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Control and Optimization of Multiscale Process Systems

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Preface

Multiscale process systems are characterized by highly coupled phenomena that occur in disparate spatial and temporal scales. Examples include the chemical vapor deposition of thin films, as well as ion-sputtering and catalytic processes where gas-phase and surface processes strongly interact. Detailed modeling of multiscale process systems naturally leads to continuum laws for the macroscopic (gas-phase) phenomena coupled with stochastic simulations for the microscopic (surface) phenomena. Control and optimization of multiscale process systems, targeting regulation of microscopic properties like thin-film surface roughness, cannot be addressed using existing methods that rely on continuum process models in the form of linear/nonlinear differential equations.

This book—the first of its kind—presents general, yet practical, methods for model-based feedback control and optimization of multiscale process systems. Beginning with an introduction to general issues on control and optimization of multiscale processes and a review of previous work in this area, the book discusses detailed modeling approaches for multiscale processes with emphasis on the theory and implementation of kinetic Monte Carlo simulation, methods for feedback control using kinetic Monte Carlo models, stochastic model construction and parameter estimation, predictive and covariance control using stochastic partial differential equation models, and both steady-state and dynamic optimization algorithms that efficiently address coupled macroscopic and microscopic objectives. The methods are applied to various multiscale/microscopic processes—including thin-film deposition processes, an ion-sputtering process, and a catalytic CO oxidation process—and their effectiveness and performance are evaluated through detailed computer simulations. The book also includes discussions of practical implementation issues that can help researchers and engineers understand the development and application of the methods in greater depth.

The book assumes a basic knowledge about differential equations, probability theory, and control theory and is intended for researchers, graduate students, and process control engineers.

In addition to our work, Dr. Dong Ni and doctoral candidate Gangshi Hu at UCLA contributed greatly to the research results included in the book and in the preparation of the final manuscript. We would like to thank them for their hard work and contributions. We would also like to thank all the other people who contributed in some way to this project. In particular, we would like to thank our colleagues at UCLA and Penn State for creating a pleasant working environment, the staff of Birkhäuser for excellent cooperation, and the United States National Science Foundation for financial support. Last, but not least, we would like to express our deepest gratitude to our families for their dedication, encouragement, and support over the course of this project. We dedicate this book to them.

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