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Artificial Intelligence-Driven Optimization of Supercritical CO_2 Extraction of Volatile Oils from Aromatic Plants: Experiments, Modeling, and Applications

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Abstract: *Volatile oils extracted from aromatic plants are widely utilized in food, pharmaceutical, cosmetic, and nutraceutical industries due to their diverse biological activities and sensory properties. Conventional extraction techniques, including hydrodistillation and solvent extraction, often suffer from thermal degradation, solvent residues, and limited selectivity. Supercritical carbon dioxide (SC-CO_2) extraction has emerged as a sustainable and efficient alternative capable of producing high-quality volatile oils under mild operating conditions. Despite significant advances in experimental studies, optimization of SC-CO_2 extraction remains challenging because of the complex interactions among pressure, temperature, CO_2 flow rate, particle size, moisture content, and extraction time. Recent developments in artificial intelligence (AI), machine learning (ML), and hybrid modeling have created new opportunities for predictive process optimization and intelligent control. This review discusses the fundamentals of SC-CO_2 extraction of volatile oils from aromatic plants, summarizes experimental findings, examines thermodynamic and kinetic models, and critically evaluates AI-based optimization approaches including artificial neural networks, support vector machines, random forests, adaptive neuro-fuzzy systems, and genetic algorithms. The integration of mechanistic and data-driven models, digital twins, and Industry 4.0 concepts for intelligent extraction systems is also explored. Future research directions emphasize explainable AI, hybrid physics-informed machine learning, real-time optimization, and sustainable industrial implementation.*

Keywords: Supercritical CO_2 extraction; Aromatic plants; Essential oils; Volatile oils; Artificial intelligence; Machine learning; Process optimization; Kinetic modeling

I. INTRODUCTION

Aromatic plants constitute an important source of volatile oils rich in terpenes, alcohols, aldehydes, ketones, esters, and phenolic compounds. These bioactive constituents possess antimicrobial, antioxidant, anti-inflammatory, and therapeutic properties. Conventional extraction methods such as hydrodistillation, steam distillation, and organic solvent extraction remain widely employed but frequently cause degradation of thermolabile compounds and loss of volatile constituents. Supercritical fluid extraction (SFE) using carbon dioxide has emerged as a green extraction technology due to its non-toxic nature, low critical temperature (31.1°C), moderate critical pressure (73.8 bar), easy solvent recovery, and excellent selectivity. SC-CO_2 extraction enables recovery of high-quality volatile oils with minimal thermal damage and negligible solvent residues. Although extensive experimental studies have been conducted on lavender, thyme, rosemary, peppermint, basil, coriander, fennel, lemongrass, and numerous medicinal plants, optimization remains challenging because extraction performance depends on multiple interacting variables. Mathematical models and AI-based predictive approaches are increasingly being adopted to address these challenges.

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1. Objectives of the Research

i. To analyze the fundamentals of SC-CO_2 extraction : Understand phase behavior, solvent properties, and extraction mechanisms.
ii. To review experimental studies on aromatic plant extraction :Evaluate the influence of key parameters such as pressure, temperature, CO_2 flow rate, particle size, and extraction time on yield and composition.
iii. To examine thermodynamic and solubility modeling approaches: Assess models such as Peng–Robinson EOS, SRK EOS, and Chrastil equation for predicting solubility of volatile compounds.
iv. To evaluate kinetic and mass transfer models : Critically compare models like Sovová model, Broken–Intact Cell model, and diffusion-based approaches for describing extraction behavior.
v. To investigate artificial intelligence techniques in extraction optimization : Review applications of ANN, SVM, Random Forest, and ANFIS in predicting yield, selectivity, and process performance..

II. Fundamentals of Supercritical CO_2 Extraction

2.1 Supercritical State of Carbon Dioxide

Above its critical point, CO_2 exhibits properties intermediate between liquids and gases:
i. Liquid-like density
ii. Gas-like diffusivity
iii. Low viscosity
iv. Tunable solvent power
These characteristics enable efficient penetration into plant matrices and enhanced solubilization of volatile compounds.

2.2 Extraction Mechanism

The extraction process generally involves:
i. Solvent penetration into plant particles
ii. Solubilization of volatile compounds
iii. Internal diffusion
iv. External mass transfer
v. Separation through pressure reduction
The extraction rate is controlled by both equilibrium and mass-transfer phenomena.

III. ARTIFICIAL INTELLIGENCE IN SC-CO_2 EXTRACTION

Traditional models often require assumptions that may not adequately represent complex nonlinear interactions.
AI provides data-driven alternatives.

3.1 Artificial Neural Networks (ANN)

Inputs: Pressure, Temperature, Flow rate, Particle size, Time Outputs: Extraction yield, Composition, Selectivity Advantages:
i. Handles nonlinear relationships
ii. High prediction accuracy Limitations:
i. Black-box behavior
ii. Data intensive

3.2 Support Vector Machines (SVM) Advantages:

i. Effective for small datasets
ii. Strong generalization capability Applications:
i. Yield prediction

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ii. Process classification

3.3 Random Forest (RF) Advantages:
i. Robustness
ii. Feature importance analysis
iii. Useful for identifying dominant process variables.

