

- | | |
|-------------------------|---|
| 1. Record Nr. | UNIORUON00279229 |
| Titolo | Spomenica posvetena na Ante Popovski, redoven clen na Makedonskata Akademija na Naukite i Umetnostite |
| Pubbl/distr/stampa | Skopje, : Makedonska Akademija na Naukite i Umetnostite, 2004 |
| Descrizione fisica | 37 p. ; 24 cm. |
| Disciplina | 891.819 |
| Soggetti | POPOVSKI ANTE |
| Lingua di pubblicazione | Macedonian |
| Formato | Materiale a stampa |
| Livello bibliografico | Monografia |
-
- | | |
|-------------------------|---|
| 2. Record Nr. | UNINA9910830887803321 |
| Autore | Liu Y. A. |
| Titolo | Integrated Process Modeling, Advanced Control and Data Analytics for Optimizing Polyolefin Manufacturing / / Y. A. Liu and Niket Sharma |
| Pubbl/distr/stampa | Weinheim, Germany : , : WILEY-VCH GmbH, , [2023]
©2023 |
| ISBN | 3-527-84383-3
3-527-84381-7 |
| Edizione | [First edition.] |
| Descrizione fisica | 1 online resource (865 pages) |
| Disciplina | 668.4234 |
| Soggetti | Polyolefins |
| Lingua di pubblicazione | Inglese |
| Formato | Materiale a stampa |
| Livello bibliografico | Monografia |
| Nota di bibliografia | Includes bibliographical references and index. |
| Nota di contenuto | Cover -- Volume 1 -- Title Page -- Copyright -- Contents -- Foreword -- Preface -- Acknowledgment -- Copyright Notice -- About the Authors -- About the Companion Website -- Chapter 1 Introduction to Integrated Process Modeling, Advanced Control, and Data Analytics in Optimizing Polyolefin Manufacturing -- 1.1 SegmentBased Modeling of |

Polymerization Processes: Component Characterization and Polymer Attributes -- 1.1.1 Component Types in Polymer Process Modeling -- 1.1.2 Concept of Moments and Some Basic Polymer Attributes -- 1.1.3 Stream Initialization and Basic Polymer Attributes -- 1.2 Workshop 1.1: Finding the Resulting Stream Attributes After Mixing Two Copolymer Streams -- 1.2.1 Objective -- 1.2.2 Problem Statement -- 1.2.3 Process Flowsheet -- 1.2.4 Unit System, Components, and Characterization of Copolymers -- 1.2.5 Property Method and Property Parameters for Components -- 1.2.6 Specifications of Streams and Blocks -- 1.3 Workshop 1.2: A Simplified Simulation Model for a Slurry HDPE Process and the Workflow for Developing a Polymer Process Simulation Model -- 1.3.1 Objective -- 1.3.2 Step 1: Problem Setup -- 1.3.3 Step 2: Component Specifications -- 1.3.4 Step 3: Property Method -- 1.3.5 Step 4: Property Parameters - Obtaining Values from Databanks and Estimating Missing Parameters -- 1.3.6 Step 5: Verification of the Accuracy of the Selected Property Method by Comparing Predicted PureComponent Property Values with Report Experimental Data -- 1.3.7 Step 6: Regress Component Liquid Density Data and Binary Vapor-Liquid Equilibrium (TPXY) Data to Estimate Missing Purecomponent and Binary Interaction Parameters of Selected Property Method and Verify Predicted VLE Results with Experimental Data -- 1.3.8 Step 7: Develop Correlations for Polymer Product Quality Indices, Such as Density and Melt Index (Melt Flow Rate) Based on Plant Data.

