

Contents

List of contributing authors — VII

Juan Gabriel Segovia-Hernández, Maricruz Juárez-García,
and Eduardo Sánchez-Ramírez

Chapter 1

**Optimization and its importance for chemical engineers: challenges,
opportunities, and innovations — 1**

José A. Caballero

Chapter 2

Deterministic optimization of distillation processes — 25

Luis Fernando Lira-Barragán, Fabricio Nápoles-Rivera,
and José María Ponce-Ortega

Chapter 3

**Optimal design of process energy systems integrating sustainable
considerations — 79**

Oscar Daniel Lara-Montaño, Manuel Toledano-Ayala, Claudia Gutiérrez-Antonio,
Fernando Israel Gómez-Castro, Elena Niculina Dragoi, and Salvador Hernández

Chapter 4

Metaheuristics for the optimization of chemical processes — 113

Mathias Neufang, Emma Pajak, Damien van de Berg, Ye Seol Lee, and
Ehecatl Antonio Del Rio Chanona

Chapter 5

**Surrogate-based optimization techniques for process systems
engineering — 159**

Daniel Rangel-Martínez and Luis A. Ricardez-Sandoval

Chapter 6

**Data-driven techniques for optimal and sustainable process integration of
chemical and manufacturing systems — 215**

Antonio Flores-Tlacuahuac

Chapter 7

Applications of Bayesian optimization in chemical engineering — 255

Seyed Reza Nabavi, Zhiyuan Wang, and Gade Pandu Rangaiah

Chapter 8

Sensitivity assessment of multi-criteria decision-making methods in chemical engineering optimization applications — 283

Kai Kruber, Siv Kinau, and Mirko Skiborowski

Chapter 9

Hybrid optimization methodologies for the design of chemical processes — 305

Urmila Diwekar

Chapter 10

Optimization under uncertainty in process systems engineering — 343

Riju De and Yogendra Shastri

Chapter 11

Optimal control of batch processes in the continuous time domain — 379

Yulissa Mercedes Espinoza-Vázquez, Nereyda Vanessa Hernández-Camacho,
Jahaziel Alberto Sánchez-Gómez, José Ezequiel Santibañez-Aguilar,
and Fernando Israel Gómez-Castro

Chapter 12

Supply chain optimization for chemical and biochemical processes — 401

David Esteban Bernal Neira, Fernando Israel Gómez-Castro,
Ehecatl Antonio del-Río-Chanona, and Vicente Rico-Ramírez

Chapter 13

Future insights for optimization in chemical engineering — 425

Index — 445