

## Contents

**About the Authors** *xiii*  
**Foreword by Lawrence B. Evans** *xv*  
**Foreword by Steven R. Cope** *xvii*  
**Preface** *xix*  
**Acknowledgments** *xxiii*  
**Scope of Textbook** *xxv*  
**Software Selection and Copyright Notice** *xxvii*

<b>1</b>	<b>Characterization and Physical and Thermodynamic Properties of Oil Fractions</b>	<b>1</b>
1.1	Crude Assay	1
1.1.1	Bulk Properties	2
1.1.2	Fractional Properties	6
1.1.3	Interconversion of Distillation Curves	7
1.2	Boiling Point-Based Hypothetical or Pseudocomponent Generation	8
1.3	Workshop 1.1 – Interconvert Distillation Curves	13
1.4	Workshop 1.2 – Extrapolate an Incomplete Distillation Curve	13
1.5	Workshop 1.3 – Calculate MeABP of a Given Assay	13
1.6	Workshop 1.4 – Represent an Oil Fraction by the Old Oil Manager in Aspen HYSYS Petroleum Refining	16
1.7	Workshop 1.5 – Represent an Oil Fraction by the New Petroleum Assay Manager in Aspen HYSYS Petroleum Refining	25
1.8	Workshop 1.6 – Conversion from the Oil Manager to Petroleum Assay Manager and Improvements of the Petroleum Assay Manager over the Oil Manager	32
1.9	Property Requirements for Refinery Process Models	33
1.10	Physical Properties	36
1.10.1	Estimating Minimal Physical Properties for Pseudocomponents	36
1.10.2	Molecular Weight	37
1.10.3	Critical Properties	38
1.10.4	Liquid Density	40
1.10.5	Ideal Gas Heat Capacity	42
1.10.6	Other Derived Physical Properties	43

1.11	Process Thermodynamics	45
1.11.1	Process Thermodynamics	47
1.11.2	Mixed or Activity Coefficient-Based Approach	47
1.11.3	Equation-of-State Approach	49
1.12	Miscellaneous Physical Properties for Refinery Modeling	50
1.12.1	Two Approaches for Estimating Fuel Properties	51
1.12.2	Flash Point	52
1.12.3	Freeze Point	52
1.12.4	PNA Composition	53
1.13	Conclusion	54
	Nomenclature	55
	Bibliography	56
<b>2</b>	<b>Atmospheric or Crude Distillation Unit (CDU)</b>	<b>59</b>
2.1	Introduction	59
2.2	Scope of the Chapter	60
2.3	Process Overview	60
2.3.1	Desalting	61
2.3.2	Preheat Train and Heat Recovery	62
2.3.3	Atmospheric Distillation	62
2.4	Model Development	65
2.4.1	MESH Equations	66
2.4.2	Overall Column Efficiency and Murphree Stage Efficiency	66
2.4.3	Recommendation for Correctly Handling the Efficiency	68
2.4.4	Inside-Out Algorithm for Distillation Column Calculation	
	Convergence	69
2.5	Feed Characterization	72
2.6	Data Requirements and Validation	73
2.7	A Representative Atmospheric Distillation Unit	76
2.8	Building the Model in Aspen HYSYS Petroleum Refining	77
2.8.1	Entering the Crude Information	78
2.8.2	Selection of a Thermodynamic Model	84
2.8.3	Crude Charge and Prefractionation Units	87
2.8.4	Atmospheric Distillation Column – Initial	88
2.8.5	Atmospheric Distillation Column – Side Strippers	95
2.8.6	Atmospheric Distillation Column – Pumparounds	98
2.8.7	Atmospheric Distillation Column – Adding Custom Stream	
	Properties	101
2.8.8	Post-Convergence	104
2.9	Results	105
2.10	Model Applications to Process Optimization	109
2.10.1	Improve the 5% Distillation Point for an Individual Cut	109
2.10.2	Change Yield of a Given Cut	109
2.10.3	Workshop 2.1 – Perform Case Studies to Quantify the Effects of	
	Stripping Steam Rate and Product Draw Rate	111
2.11	Workshop 2.2 – Rebuild Model Using “Backblending” Procedure	114
2.11.1	Import Distillation Data into Aspen HYSYS Oil Manager	115