1.3.9 Step 8: Define the Polymerization Reactions and Enter the Initial Reaction Rate Constants -- 1.3.10 Step 9: Draw the OpenLoop Process Flowsheet and Enter the Inputs for Streams and Blocks -- 1.3.11 Step 10: Run the Initial Openloop Process Simulation and Check if the Simulation Results Are Reasonable -- 1.3.12 Step 11: Close the Recycled Loops, Finalize a Converged Closedloop Steadystate Simulation Model, and Investigate Applications to Improving Process Operations and Identifying Operating Conditions for New Product Design -- 1.3.13 Step 12: Convert the Steadystate Simulation Model in Aspen Plus to a Dynamic Simulation Model in Aspen Plus Dynamics -- Add Appropriate Controllers -- and Investigate Process Operability, Control, and Grade Changes -- 1.4 Industrial and Potential Applications of Integrated Process Modeling, Advanced Control, and Data Analytics to Optimizing Polyolefin Manufacturing -- 1.4.1 Industrial and Potential Applications of Process Modeling to Optimizing Polyolefin Manufacturing -- 1.4.2 Industrial and Potential Applications of Advanced Process Control to Optimizing Polyolefin Manufacturing -- 1.4.3 Industrial and Potential Applications of Data Analytics to Optimizing Polyolefin Manufacturing -- 1.4.4 Hybrid Modeling: Integrated Applications of Process Modeling, Advanced Control, and Data Analytics to Optimizing Polyolefin Manufacturing -- References -- Chapter 2 Selection of Property Methods and Estimation of Physical Properties for Polymer Process Modeling -- 2.1 Property Methods and Thermophysical Parameter Requirements for Process Simulation -- 2.2 Polymer Activity Coefficient Models (ACM): Polymer Nonrandom Two liquid (POLYNRTL) Model -- 2.2.1 Vapor-Liquid Equilibrium for an Ideal Vapor Phase and a Nonideal Liquid Phase.

2.2.2 General Vapor-Liquid Equilibrium Relationships Based on Fugacity Coefficient and Liquidphase Activity Coefficient -- 2.2.3 Segment based Mole Fraction Versus Speciesbased Mole Fraction -- 2.2.4 POLYNRTL: Polymer Nonrandom Twoliquid Activity Coefficient Model -- 2.2.5 Concept of Henry Components for Vapor-Liquid Equilibrium for a Vapor Phase and a Nonideal Liquid Phase Involving Supercritical Components -- 2.3 Workshop 2.1. Estimating POLYNRTL Binary

