Contents

1 Introduction to Optimization Modeling for Petroleum Refineries *1*

1.1 Background *1*
1.2 Overview of Refining Processes *4*
1.2.1 Atmospheric Crude Oil Distillation *5*
1.2.2 Hydroprocessing *5*
1.2.3 Sulfur Recovery *9*
1.2.4 Reforming *9*
1.2.5 Isomerization *10*
1.2.6 Blending *11*
1.3 Overview of Refinery Optimization Modeling *12*
1.3.1 Refinery Optimization Systems, Techniques, and Tools *12*
1.3.2 Modeling for Advanced Process Control *14*
1.3.3 Modeling for Real-Time Optimization *15*
1.3.4 Modeling for Process Simulation *17*
1.3.4.1 Modeling for Dynamic Simulation *18*
1.3.4.2 Modeling for Operator Training Simulation *19*
1.3.5 Modeling for Planning and Scheduling *19*
1.3.5.1 Systems Implementation *23*
1.3.5.2 Optimization of Crude Oil Scheduling *24*
1.3.5.3 Refinery Management *25*
1.4 Concluding Remarks *25*
References *26*

2 Basic Petroleum Refinery Economics *31*

2.1 Refinery Economics Overview *31*
2.1.1 Refinery Profitability *31*
2.1.2 Refinery Margins *32*
2.1.3 Refinery Margin Calculations *33*
2.1.4 Refinery Margin Trends *34*
2.1.5 Refinery Margin Improvement *34*
2.2 Marginal Economics for Incremental Optimization *34*

2.3 Refinery Economic Analysis *36*
2.3.1 Refinery Value Determination *36*
2.3.2 Refinery Economic Evaluation *37*
2.3.2.1 Simple Example *37*
2.3.2.2 Advanced Example *38*
2.3.2.3 Further Example *40*
2.3.3 Refinery Contracts *41*
2.4 Concluding Remarks *41*
References *41*

3 Superstructure Representation *43*
3.1 Introduction to Superstructures *43*
3.2 Types of Superstructure Representation *43*
3.3 State–Task Network Superstructure Representation *44*
3.4 State–Equipment Network Superstructure Representation *45*
3.5 Resource–Task Network Superstructure Representation *46*
3.6 Superstructure Generation *47*
3.7 Other Superstructure Representations *48*
3.7.1 State–Space Network Superstructure Representation *48*
3.7.2 Unit Operation–Port–State Superstructure Representation *48*
3.7.3 Bond Graph Superstructure Representation *48*
3.8 Superstructure Representation Example for Naphtha Processing *49*
3.9 Chapter Summary *53*
References *53*

4 Modeling Framework *57*
4.1 Modeling of Mixed Continuous and Integer Decision Variables *57*
4.2 Superstructure Optimization Modeling *58*
4.3 Constructing Superstructures *58*
4.4 Modeling of Superstructure Representations *59*
4.5 Modeling of Discrete Decisions and Logical Relations *60*
4.5.1 Propositional Logics for Superstructure Optimization Modeling *61*
4.5.2 Logical Binary Variables *62*
4.5.3 Yes/No Type Binary Variables *62*
4.5.4 Disjunctive Optimization Modeling *63*
4.6 Modeling of Process Units and Operations *67*
4.6.1 Process Design Procedure *67*
4.6.2 Selecting Modeling Variables *67*
4.6.3 Formulating Simple Models *68*
4.6.4 Basic Unit Models *68*
4.6.4.1 Mixer *68*
4.6.4.2 Splitter *69*
4.6.4.3 Separator *70*
4.6.4.4 Valve *70*
4.6.4.5 Multicomponent Splitter *70*

4.6.5 Unit Operation Models *72*
4.6.5.1 Compressor *72*
4.6.5.2 Furnace *72*
4.6.5.3 Conversion Reactor *72*
4.6.5.4 Heat Exchanger *75*
4.6.6 Information Flow Modeling *75*
4.6.6.1 Information Flow Diagram *77*
4.6.6.2 Choice of Design Variables *79*
4.6.6.3 Equation Ordering *79*
4.7 Modeling for Numerical Studies *84*
4.8 Chapter Summary *86*
References *86*

5 Model Formulation and Implementation *89*
5.1 Mathematical Formulation *89*
5.2 Generic Optimization Model Formulation for Refinery Planning *90*
5.2.1 Objective Function *91*
5.2.2 Production Capacity and Expansion Constraints *91*
5.2.3 Mass Balances *92*
5.2.4 Demand Constraints *92*
5.2.5 Availability Constraints *92*
5.2.6 Non-Negativity Constraints *92*
5.3 Generic Optimization Model Formulation for Refinery Design *93*
5.3.1 Material Balances *93*
5.3.2 Mixed-Integer Logical Constraints *93*
5.3.3 Logical Constraints on Design and Structural Specifications *94*
5.3.4 Logic Propositional Constraints on Design Specifications *95*
5.3.4.1 Example 1 *95*
5.3.4.2 Example 2 *100*
5.3.5 Logic Propositional Constraints on Structural Specifications *101*
5.3.6 Generalized Disjunctive Programming *101*
5.4 Numerical Implementation for Computational Experiments *106*
5.5 Computational Experiment Examples *110*
5.5.1 MILP Model Results *113*
5.5.2 GDP Model Results *114*
5.6 Chapter Summary *123*
References *123*

