas exchange in fruit.

Marquez-Lago and Marchisio in Chapter 15 consider dynamic modeling in synthetic biology, that is, the engineering of novel biological functions and systems. These authors adopt a detailed modeling methodology based on the concept of composable parts. Further, they pay special attention to the selection of a correct simulation regime, highlighting the problems of using deterministic approaches, and discussing alternative stochastic simulation methods. These topics and techniques are illustrated considering a synthetic oscillator made of three genes.

In Chapter 16, Bezzo and coworkers reviewed the role of the optimal model-based design of experiments techniques with reference to the problem of individual parameter identification for complex physiological models of glucose homeostasis. It was emphasized that the parameter identification problem is a tradeoff between several issues: acquisition of a high information content from a clinical test, compliance to a number of constraints in the system inputs and outputs, practical applicability of the test. It was showed that model-based design of experiments does allow designing effective and safe clinical tests, where the administration of carbohydrates (i.e., glucose) and possibly insulin is exploited to provide dynamic excitation to the body system, and a proper schedule of blood samples is used to collect the information generated during the test.

This collection represents a set of stand-alone works that captures recent research trends in the development and application of modeling frameworks techniques of various process and biosystems. We hope that by the end of the book, the reader will have developed a commanding comprehension of the main aspects of dynamic process modeling, the ability to critically access the key characteristics and elements related to the construction and application of detailed models and the capacity to implement the new technology in practice.

We are extremely grateful to the authors for their outstanding contributions and for their patience, which have led to a final product that far exceeded our expectations.

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