Parameters Using UNIFAC -- 2.3.1 Objective -- 2.3.2 Estimating POLYNRTL Binary Parameters Using UNIFAC for Polystyrene Manufacturing -- 2.4 Prediction of Polymer Physical Properties by Van Krevelen Functional Group Method -- 2.5 Workshop 2.2. Estimating the Physical Properties of a Copolymer Using the Van Krevelen Group Contribution Method -- 2.5.1 Objective -- 2.5.2 Draw the Process Flowsheet and Specify the Unit Set and Global Options -- 2.5.3 Define Components, Segments, and Polymer and Characterize Their Structures -- 2.5.4 Choosing Property Method and Entering or Estimating Property Parameters -- 2.5.5 Specifications of Feed Stream and Flash Block -- 2.5.6 Creating Property Sets -- 2.5.7 Defining Property Analysis Run to Create Property Tables -- 2.6 Polymer Sanchez-Lacombe Equation of State (POLYSL) -- 2.7 Workshop 2.3. Estimating Property Parameters Using Data Regression Tool -- 2.7.1 Objective -- 2.7.2 Defining a DRS Run -- 2.7.3 Specifying a Unit Set and Global Options -- 2.7.4 Defining Components, Segments, Oligomers, and Polymer -- 2.7.5 Choose Property Method and Enter Known Property Parameters from Aspen Enterprise Databanks -- 2.7.6 Enter Experimental Data for Data Regression, Run the Regression, and Examine the Results -- 2.7.7 Specifying a Regression Run and the Parameters to be Regressed -- 2.7.8 Running the Regression Case and Examining the Results. 2.8 Polymer Perturbedchain Statistical Fluid Theory (POLYPCSF) Equation of State -- 2.9 Workshop 2.4. Regression of Property Parameters for POLYPCSF EOS -- 2.9.1 Objective and Data Sources -- 2.9.2 Regression of Pure Component Parameters for POLYPCSF EOS -- 2.10 Correlation of Polymer Product Quality Indices and Structure-Property Correlations -- 2.10.1 Polyolefin Product Quality Indices -- 2.10.2 Empirical Correlations of Polymer Product Quality Targets -- 2.10.3 Estimation of Apparent Newtonian Viscosity from MIMWW Measurement -- References -- Chapter 3 Reactor Modeling, Convergence Tips, and DataFit Tool -- 3.1 Kinetic or RateBased Reactors -- 3.2 Continuous StirredTank Reactor Model (RCSTR) -- 3.2.1 RCSTR Configurations -- 3.2.2 RCSTR Specifications -- 3.3 Plug Flow Reactor Model (RPLUG) -- 3.3.1 RPLUG Configurations -- 3.3.2 RPLUG Specifications -- 3.4 Batch Reactor Model (RBATCH) -- 3.4.1 RBATCH Configuration -- 3.4.2 RBATCH Specifications -- 3.5 Representation of Nonideal Reactors -- 3.6 RCSTR Convergence -- 3.6.1 Initialization -- 3.6.2 Scaling Factors -- 3.6.3 Residence Time Loop -- 3.6.4 Energy Balance Loop -- 3.6.5 Mass Balance Loop -- 3.6.6 Flash Loop -- 3.6.7 Recommendation for RCSTR Mass Balance Algorithm for Polyolefin Process Simulation -- 3.7 RPLUG/RBATCH Model Convergence -- 3.8 Data Fit (Simulation Data Regression) -- 3.9 Workshop 3.1: Data Fit of Kinetic Parameters for Styrene Polymerization Using Concentration Profile Data -- 3.9.1 Objective -- 3.9.2 A Simplified Kinetic Model for Styrene Polymerization -- 3.9.3 Datasets -- 3.9.4 Simulation Data Regression (Data Fit) -- 3.10 Workshop 3.2: Data Fit of Kinetic Parameters for Styrene Polymerization Using Point Data -- 3.10.1 Objective -- 3.10.2 Dataset -- 3.10.3 Simulation Data Regression (Data Fit) -- References -- Chapter 4 Free Radical Polymerizations: LDPE and EVA. 4.1 Polymers by Free Radical Polymerization -- 4.2 Kinetics of Free Radical Polymerization -- 4.2.1 Initiator and Its DecompositionRate Parameters -- 4.2.2 Chain Initiation Reactions -- 4.2.3 Chain Propagation Reactions -- 4.2.4 Chain Transfer Reactions -- 4.2.5 Termination Reactions -- 4.2.6 Autoacceleration, Trommsdorff Effect, or Gel Effect -- 4.2.7 Other Free Radical Polymerization Reactions -- 4.3 Thermodynamic Methods and Property Parameter Requirements -- 4.4 Workshop 4.1: Simulation of an Autoclave Highpressure LDPE

Process -- 4.4.1 Objectives -- 4.4.2 Process Flowsheet and Simulation Representation -- 4.4.3 Unit System, Components, and Characterization of Polymer -- 4.4.4 Thermodynamic Methods and Property Parameters for Components, Segment, and Polymer -- 4.4.5 PCES (Physical Constant Estimation System) for Estimating Missing Property Parameters -- 4.4.6 Defining Free Radical Polymerization Reactions for LDPE -- 4.4.7 Specifications of Inlet Process Streams and Unit Operation and Reactor Blocks -- 4.4.8 Methodology for Improving Simulation Convergence and for Kinetic Parameter Estimation -- 4.4.9 BaseCase Simulation Results -- 4.4.10 Model Applications -- 4.4.11 Separation Section -- 4.5 Workshop 4.2: Simulation of Tubular Reactors for HP LDPE Process -- 4.5.1 Objectives -- 4.5.2 Process Flowsheet and Simulation Representation -- 4.5.3 Unit System, Components, and Characterization of Polymer -- 4.5.4 Thermodynamic Method and Property Parameters for Components -- 4.5.5 PCES (Physical Constant Estimation System) for Estimating MissingProperty Parameters -- 4.5.6 Free Radical Polymerization Reactions for LDPE -- 4.5.7 Specifications of Inlet Process Streams and Unit Operation and Reactor Blocks -- 4.5.8 User FORTRAN Subroutine for Heat Transfer Calculations for the LDPE Reactor.
4.5.9 BaseCase Simulation Targets and Kinetic Parameter Estimation.