2.11.2	Define a New Blend of the Backblended Crude Feed	116
2.11.3	Build the CDU Model Based on the Backblended Feed	120
2.11.4	Converging Column Model	120
2.11.5	Comparison of Results	123
2.12	Workshop 2.3 – Investigate Changes in Product Profiles with New Product Demands	126
2.12.1	Update Column Specifications	126
2.12.2	Vary Draw Rate of LGO	127
2.13	Workshop 2.4 – Investigate the Effects of Process Variables on Product Qualities	129
2.14	Workshop 2.5 – Application of Column Internal Tools (Column Hydraulic Analysis)	131
2.15	Workshop 2.6 – Application of the Petroleum Distillation Column	140
2.16	Conclusions	144
	Nomenclature	145
	Bibliography	145
<b>3</b>	<b>Vacuum Distillation Unit</b>	<b>147</b>
3.1	Process Description	147
3.2	Plant Data Reconciliation	149
3.2.1	Required Data	149
3.2.2	Representation of the Atmospheric Residue	149
3.2.3	Makeup of Gas Streams	152
3.3	Model Implementation	154
3.3.1	Plant Data and Modeling Approaches	155
3.3.2	Workshop 3.1 – Build the Simplified VDU Model	157
3.3.3	Workshop 3.2 – Build the Rigorous Model from a Simplified Model	165
3.4	Model Application – VDU Deep-Cut Operation	172
3.5	Workshop 3.3 – Simulation of the VDU Deep-Cut Operation	176
	Bibliography	180
<b>4</b>	<b>Predictive Modeling of the Fluid Catalytic Cracking (FCC) Process</b>	<b>183</b>
4.1	Introduction	184
4.2	Process Description	185
4.2.1	Riser–Regenerator Complex	185
4.2.2	Downstream Fractionation	187
4.3	Process Chemistry	188
4.4	Literature Review	190
4.4.1	Kinetic Models	190
4.4.2	Unit-Level Models	193
4.5	Aspen HYSYS Petroleum Refining FCC Model	195
4.5.1	Slip Factor and Average Voidage	196
4.5.2	21-Lump Kinetic Model	197
4.5.3	Catalyst Deactivation	198

4.6	Calibrating the Aspen HYSYS Petroleum Refining FCC Model	199
4.7	Fractionation	200
4.8	Mapping Feed Information to Kinetic Lumps	203
4.8.1	Fitting Distillation Curves	203
4.8.2	Inferring Molecular Composition	205
4.8.3	Convert Kinetic Lumps to Fractionation Lumps	208
4.9	Overall Modeling Strategy	209
4.10	Results	211
4.11	Applications	220
4.11.1	Improving Gasoline Yield	220
4.11.2	Increasing Unit Throughput	223
4.11.3	Sulfur Content in Gasoline	224
4.12	Refinery Planning	225
4.13	Workshop 4.1 – Guide for Modeling FCC Units in Aspen HYSYS Petroleum Refining	231
4.13.1	Introduction	231
4.13.2	Process Overview	231
4.13.3	Process Data	231
4.13.4	Aspen HYSYS and Initial Component and Thermodynamics Setup	231
4.13.5	Basic FCC Model	238
4.13.6	FCC Feed Configuration	241
4.13.7	FCC Catalyst Configuration	246
4.13.8	FCC Operating Variable Configuration	250
4.13.9	Initial Model Solution	252
4.13.10	Viewing Model Results	253
4.14	Workshop 4.2 – Calibrating Basic FCC Model	258
4.15	Workshop 4.3 – Build the Model for Main Fractionator and Gas Plant System	267
4.15.1	T201_MainFractionator	267
4.15.2	Overhead Wet Gas System, Primary Stripper Column T302_Stripper, and Debutanizer or Gasoline Stabilization Column T304_Stabilizer	275
4.15.3	T301_Absorber, Primary Absorber and T303_ReAbsorber, Sponge Oil Absorber, or Reabsorption Column	281
4.16	Workshop 4.4 – Perform Case Studies to Quantify Effects of Key FCC Operating Variables	285
4.17	Workshop 4.5 – Generate Delta-Base Vectors for Linear Programming (LP)-Based Planning	291
4.18	Conclusions	297
	Nomenclature	298
	Bibliography	299
5	<b>Predictive Modeling of Continuous Catalyst Regeneration (CCR) Reforming Process</b>	303
5.1	Introduction	304
5.2	Process Overview	304

