THERMODYNAMIC MODELLING OF LIQUID-LIQUID EXTRACTION OF LIMONOIDS FROM *Azadirachta indica*

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A DISSERTATION SUBMITTED TO THE SCHOOL OF POSTGRADUATE STUDIES IN PARTIAL FULFILMENT OF THE REQUIREMENTS FOR THE AWARD OF THE DEGREE OF MASTER OF ENGINEERING (M.Eng) IN THE DEPARTMENT OF CHEMICAL ENGINEERING, COLLEGE OF ENGINEERING, COVENANT UNIVERSITY.

JULY, 2022

ACCEPTANCE

This is to attest that this dissertation is accepted in partial fulfillment for the degree of Master of Engineering in the Department of Chemical Engineering, College of Engineering, Covenant University, Ota, Ogun State, Nigeria.

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DECLARATION

I, **NKONGHO SONIA (2OPCF02279)**, declare that this dissertation is a representation of my work, and is written and implemented by me under the supervision of Doctor Olayemi A. Odunlami of the Department of Chemical Engineering, Covenant University, Ota, Nigeria. I attest that this dissertation has in no way been submitted either wholly or partially to any other University or institution of higher learning for the award of a masters' degree. All information cited from published and unpublished literature has been duly referenced.

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Signature and Date

CERTIFICATION

This is to certify that the research work titled "**THERMODYNAMIC MODELLING OF LIQUID-LIQUID EXTRACTION OF LIMONOIDS FROM *Azadirachta indica*",** is an original research work carried out by **NKONGHO SONIA** meets the requirements and regulations governing the award of Master of Engineering (M.Eng) degree in Chemical Engineering from the Department of Chemical Engineering, College of Engineering, Covenant University, Ota, and is approved for its contribution to knowledge and literary presentation.

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DEDICATION

This work is dedicated to the Almighty God for His divine direction and favor throughout this work. It is only by His grace this work was completed. I also dedicate this work to my mother, Tambe Cecilia Nkongho, and my sister Agbor Pamela Tambe for their constant prayers, moral and financial support. May God replenish the source abundantly.

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LIST OF ABBREVIATIONS

FDA	Food and Development Association
WHO	World Health Organization.
ACT	Active Ingredients in Artemether
GMP	Good Manufacturing Practice
SA	Structural Alerts
SFE	Supercritical Fluid Extraction
QSAR	Quantitative Structural-Activity Relationship
EC	Effective Constituents
TM	Traditional Medicine
WM	Western Medicine
NRTL	Non -random two liquids
UNIFAC	UNIQUAC Functional-group Activity Coefficient
UNIQUAC	Universal Quasichemical activity Coefficient
LLE	Liquid-liquid Extraction
GC	Gas Chromatography
FID	Flame Ionization Detector
BIP	Binary Interaction Parameter
RMSD	Root Mean Square Deviation

ABSTRACT

Limonoids from *Azadirachta indica* (also known as dongoyaro in Nigeria) leaves are separated using features of phase equilibrium including partition coefficients pressure, temperature, compositions, and partition coefficients when constructing chemical separation operations for limonoids from the leaves. In order to determine the thermodynamic properties, the ternary liquid-liquid behaviors in the system (n-hexane + limonoids + water) at 323.15 K and 373.15 K, and constant pressure of 101.3 kPa was modeled and simulated. Comparisons were made between the effects of extraction and the system's calculated partition coefficient (D) and selectivity (S). The Othmer-Tobias correlation was employed to evaluate the regularity and dependability of empirical liquid-liquid equilibrium (LLE) data. The empirical data were compared utilizing the Non-Random Two-Liquids (NRTL) and Universal Quasichemical (UNIQUAC) models, whereas the binary interaction parameters (BIPs) specified for each model were derived utilizing regression in the ASPEN plus software. The separation factor values which ranged from 0.9110 to 18.2177 demonstrated to be temperature and concentration of limonoid dependent. In accordance with the Othmer-Tobias equation, the authenticity of the LLE data had a regression coefficient greater than 0.8553. Equally, the NRTL model was the best fit for the prediction of the extraction of limonoids from neem leaves since the Root Mean Square Regression Deviation (RMSD) values between the experimental and calculated LLE data of less than 0.1847 percent as compared to 0.7501 percent using UNIQUAC model. The results obtained can be used in pharmaceutical industries in the design of the extraction column to produce high purity limonoids for the treatment of malaria which will influence the design, procedure, and enhancement of the process.

Keywords: ***Thermodynamic liquid-liquid equilibrium, Azadirachta indica, Aspen Plus, NRTL, UNIQUAC***