

1. Record Nr.	UNINA9910555162903321
Autore	Manan Zainuddin Abdul
Titolo	Modeling, simulation, and optimization of supercritical and subcritical fluid extraction processes // Zainuddin Abdul Manan, Gholamreza Zahedi, Ana Najwa Mustapa
Pubbl/distr/stampa	Hoboken, New Jersey : , : Wiley : , : American Institute of Chemical Engineers, , [2022] ©2022
ISBN	1-119-30320-6 1-119-30319-2 1-119-30321-4
Descrizione fisica	1 online resource (291 pages)
Disciplina	660.284248
Soggetti	Supercritical fluid extraction - Simulation methods Electronic books.
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Nota di bibliografia	Includes bibliographical references and index.
Nota di contenuto	Cover -- Title Page -- Copyright Page -- Contents -- Preface -- Nomenclature -- Chapter 1 Fundamentals of Supercritical and Subcritical Fluid Extraction -- 1.1 Introduction -- 1.2 Supercritical Fluid Properties -- 1.3 Subcritical Condition -- 1.4 Physical Properties of Subcritical Fluid -- 1.5 Principles of Sub- and Supercritical Extraction Process -- 1.5.1 Solid Sample Extraction -- 1.5.2 Liquid Sample Extraction -- 1.6 Applications of SCF Extraction -- 1.6.1 Decaffeination of Coffee and Tea -- 1.6.2 Removal of FFA in Fats and Oils -- 1.6.3 Enrichment of Tocopherols -- 1.6.4 Carotenes from Crude Palm Oil and from Palm Fatty Acid Esters -- 1.7 Solubility of Solutes in SCFs -- 1.8 Solute-Solvent Compatibility -- 1.9 Solubility and Selectivity of Low-Volatility Organic Compounds in SCFs -- 1.10 Method of Solubility Measurement -- 1.10.1 Static Method -- 1.10.2 Dynamic Method -- 1.11 Determination of Solvent -- 1.11.1 Carbon Dioxide (CO2) -- 1.11.2 1,1,1,2-Tetrafluoroethane (R134a) as a Solvent -- 1.12 Important Parameter Affecting Supercritical Extraction Process -- 1.12.1 Pressure and Temperature -- 1.12.2 Solvent Flowrate -- 1.12.3 Cosolvent -- 1.12.4 Moisture Content -- 1.12.5 Raw Material -- 1.13

Profile of Extraction Curves -- 1.14 Design and Scale Up -- Chapter 2
Modeling and Optimization Concept -- 2.1 SFE Modeling -- 2.1.1
Importance of Knowing the Solid Matrix and Selecting a Suitable Model
-- 2.1.2 Different Modeling Approaches in SFE -- 2.1.2.1 Experimental
Models -- 2.1.2.2 Models Which Are Based on Similarity between Heat
and Mass Transfer -- 2.1.2.3 Models Based on Conservation Balance
Equations -- 2.2 First Principle Modeling -- 2.2.1 The Equation of
Continuity -- 2.2.2 The Equation of Motion in Terms of -- 2.2.3 The
Equation of Energy in Terms of q -- 2.3 Hybrid Modeling or Gray Box
-- 2.4 ANN.