5.3	Process Chemistry	311
5.4	Literature Review	313
5.4.1	Kinetic Models and Networks	314
5.4.2	Unit-Level Models	317
5.5	Aspen HYSYS Petroleum Refining Catalytic Reformer Model	319
5.6	Thermophysical Properties	323
5.7	Fractionation System	323
5.8	Feed Characterization	324
5.9	Model Implementation	328
5.9.1	Data Consistency	329
5.9.2	Feed Characterization	330
5.9.3	Calibration	330
5.10	Overall Modeling Strategy	333
5.11	Results	335
5.12	Applications	340
5.12.1	Effect of Reactor Temperature on Process Yields	341
5.12.2	Effect of Feed Rate on Process Yields	344
5.12.3	Combined Effects on Process Yields	345
5.12.4	Effect of Feedstock Quality on Process Yields	346
5.12.5	Chemical Feedstock Production	347
5.12.6	Energy Utilization and Process Performance	349
5.13	Refinery Production Planning	350
5.14	Workshop 5.1 – Guide for Modeling CCR Units in Aspen HYSYS Petroleum Refining	354
5.14.1	Introduction	354
5.14.2	Process Overview and Relevant Data	354
5.14.3	Aspen HYSYS and Initial Component and Thermodynamic Setup	356
5.14.4	Basic Reformer Configuration	358
5.14.5	Input Feedstock and Process Variables	362
5.14.6	Solver Parameters and Running the Initial Model	368
5.14.7	Viewing Model Results	370
5.14.8	Updating Results with Molecular Composition Information	372
5.15	Workshop 5.2. – Model Calibration	376
5.16	Workshop 5.3 – Build a Downstream Fractionation System	387
5.17	Workshop 5.4. – Case Study to Vary RON and Product Distribution Profile	395
5.18	Conclusion	400
	Nomenclature	400
	Bibliography	402
<b>6</b>	<b>Predictive Modeling of the Hydroprocessing Units</b>	<b>405</b>
6.1	Introduction	406
6.2	Aspen HYSYS Petroleum Refining HCR Modeling Tool	411
6.3	Process Description	416
6.3.1	MP HCR Process	416
6.3.2	HP HCR Process	419

6.4	Model Development	419
6.4.1	Workflow of Developing an Integrated HCR Process Model	419
6.4.2	Data Acquisition	421
6.4.3	Mass Balance	421
6.4.4	Reactor Model Development	424
6.4.4.1	MP HCR Reactor Model	424
6.4.4.2	HP HCR Reactor Model	430
6.4.5	Delumping of the Reactor Model Effluent and Fractionator Model Development	435
6.4.5.1	Applying the Gauss–Legendre Quadrature to Delump the Reactor Model Effluent	438
6.4.5.2	Key Issue of the Building Fractionator Model – Overall Stage Efficiency Model	440
6.4.5.3	Verification of the Delumping Method – Gaussian–Legendre Quadrature	440
6.4.6	Product Property Correlation	442
6.5	Modeling Results of MP HCR Process	444
6.5.1	Performance of the Reactor and Hydrogen Recycle System	444
6.5.2	Performance of Fractionators	445
6.5.3	Product Yields	447
6.5.4	Distillation Curves of Liquid Products	449
6.5.5	Product Property	451
6.6	Modeling Results of HP HCR Process	454
6.6.1	Performance of the Reactor and Hydrogen Recycle System	454
6.6.2	Performance of Fractionators	455
6.6.3	Product Yields	455
6.6.4	LPG Composition and Distillation Curves of Liquid Products	459
6.6.5	Product Property	462
6.7	Model Applications	464
6.7.1	$H_2$ -to-Oil Ratio versus Product Distribution, Remained Catalyst Life, and Hydrogen Consumption	464
6.7.2	WART Versus Feed Flow Rate Versus Product Distribution	466
6.8	Model Application – Delta-Base Vector Generation	468
6.9	Workshop 6.1 – Build a Preliminary Reactor Model of HCR Process	471
6.10	Workshop 6.2 – Calibrate Preliminary Reactor Model to Match Plant Data	481
6.11	Workshop 6.3 – Case Studies	497
6.12	Workshop 6.4 – Fractionation System for HCR Reactor	505
6.13	Conclusion	512
	Nomenclature	513
	Bibliography	514
7	<b>Alkylation, Delayed Coking, and Refinery-Wide Simulation</b>	517
7.1	Alkylation	517
7.1.1	Process Description	517

7.1.2	Feed Components and Alkylation Kinetics	518
7.1.3	Workshop 7.1 – Hydrofluoric Acid Alkylation Process	
	Simulation	519
7.2	Delayed Coking	528
7.2.1	Process Description	528
7.2.2	Feed Characterization, Kinetic Lumps, and Coking Reaction	
	Kinetics	529
7.2.3	Workshop 7.2 – Simulation and Calibration of a Delayed Coking	
	Process	530
7.2.4	Workshop 7.3 – Simplified Model of Delayed Coker by Petroleum Shift	
	Reactor for Production Planning Applications	542
7.3	Refinery-Wide Process Simulation	548
7.3.1	Refinery-Wide Process Model: A Key to Integrating Process Modeling	
	and Production Planning	548
7.3.2	An Example of a Refinery-Wide Process Simulation Model	549
7.3.3	Tools for Developing Refinery-Wide Process Models	551
7.3.4	Deployment and Applications of the Refinery-Wide Process Models	
	for Process Engineering and Production Planning	551
7.4	Conclusions	553
	Bibliography	554
	<b>List of Computer Files</b>	555
	<b>Index</b>	559