3.4 Adaptive Neuro-Fuzzy Inference Systems (ANFIS) Combines:
i. Neural networks
ii. Fuzzy logic
iii. Suitable for uncertain and noisy extraction data.

IV. RESULT AND DISCUSSION

1. Effect of Operating Parameters on Extraction Yield and Composition

Analysis of experimental studies across various aromatic plants indicates that pressure is the most influential parameter in SC-CO_2 extraction. Increasing pressure from 100 to 300 bar significantly enhances CO_2 density, thereby improving solvent strength and extraction yield. However, beyond an optimal pressure range (typically 250–300 bar), the increase in yield becomes marginal due to saturation effects.

Temperature exhibits a dual influence on extraction efficiency. At lower pressures, increasing temperature reduces CO_2 density and extraction yield, whereas at higher pressures, increased solute vapor pressure dominates, leading to improved extraction. This phenomenon, known as the crossover effect, is consistently reported in studies involving lavender, peppermint, and basil.

Particle size reduction enhances extraction efficiency by increasing surface area and reducing internal diffusion resistance. However, excessively fine particles may lead to bed compaction, reduced permeability, and increased pressure drop, thereby negatively affecting extraction performance.

CO_2 flow rate primarily affects mass transfer rates. Higher flow rates improve extraction kinetics but may reduce solvent utilization efficiency, indicating the need for optimal flow conditions.

2. Extraction Kinetics and Mass Transfer Behavior The extraction process typically follows three distinct stages: Constant Extraction Rate (CER):

i. Rapid removal of easily accessible solutes from broken cells.

Falling Extraction Rate (FER):

ii. Controlled by internal diffusion resistance.
iii. Diffusion-Controlled Period (DCP): Slow extraction from intact plant cells.

Among the available models, the Sovová model demonstrates the best agreement with experimental data due to its ability to account for both external mass transfer and internal diffusion. The Broken–Intact Cell model further supports the existence of two distinct solute fractions, reinforcing the biphasic extraction behavior.

Model validation studies show that kinetic models can predict extraction yield with reasonable accuracy (typically within 5–10% deviation), although parameter estimation remains a challenge.

3. Thermodynamic and Solubility Modeling

Thermodynamic modeling using Peng–Robinson and SRK equations of state provides reliable predictions of phase equilibrium behavior in SC-CO_2 systems. However, these models require binary interaction parameters, which are not always readily available for complex essential oil mixtures.

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The Chrastil model has been widely used for correlating solubility data due to its simplicity and ability to capture the relationship between solubility, temperature, and CO_2 density. Comparative studies indicate that semi-empirical models often outperform EOS-based approaches for practical applications due to reduced computational complexity.

4. Performance of Artificial Intelligence Models

AI-based models have demonstrated superior predictive capability compared to traditional statistical methods.
Artificial Neural Networks (ANN):
Achieve high prediction accuracy ($R^2 > 0.98$ in many studies) for extraction yield and composition.
Capable of capturing nonlinear relationships among process variables. Support Vector Machines (SVM):
Perform well with smaller datasets and exhibit strong generalization ability. Random Forest (RF):
Provide insights into feature importance, identifying pressure and temperature as dominant variables.
ANFIS models:
Effectively handle uncertainty and noisy experimental data.
Overall, AI models significantly reduce the need for extensive experimental trials by enabling data-driven prediction of optimal conditions.

5. Comparison of RSM and AI-Based Optimization

Response Surface Methodology (RSM) has been widely used for experimental design and optimization. While RSM provides useful statistical relationships and interaction effects, it is limited by:
Assumption of quadratic relationships Reduced accuracy for highly nonlinear systems In contrast, AI-based models:
Capture complex nonlinear interactions Provide higher prediction accuracy Adapt better to large datasets
However, AI models require large datasets and lack interpretability, which remains a key limitation.

6. Hybrid Modeling Approaches

Hybrid models combining mechanistic and AI approaches show significant promise. Examples include:
ANN integrated with kinetic models for parameter estimation Machine learning correction of mass transfer coefficients Physics-informed neural networks (PINNs)
These approaches improve prediction accuracy while maintaining physical interpretability. Hybrid models are particularly useful for scale-up and industrial applications.

7. Industrial Relevance and Scale-Up Considerations

SC-CO_2 extraction is increasingly applied at industrial scale for the production of high-value essential oils. However, scale-up remains challenging due to:
Complex mass transfer phenomena Equipment design limitations
High capital costs
Modeling and AI tools can assist in optimizing process conditions, reducing operational costs, and improving process efficiency.
The integration of experimental studies, mechanistic modeling, and artificial intelligence provides a comprehensive framework for optimizing SC-CO_2 extraction of volatile oils. While traditional models offer mechanistic understanding, AI enhances predictive accuracy and optimization efficiency. The future of this field lies in hybrid, intelligent, and sustainable extraction systems that combine the strengths of both approaches.

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