2.4.1 Simple Neural Network Structure -- 2.4.1.1 Transfer Function --
2.4.1.2 Activation Functions -- 2.4.1.3 Learning Rules -- 2.4.2
Network Architecture -- 2.5 Fuzzy Logic -- 2.5.1 Boolean Logic and
Fuzzy Logic -- 2.5.2 Fuzzy Sets -- 2.5.3 Membership Function --
2.5.3.1 Membership Function Types -- 2.5.4 Fuzzy Rules -- 2.5.4.1
Classical Rules and Fuzzy Rules -- 2.5.5 Fuzzy Expert System and
Fuzzy Inference -- 2.5.5.1 Mamdani FIS -- 2.5.5.1.1 Fuzzification --
2.5.5.1.2 Fuzzy Logical Operation and Rule Evaluation -- 2.5.5.1.3
Implication Method -- 2.5.5.1.4 Aggregation of the Rule Outputs --
2.5.5.1.5 Defuzzification -- 2.5.5.2 Sugeno Fuzzy Inference -- 2.6
Neuro Fuzzy -- 2.6.1 Structure of a Neuro Fuzzy System -- 2.6.2
Adaptive Neuro Fuzzy Inference System (ANFIS) -- 2.6.2.1 Learning in
the ANFIS Model -- 2.7 Optimization -- 2.7.1 Traditional Optimization
Methods -- 2.7.2 Evolutionary Algorithm -- 2.7.3 Simulated Annealing
Algorithm -- 2.7.4 Genetic Algorithm -- 2.7.4.1 Genetic Algorithm
Definitions -- 2.7.4.2 Genetic Algorithms Overview -- 2.7.4.3
Preliminary Considerations -- 2.7.4.4 Overview of Genetic
Programming -- 2.7.4.5 Implementation Details -- 2.7.4.5.1 Selection
Operator -- 2.7.4.5.2 Crossover Operator -- 2.7.4.5.3 Mutation
Operator -- 2.7.4.6 Effects of Genetic Operators -- 2.7.4.7 The
Algorithms -- Chapter 3 Physical Properties of Palm Oil as Solute -- 3.1
Introduction -- 3.2 Palm Oil Fruit -- 3.3 Palm Oil Physical and Chemical
Properties -- 3.3.1 Palm Oil Triglycerides -- 3.3.2 Minor Components
in Palm Oil -- 3.4 Vegetable Oil Refining -- 3.5 Conventional Palm Oil
Refining Process -- 3.5.1 Chemical Refining -- 3.5.2 Physical Refining
-- 3.5.3 Effect of Palm Oil Refining -- 3.6 Conclusions -- Chapter 4
First Principle Supercritical and Subcritical Fluid Extraction Modeling:
Part I: Modeling Methodology -- 4.1 Introduction.
4.2 Phase Equilibrium Modeling -- 4.3 The Redlich-Kwong-Aspen
Equation of State -- 4.3.1 Calculations of Pure Component Parameters
for the RKA-EOS -- 4.3.2 Binary Mixture Calculations -- 4.4 Palm Oil
System Characterization -- 4.4.1 Palm Oil Triglycerides -- 4.4.2 Free
Fatty Acids -- 4.4.3 Palm Oil Minor Components -- 4.5 Development of
Aspen Plus® Physical Property Database for Palm Oil Components --
4.5.1 Vapor Pressure Estimation -- 4.5.2 Estimation of Pure
Component Critical Properties -- 4.5.2.1 Critical Properties Estimation
Using Normal Boiling Point -- 4.5.2.2 Critical Properties Estimation
Using One Vapor Pressure Point -- 4.6 Binary Interaction Parameters
Calculations -- 4.7 Supercritical Fluid Extraction Process Development
-- 4.7.1 Hydrodynamics of Countercurrent SFE Process -- 4.7.2
Solubility of Palm Oil in Supercritical CO₂ -- 4.7.3 Process Modeling
and Simulation -- 4.7.3.1 Simple Countercurrent Extraction -- 4.7.3.2
Countercurrent Extraction with External Reflux -- 4.7.4 Process
Analysis and Optimization -- Part II: Results and Discussion -- 4.8
Palm Oil Component Physical Properties -- 4.8.1 Vapor Pressure of
Palm Oil Components -- 4.8.2 Pure Component Critical Properties --
4.9 Regression of Interaction Parameters for the Palm Oil Components-
Supercritical CO₂ Binary System -- 4.9.1 Binary System: Triglyceride -

Supercritical CO₂ -- 4.9.2 Binary System: Oleic Acid - Supercritical CO₂
-- 4.9.3 Binary System: -Tocopherol - Supercritical CO₂ -- 4.9.4
Binary System: -Carotene - Supercritical CO₂ -- 4.9.5 Temperature-
Dependent Interaction Parameters -- 4.10 Phase Equilibrium
Calculation for the Palm Oil -Supercritical CO₂ System -- 4.11 Ternary
System: CO₂ - Triglycerides - Free Fatty Acids -- 4.12 Distribution
Coefficients of Palm Oil Components -- 4.13 Separation Factor Between
Palm Oil Components.