6 Solution Strategies *125*
6.1 Convex Relaxation *125*
6.2 Lagrangean Decomposition *126*
6.3 Global Optimization Techniques *126*
6.3.1 Branch and Reduce *128*
6.3.2 Spatial Branch and Bound *128*
6.3.3 Hybrid Branch and Bound *128*

6.3.4 Interval Analysis *129*
6.3.5 Extended Cutting Plane *129*
6.4 Advancements in Commercial Integer Optimization Solvers *130*
6.4.1 Overview *130*
6.4.2 Computational Performance of Commercial Integer Optimization Solvers *130*
6.4.3 A Commercial Success Story: CPLEX Integer Optimization Solver *130*
6.4.4 Solution Methods and Algorithms *131*
6.4.4.1 Integer Optimization Algorithms *131*
6.4.4.2 Branch and Bound *132*
6.4.4.3 Presolve and Cutting Planes *134*
6.4.4.4 Heuristics *135*
6.4.4.5 Combined Local Search and Heuristics *136*
6.4.4.6 Parallelization *136*
6.4.4.7 Solution Pools *136*
6.4.4.8 Tuning Tools *136*
6.4.5 Application Examples *136*
6.4.5.1 Example 1: Energy Optimization *137*
6.4.5.2 Example 2: Financial Optimization *137*
6.4.5.3 Example 3: Manufacturing Optimization *137*
6.4.5.4 Concluding Remarks *138*
6.5 Chapter Summary *139*
References *139*

7 Industrial Case Studies with Business-Centric Techno-Commercial Considerations *145*
7.1 Industrial Case Study 1: Refinery Configuration for Heavy Oil Processing *145*
7.1.1 Background *145*
7.1.2 Problem Statement *146*
7.1.3 Model Formulation *147*
7.1.4 Numerical Example *148*
7.1.5 Concluding Remarks *151*
7.2 Industrial Case Study 2: Refinery Configuration for Whole Complex Processing *152*
7.2.1 Model Formulation *152*
7.2.1.1 Superstructure Representation *156*
7.2.1.2 Logic Propositions *162*
7.2.1.3 Objective Function *164*
7.2.2 Computational Results *165*
7.2.2.1 Computational Results and Discussion *166*
7.2.2.2 Model Validation *171*
7.2.2.3 Application Extension to Refinery Upgrade Studies *176*
7.2.2.4 Sensitivity Analysis *176*

7.2.3 Concluding Remarks *176*
7.3 Industrial Case Study 3: Refinery Configuration for Naphtha Upgrading *177*
7.3.1 Problem Statement *178*
7.3.2 Propositional Logics and Logic Cuts in Process Synthesis Problems *178*
7.3.3 Logical Constraints *178*
7.3.3.1 General Formulation *178*
7.3.3.2 Logical Constraints on Processing Alternatives of Naphtha for Petroleum Refineries *182*
7.3.4 Computational Experience *182*
7.3.5 Concluding Remarks *183*
7.4 Chapter Summary *186*
References *186*

8 Industrial Case Studies with Environmental-Centric Techno-Commercial Considerations *191*
8.1 Industrial Case Study 1: Refinery Configuration with Environmental Considerations *191*
8.1.1 Background *191*
8.1.2 Problem Statement *192*
8.1.3 Model Formulation *192*
8.1.3.1 Superstructure Representation *192*
8.1.3.2 Material Balance Constraints *192*
8.1.3.3 Logical Constraints *194*
8.1.3.4 Logic Propositions *194*
8.1.3.5 Environmental Performance Assessment for Risk Evaluation of Flowsheets *196*
8.1.3.6 Objective Function *197*
8.1.4 Numerical Example *197*
8.1.5 Concluding Remarks *198*
8.2 Industrial Case Study 2: Refinery Configuration with Heat Integration *198*
8.2.1 Problem Statement *198*
8.2.2 Superstructure Representation *199*
8.2.3 Modeling and Computational Strategy *201*
8.2.4 Model Formulation *202*
8.2.4.1 Flowsheet Optimization *202*
8.2.4.2 Heat Integration Constraints *205*
8.2.4.3 Objective Function *206*
8.2.5 Computational Results *206*
8.2.6 Concluding Remarks *209*
8.3 Chapter Summary *211*
References *212*

9 Industrial Case Studies with Engineering-Centric Techno-Commercial Considerations *215*
9.1 Industrial Case Study 1: Refinery Configuration for High-Octane Fuel Production *215*
9.1.1 Catalytic Reforming Process *216*
9.1.2 Data Reconciliation Method *216*
9.1.3 Problem Statement *217*
9.1.4 Model Formulation *217*
9.1.4.1 Data Reconciliation Model *218*
9.1.4.2 Feed Characterization *219*
9.1.4.3 Reactor Representation *220*
9.1.4.4 Reactor Pressure Balance *221*
9.1.4.5 Reaction Kinetic Tuning *221*
9.1.4.6 Reactor Switch in Cyclic Reformer *221*
9.1.4.7 Measurement Models *223*
9.1.5 Results and Discussion *224*
9.1.5.1 Key Process Variables *224*
9.1.5.2 Tuning Strategies *225*
9.1.5.3 Reformate Yields *226*
9.1.5.4 Reactor Total Endotherms *226*
9.1.6 Concluding Remarks *226*
9.2 Industrial Case Study 2: Refinery Configuration for Low-Benzene Fuel Production *227*
9.2.1 Problem Statement *227*
9.2.2 Superstructure Representation *227*
9.2.3 Model Formulation *229*
9.2.4 Preliminary Computational Results *234*
9.3 Chapter Summary *234*
References *234*

Summary and Conclusions *237*
Index *239*