4.13.1 Separation Factor Between Fatty Acids and Triglycerides --
4.13.2 Separation Factor Between Fatty Acids and -Tocopherols --
4.14 Base Case Process Simulation -- 4.14.1 Palm Oil Deacidification
Process -- 4.14.1.1 Solubility of Palm Oil in Supercritical CO₂ --
4.14.1.2 Palm Oil Deacidification Process: Comparison to Pilot Plant
Results -- 4.15 Conclusion -- Chapter 5 Application of Other
Supercritical and Subcritical Modeling Techniques -- 5.1 Mass Transfer,
Correlation, ANN, and Neuro Fuzzy Modeling of Sub- and Supercritical
Fluid Extraction Processes -- 5.2 Mass Transfer Model -- 5.3 ANN
Modeling -- 5.4 Neuro Fuzzy Modeling -- 5.5 ANFIS and Gray-box
Modeling of Anise Seeds -- 5.6 White Box SFE Modeling of Anise --
5.6.1 Gray Box Parameters -- 5.6.2 ANFIS -- 5.6.2.1 Preprocessing --
5.6.3 Gray Box -- 5.7 Results and Discussion -- 5.7.1 ANFIS -- 5.7.2
Gray Box Modeling Results -- 5.7.2.1 Black Box -- 5.7.3 Comparison of
ANFIS and Gray Box Models with ANN and White Box Models -- 5.8
Introduction - Statistical versus ANN Modeling -- 5.9 Supercritical
Carbon Dioxide Extraction of Q. infectoria Oil -- 5.9.1 Materials and
Methods -- 5.9.2 Experimental Design -- 5.9.3 Artificial Neural
Network Modeling -- 5.10 Subcritical Ethanol Extraction of Java Tea Oil
-- 5.10.1 Artificial Neural Network Modeling -- 5.11 SFE of Oil from
Passion Fruit Seed -- 5.11.1 Experimental Procedures -- 5.11.2 RSM
Statistical Modeling -- 5.11.3 ANN Modeling of Passion Fruit Seed Oil
Extraction with Supercritical Carbon Dioxide -- Chapter 6 Experimental
Design Concept and Notes on Sample Preparation and SFE Experiments
-- 6.1 Introduction -- 6.2 Experimental Design -- 6.3 Statistical
Optimization -- 6.4 Optimization of Palm Oil Subcritical R134a
Extraction -- 6.4.1 Effect of Temperature and Pressure -- 6.4.2 Model
Fitting -- 6.4.3 Process Optimization.
6.5 Comparison of Subcritical R134a and Supercritical CO₂ Extraction
of Palm Oil -- 6.5.1 Extraction Performance -- 6.5.2 Economic Factor
-- 6.6 Sample Pretreatment -- 6.6.1 Moisture Content Reduction --
6.6.2 Sample Size Reduction -- 6.7 New Trends in Pretreatment -- 6.8
Optimal Pretreatment -- Chapter 7 Supercritical and Subcritical
Optimization: Part I: First Principle Optimization -- 7.1 Introduction --
7.2 Evaluation of Separation Performance -- 7.2.1 Effects of
Temperature and Pressure -- 7.2.2 Effect of the Number of Stages --
7.2.3 Effect of Solvent-to-Feed Ratio -- 7.2.4 Effect of Reflux Ratio --
7.3 Parameter Optimization of Palm Oil Deacidification Process -- 7.3.1
Simple Countercurrent Extraction (Without Reflux) -- 7.3.2
Countercurrent Extraction with Reflux -- 7.4 Proposed Flowsheet for
Palm Oil Refining Process -- 7.5 Conclusions -- Part II: ANN, GA
Statistical Optimization -- 7.6 Introduction -- 7.7 Traditional
Optimization -- 7.8 Nimbin Extraction Process Optimization -- 7.9
Genetic Algorithm for Mass Transfer Correlation Development -- 7.10
Optimizing Chamomile Extraction -- 7.11 Statistical and ANN
Optimization -- 7.12 Conclusion -- Appendix A Calculation of the
Composition for Palm Oil TG (Lim et al. 2003) -- Appendix B
Calculation of Distribution Coefficient and Separation Factor (Lim et al.
2003) -- Appendix C Calculation of Palm Oil Solubility in Supercritical
CO₂ (Lim et al. 2003) -- References -- Index -- EULA.
